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# RESEARCH MEMORANDUM

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# THEORETICAL PERFORMANCE OF DIBORANE AS A ROCKET FUEL

By Vearl N. Huff, Clyde S. Calvert and Virginia C. Erdmann

Lewis Flight Propulsion Laboratory Cleveland, Ohio

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# RESEARCH MEMORANDUM

# THEORETICAL PERFORMANCE OF DIBORANE AS A ROCKET FUEL

# By Vearl N. Huff, Clyde S. Calvert and Virginia C. Erdmann

# SUMMARY

Theoretical performance data based on equilibrium isentropic expansion and constant-composition (frozen) isentropic expansion from a combustion-chamber pressure of 20.4 atmospheres (300 lb/sq in. absolute) to an ambient pressure of 1 atmosphere are presented for a range of mixtures for four rocket-propellant combinations of diborane with liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide. The theoretical data include combustion-chamber and nozzle-exit temperatures, specific impulse, and volume specific impulse. Composition and mean molecular weight of the reaction products are given for both the combustion chamber and the nozzle exit.

The maximum specific impulse for all the combinations occurred in the fuel-rich region. On the basis of maximum specific impulse, the four oxidants reacting with diborane assumed the following order: liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide. On the basis of calculated maximum volume specific impulse, the order of the four oxidants reacting with diborane was: liquid fluorine oxide, liquid fluorine, 100-percent hydrogen peroxide, and liquid oxygen.

# INTRODUCTION

Considerable interest has been shown in some of the boron compounds as rocket propellants because their high heat of combustion per unit weight indicates a high specific impulse.

Pentaborane and diborane are two of the more significant of the boron hydrides under consideration because chemically they are sufficiently stable to permit synthesis and use. Pentaborane has several advantages over diborane including higher density and boiling point, but diborane is more readily available and more data on its heat of combustion exist.

Computed performance of diborane and liquid oxygen for three mixture ratios under equilibrium-expansion conditions and for a range of mixture ratios under frozen-expansion conditions is presented in reference 1. A theoretical and experimental investigation of boron compounds as rocket fuels is being conducted at the NACA Lewis laboratory and calculations are reported herein that were made from December 1947 to May 1948. These computations extend the mixture range of reference 1 for diborane and liquid oxygen and, in addition, give performance over a considerable mixture range of diborane with liquid fluorine, liquid fluorine oxide, and hydrogen peroxide. The results include combustion-chamber temperature, nozzle-exit temperature, specific impulse, volume specific impulse, composition, and mean molecular weight as functions of mixture ratio.

# METHOD OF CALCULATION

The calculation of specific impulse involves the determination of the gas composition and the temperature in the combustion chamber and at the nozzle exit. The products of reaction were assumed to expand from a combustion-chamber pressure of 20.4 atmospheres (300 lb/sq in. absolute) to an ambient pressure of 1 atmosphere. The ideal gas laws were used.

The molecules considered to be present in the gas phase for the appropriate reactions were: atomic hydrogen H, hydrogen H<sub>2</sub>, water vapor H<sub>2</sub>O, hydroxyl radical OH, hydrogen fluoride HF, boron hydride BH, atomic oxygen O, oxygen O<sub>2</sub>, boron trioxide B<sub>2</sub>O<sub>3</sub>, boron oxide BO, atomic fluorine F, fluorine F<sub>2</sub>, boron trifluoride EF<sub>3</sub>, boron fluoride EF, atomic boron B, and diatomic boron B<sub>2</sub>. At nozzle-exit temperatures below 2000<sup>o</sup> K, liquid boron trioxide B<sub>2</sub>O<sub>3</sub> was also included but boron B in the liquid and solid states, which could also be present, was neglected. The boiling point of boron is given as 2823<sup>o</sup> K in reference 2 (p. 1750). For many of the calculations, the liquid and solid states of boron would not be present and, for the remaining calculations, the effect on specific impulse is probably small.

The theoretical performance was calculated on the basis of constant enthalpy from the fuel and the oxidant at the assumed initial state of the propellants (tank conditions) to the state of the reaction products in the combustion chamber. The term enthalpy  $H_{\Gamma}^{\sigma}$  is defined by



where

 $E_0^{O}$  heat of formation at  $0^{O}$  K, calories per mole

T temperature, <sup>o</sup>K

 $c_n$  specific heat at constant pressure, calories per mole per  ${}^{O_{K}}$ 

The superscript o denotes the thermodynamic standard reference state of unit activity; the subscript T denotes the absolute temperature in degrees Kelvin. After the enthalpy of the fuel plus the oxidant at initial states was calculated, the combustion temperature was obtained by simultaneously solving the equations for equilibrium, mass balance, and enthalpy by a method of successive approximations. The equation for enthalpy of the reaction is

 $E_T^O$  (reactants) =  $\sum_{i=1}^{n} (E_T^O)_i$  (products of reaction)

where

n

(**E**C)

 $H_m^O$  (reactants) enthalpy of reactants at initial states, calories

moles of product i

enthalpy of product i, calories per mole

The nozzle-exit temperature was calculated on the assumption that chemical equilibrium prevailed throughout expansion (equilibrium expansion) and on the assumption that no chemical recombination took place (frozen expansion). In each case, isentropic expansion was assured by comparing the entropy of the fluid at the exit  $S_{\Theta}$ to the entropy of the fluid in the combustion chamber  $S_{c}$ .

$$S_{c} = S_{\theta} = \frac{1}{\sum_{i=1}^{n} M_{i}} \left[ \sum_{i=1}^{n} (S_{T}^{0})_{i} - R\sum_{i=1}^{n} p_{i} \log_{\theta} p_{i} \right]$$

where

M, molecular weight of product i

(s\_T^o)\_i

absolute entropy of product i, calories per mole per <sup>O</sup>K i

R gas constant, 1.98714 calories per mole per <sup>O</sup>K

p, partial pressure of product i, atmospheres

Specific impulse I (lb-sec/lb) was calculated from the difference in enthalpy between the combustion chamber and the nozzle exit by the equation

I = 9.328 
$$\sqrt{\left(\frac{H_T^o}{\sum n_i M_i}\right)_c - \left(\frac{H_T^o}{\sum n_i M_i}\right)_e}$$

Volume specific impulse  $I_d$  (lb-sec/(cu ft)(62.43) or gram-sec/cc) is also included.

# THERMOCHEMICAL DATA

The heats of formation of diborane  $B_2H_6$ , boron trioxide  $B_2O_3$ , and boron trifluoride  $BF_3$  were taken from reference 3. Some uncertainty exists concerning the thermochemical data for the various states of boron and its compounds. The heat of combustion of diborane with oxygen, however, is not subject to so much question and is given by reference 3 as 510 kilocalories per mole. The value of the heat of formation of B<sub>2</sub>H<sub>6</sub> has been given as -44 kilocalories per mole in reference 3, -29.5 kilocalories per mole in reference 4, and recently a value of 26 kilocalories per mole in reference 5. (Heat liberated is considered to be negative.) All the data presented herein are based on a heat of formation of -44 kilocalories per mole for diborane. One calculation, however, was made for the stoichiometric mixture of diborane and liquid oxygen using the value of 26 kilocalories per mole and the specific impulse was 2.5 percent lower than by using the value of -44 kilocalories. The heat of transition of  $B_2O_3$  (amorphous) to  $B_2O_3$  (crystalline) was neglected. The effect of this assumption is small and will change the specificimpulse values on the order of 0.7 percent.

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The heats of formation of hydrogen fluoride HF and atomic fluorine F were taken from reference 6. The lower value ((1/2)(63.5 k-cal)) given for F was used because it is the basis of the thermodynamic properties of F and F<sub>2</sub> (reference 6). The heats of formation of H<sub>2</sub>O, O, OH, and H were obtained from reference 7. The sensible enthalpies and entropies of HF, F, and F<sub>2</sub> were taken from reference 6 and those of H<sub>2</sub>O, O, O<sub>2</sub>, OH, H, and H<sub>2</sub> from reference 7.

The heats of fusion and vaporization of B and  $B_2O_3$ , the heats of formation of BO and B, and the sensible enthalpies and free energies of  $B_2O_3$ , B,  $B_2$ , and BO to  $5000^{\circ}$  K were taken from reference 8. The functions for B were extended to  $6000^{\circ}$  K in the same manner in which the calculations were made in reference 8. Free energy, sensible enthalpy, and entropy of  $BF_3$  in the ideal gas state from 298.16° to  $1000^{\circ}$  K were taken from reference 9 and extended to  $6000^{\circ}$  K from spectroscopic data of reference 10, by assuming that the BF<sub>3</sub> molecule is a rigid rotator and a harmonic oscillator.

Similar calculations were also made for BH and BF from the spectroscopic data of reference 11. The  $3_{\pi}$  state was considered the ground state for BF because no other information was found in the literature. The values of enthalpy, entropy, and free energy for BF<sub>3</sub>, BF, BH, and B are listed in tables I, II, and III, respectively.

The propellants were taken as liquids at the following initial temperatures:

Propellant (100 percent)	Initial temperature (°K)
Diborane	298.16
Fluorine	85.16
Fluorine oxide	128.30
Oxygen	90.10
Hydrogen peroxide	298.16

Liquid  $B_2H_6$  was used at 298.16 <sup>O</sup>K because no specific-heat data were available to adjust the initial temperature to or below the boiling point. The effect on specific impulse of using this

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initial temperature for  $B_2H_6$  is small and an error in the opposite direction and of the same order of magnitude was introduced when the heat of transition of  $B_2O_3$  (amorphous) to  $B_2O_3$  (crystalline) was neglected.

The density of diborane increases as the temperature is lowered and therefore the highest density reported in reference 12 (0.4818 gram/cc at  $-129^{\circ}$  C) was used for the computation of volume specific impulse. Additional physical and thermochemical properties of diborane and the oxidants considered were taken from references 13 to 16 and are given in table IV.

# RESULTS AND DISCUSSION

The performance parameters of diborane reacting with liquid fluorine, liquid fluorine oxide, liquid oxygen, and loo-percent hydrogen peroxide are plotted against the percent by weight of fuel in the mixture in figure 1. The quantities plotted for each combination for both frozen and equilibrium expansions are combustionchamber temperature  $T_c$ , nozzle-exit temperature  $T_e$ , specific impulse I, volume specific impulse  $I_d$ , and mean molecular weight in combustion chamber  $M_c$ . The mean molecular weight at the nozzle exit  $M_e$  was also included for equilibrium expansion.

The curves of combustion-chamber temperature for the combinations considered reached a maximum near the stoichiometric mixture for all of the cases except fluorine oxide, which did not reach a maximum in the range considered. The highest combustion-chamber temperature obtained was  $5380^{\circ}$  K for the fluorine-diborane reaction (figs. 1(a) and (b)). The hydrogen peroxide (figs 1(g) and (h)) and oxygen (figs. 1(e) and (f)) combinations gave temperatures substantially lower than the fluorine. The combustion-chamber temperatures reached maximum computed values of  $4750^{\circ}$ ,  $4022^{\circ}$ , and  $3230^{\circ}$  K for fluorine oxide, oxygen, and hydrogen peroxide, respectively. The nozzle-exit-temperature curves for both the frozen and the equilibrium expansions follow a trend similar to those of the combustionchamber temperature and reach a maximum in the region of the stoichiometric mixture.

The specific-impulse curves for all the combinations considered reached maximum values in the fuel-rich region as a result of the liberation of free hydrogen, which reduces the average molecular weight of the products of combustion. The trends of the specificimpulse curves based on both frozen and equilibrium expansions are similar. The maximum deviation between the equilibrium-expansion and the frozen-expansion specific-impulse values was 8.08 percent of the equilibrium values.

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The maximum specific-impulse values that were calculated for equilibrium expansion are listed in the following table, together with the corresponding volume specific impulse.

Oxidant	Fuel (percent by wt)	Maximum specific impulse, I (lb-sec/lb)	Volume specific impulse, I <sub>d</sub> [lb-sec [(cu ft)(62.43)]	Combustion- chamber temperature, T <sub>o</sub> (°K)	c
Fluorine Fluorine oxide Oxygen Hydrogen peroxide	13.63 20.41 36.58 35.18	322.4 316.2 311.4 289.0	309.8 375.3 236.7 245.3	5240 4460 3740 2850	

Because the densities of liquids  $F_2$ ,  $F_20$ ,  $O_2$ , and  $H_2O_2$ are greater than that of liquid  $B_2H_6$ , the maximum volume specific impulse occurred at a mixture ratio less fuel rich than that required for maximum specific impulse. The general trend of the volumespecific-impulse curves is similar for both the equilibrium and frozen expansions for all the fuel-oxidant combinations. For the fluorine compounds, the maximum volume specific impulse occurs at a lower percentage of fuel than was considered. The maximum volumespecific-impulse values that were calculated for equilibrium expansion are listed in the following table, together with the corresponding specific impulse values.

Oxidant	Fuel (percent by wt)	Maximum volume specific impulse, I <sub>d</sub> [lb-sec (cu ft)(62.43)]	Specific impulse, I (lb-sec/lb)	Combustion- chamber temperature, T <sub>c</sub> ( <sup>O</sup> K)
Fluorine	12.030	424.2	302.3	<b>47</b> 50
Fluorine	9.853	317.0	315.5	5 <b>380</b>
Hydrogen peroxide	11.950	300.9	259.0	3218
Oxygen	25.710	243.2	288.2	4022

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The mean molecular weight at both the combustion chamber and the exit decreased as the percent by weight of fuel increased. In the case of the  $H_2O_2$  reaction with greater than 35 percent fuel, liquid  $B_2O_3$  appeared at the exit condition and caused the molecular weight to increase. For all propellant combinations considered, the mean molecular weight was from 12.0 to 1.7 percent higher at the exit than in the combustion chamber.

The calculated values of the various performance parameters for each of the propellant combinations and for several mixture ratios are listed in table V.

The compositions of the products of combustion in the combustion chamber and at the nozzle exit are shown in figure 2. The mole fraction of each product present in the gas mixture for each of the combinations is plotted against the percent by weight of fuel.

The curves of composition are similar for the combustion-chamber and nozzle-exit conditions for any one propellant combination (fig. 2). The general trend of a given molecule is the same for all propellant combinations. As the mixture becomes more fuel rich, B<sub>2</sub>, B, and H<sub>2</sub> increase and F<sub>2</sub>, F, O<sub>2</sub>, and O decrease. The molecules H<sub>2</sub>O and HF are principal constituents throughout most of the mixture range considered, but are reduced by boron at the extreme fuel-rich region. The molecules BF<sub>3</sub> and B<sub>2</sub>O<sub>3</sub> are comparatively constant throughout the range of mixture ratios considered. Certain molecules reach a maximum (for example, H) or a minimum (for example, BF<sub>3</sub>) because of the opposing effects of the variation of temperature and mixture ratio.

# SUMMARY OF RESULTS

Theoretical performance data, which were based on both frozen and equilibrium expansions, obtained over a range of mixtures for the four rocket propellant combinations of diborane with liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide at a reaction pressure of 20.4 atmospheres (300 lb/sq in. absolute) and a nozzle-exit pressure of 1 atmosphere, are summarized as follows:

1. The maximum calculated specific-impulse values in pound-seconds per pound for diborane reacting with liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide, were 322.4, 316.2, 311.4, and 289.0, respectively, for equilibrium expansion.

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2. The maximum specific impulse for all the propellant combinations occurred in the fuel-rich region at a combustion-chamber temperature less than maximum.

3. The specific impulse for equilibrium expansion was a maximum of 8.08 percent greater than that for frozen expansion.

4. The maximum calculated volume-specific-impulse values (lb-sec/(cu ft)(62.43)) for the mixture range considered were 424.2, 317.0, 300.9, and 243.2 for liquid fluorine oxide, liquid fluorine, 100-percent hydrogen peroxide, and liquid oxygen, respectively, for equilibrium expansion.

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### REFERENCES

- 1. Anon.: A Compilation of Computed Specific Impulse Values. Project RAND, RA - 15049, Battelle Memorial Inst., Sept. 2, 1947. (Subcontract under AAF Contract No. W33-038 ac-14105 to Douglas Aircraft Co., Inc.)
- 2. Anon.: Handbook of Chemistry and Physics. Charles D. Hodgman, ed., Chem. Rubber Pub. Co. (Cleveland), 29th ed., 1945.
- Roth, W. A., und Börger, Erika: Zur Thermochemie des Bors. Berichte d. D. Chemischen Gesellschaft, Jahrg. 70, Nr. 2, Jan. 6, 1937, S. 48-54.
- 4. Roth, W. A.: The Thermochemistry of Boron. Chem. Abs., vol. 41, no. 17, Sept. 10, 1947, column 5373f. (Abs. from Z. Naturforsch, Vol. 1, 1946, pp. 574-576.)
- 5. Eggersgluess, W., Mazurkiewicz, A., and Parker, W. G.: The Heat of Formation of Boron Trioxide. Rep. No. CHEM. 433, R.A.E., July 1947.
- 6. Kiehl, S. J., Jr., and Moore, J. R.: Propellants for Supersonic Vehicles: Liquid Fluorine. Project RAND, RA - 15407, Battelle Memorial Inst., Aug. 12, 1947. (Subcontract under AAF Contract No. W33-038-ac-14105 to Douglas Aircraft Co., Inc.)

CONFIDENTIAL

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- 7. Hirschfelder, J. O., McClure, F. T., Curtiss, C. F., and Osborne, D. W.: Thermodynamic Properties of Propellant Gases. NDRC Rep. No. A-116, Nov. 23, 1942. (Abs. Bib. Sci. Ind. Reps., vol. 2, no. 10, Sept. 6, 1946, p. 743, PB 28531.)
- 8. Wacker, Paul F., Wooley, Harold W., and Fair, Myron F.: Thermodynamic Properties and Gaseous Equilibria of Boron, Oxygen and the Oxides of Boron. Tech. Rep., Heat and Power Div., Nat. Bur. Standards, Jan. 25, 1945. (Bur. Aero., Navy Dept.)
- 9. Spencer, Hugh M.: Thermodynamic Properties of Gaseous Boron Trifluoride, Boron Trichloride, and Boron Tribromide. Jour. Chem. Phys., vol. 14, no. 12, Dec. 1946, pp. 729-732.
- 10. Herzberg, Gerhard: Infrared and Raman Spectra of Polyatomic Molecules. D. Van Nostrand Co., Inc. (New York), 1945.
- 11. Herzberg, Gerhard: Molecular Spectra and Molecular Structure. I. Diatomic Molecules, ch. VIII. Prentice-Hall, Inc. (New York), 1939, p. 484.
- 12. Laubengayer, A. W., Ferguson, R. P., and Newkirk, A. E.: The Densities, Surface Tensions and Parachors of Diborane, Boron Triethyl and Boron Tribromide. The Atomic Parachor of Boron. Jour. Am. Chem. Soc., vol. 63, no. 2, Feb. 1941, pp. 559-561.
- Maass, O., and Hatcher, W. H.: The Properties of Pure Peroxide.
   I. Jour. Am. Chem. Soc., vol. XLII, July-Dec. 1920, pp. 2538-2569.
- 14. Anon.: Tables of Selected Values of Chemical Thermodynamic Properties. Nat. Bur. Standards, Dec. 31, 1947.
- 15. Bichowsky, F. Russell, and Rossini, Frederick D.: The Thermochemistry of the Chemical Substances. Reinhold Pub. Corp. (New York), 1936.
- 16. Anon.: International Critical Tables. Vol. 3. McGraw-Hill Book Co., Inc., 1928, pp. 20, 203, 214; vol. 7, 1930, pp.11, 212.

		Enthalpy, HT	$-H_0^0$ , cal	mole
Temperature	BF3	BF	BH	В
(°K)				
1000	14.007	7.617	7,188	4,997
1100	15.833	8,465	7,972	5,494
1200	17.683	9.319	8,767	5,991
1300	19.551	10,179	9.574	6,487
1400	21.435	11.043	10.387	6,984
1500	23,332	11.911	11,213	7,481
1600	25.239	12,782	12.043	7,978
1700	27,154	13,656	12,880	8,475
1800	29,077	14,532	13,721	8.971
1900	31,007	15,409	14,568	9.468
2000	32,942	16,288	15,419	9,965
2100	34,882	17,169	16,273	10,462
2200	36,825	18,050	17,130	10,959
2300	38,773	18,933	17,990	11,455
2400	40,723	19,817	18,853	11,952
2500	42,677	20,701	19,718	12,449
2600	44,632	21,587	20,586	12,946
2700	46,591	22,473	21,455	13,443
2800	48,551	23,359	22,325	13,939
2900	50,512	24,246	23,197	14,436
3000	52,476	25,133	24,071	14,933
3100	54,440	26,021	24,946	15,430
3200	56,407	26,910	25,822	15,927
3300	58,374	27,798	26,699	16,423
3400	60,342	28,687	27,577	16,920
3500	62,312	29,576	28,456	17,417
3600	64,283	30,466	29,335	17,914
3700	66,254	31,356	30,216	18,411
3800	68,226	32,246	31,097	18,907
3900	70,198	33,136	31,979	19,404
4000	72,172	34,026	32,861	19,901
4100	74,140	34,917	33,744	20,398
4200	70,121	35,808	34,627	20,895
4400	10,091	37 500	35,511	21,391
4500	82 045	39,090	37,000	21,888
4600	84 025	30 372	39 166	22,000
4700	86,001	40 264	39,100	22,002
4800	87 977	41 155	30 037	23,075
4900	89,957	42 047	40,823	24 379
5000 .	91 935	42 939	41 710	24,860
5100	93,913	43,831	42.597	25 366
5200	95,893	44,723	43,484	25 863
5300	97,872	45,615	44.371	26,360
5400	99,851	46,507	45,259	26,857
5500	101.831	47, 399	46,147	27,354
5600	103,810	48,291	47,035	27,851
5700	105,792	49,184	47,923	28,349
5800	107,771	50,076	48,812	28,845
5900	109.751	50,968	49 700	20 343
6000	111,736	51,861	50,589	29,840

TABLE I - ENTHALPY OF GASES

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		Entropy, S <sub>T</sub> <sup>o</sup> ,	cal/mole -	• • K
Temperature ( <sup>O</sup> K)	BF3	Bŕ	BH	В
1000	79,293	61 764	40 505	
1100	81.033	62 570	49.703	42.662
1200	82.642	62 316	50.450	43.112
1300	84,138	64 003	51.145	43.538
1400	85.534	64.644	51.792	43.941
1500	86.842	65 043	52.392	44.320
1600	88.073	65 905	52.960	44.676
1700	89,234	66 334	53.495	45.009
1800	90.333	66.935	54.003	45.318
1900	91,377	67.300	54.484	45.604
2000	92,369	67 760	54.942	45.866
2100	93.316	69 100	55.078	46.105
2200	94,220	69 600	55.795	46.342
2300	95.085	69 003	50.194	46.573
2400	95,915	60 360	50.577	46.795
2500	96.713	60 730	50.944	47.008
2600	97.480	70 077	57.297	47.214
2700	98,210		57.637	47.411
2800	98.939		57.965	47.600
2900	99.620	71 045	58.287	47.781
3000	100.286		58.588	47.955
3100	100.030		58.884	48.119
3200	101 554	71.007	59.171	48.276
3300	101.004	71.919	59.449	48.431
3400		72.192	59.719	48.582
3500	102.141	72.458	59.981	48.729
3600		72.715	60.236	48.875
3700	103.073	72.900	60.483	49.015
3800	104.940	73.447	60.725	49.154
3900	104.940	10.447	60.959	49.288
4000	105 051	73.078	61.189	49.421
4100	106 430	73.904	61.412	49.549
4200	106 015	74+124	61.630	49.675
4300	107.380	74.000	61.845	49.796
4400	107.834	74.040	62.051	49.916
4500	108.278	74 053	60 450	50.031
4600	108.712	75,140	62.40	50.143
4700	109,137	75,341	60 020	50.252
4800	109.553	75,590	63 005	1 5U-359
4900	109,962	75 710	67 007	50.461
5000	110.361	75 203	63 300	· 50.561
5100	110.753	76,060	63 560	50.057
5200	111,138	76.243	63 734	50.755
5300	111.514	76.412	63.003	50.852
5400	111.884	76.570	64 060	50.947
5500	112.248	76.743	64 020	
5600	112.604	76,903	64.300	51 001
5700	112,955	77.062	64.540	51 300
5800	113,299	77,217	64 704	51 305
5900	113.637	77.369	64 056	51.095
6000	113.972	77.519	65 005	51 564

TABLE II - ENTROPY OF GASES AT 1 ATMOSPHERE

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	Free-e	nergy function	of gases, $-\frac{F_1}{T_1}$	$\frac{P_{\rm c}}{T} - H_{\rm O}^{\rm o}$
		cal/mole	э <b>-</b> <sup>о</sup> К	
Temperature (°K)	BF3	BF	BH	В
Temperature (°K) 1000 1100 1200 1300 1400 1500 1600 1700 1800 2000 2100 2200 2300 2400 2500 2600 2700 2600 2500 2600 2500 2600 2500 2600 2500 2600 2500 2600 2500 2600 2500 2600 2700 2600 2700 2600 2700 2600 2700 2600 2700 2600 2700 2600 2700 2800 2900 2900 2900 2900 2900 2900 29	BF <sub>3</sub> 65.286 66.639 67.907 69.098 70.223 71.288 72.299 73.261 74.179 75.057 75.898 76.705 77.481 78.228 78.947 79.642 80.314 80.963 81.600 82.202 82.794 83.369 83.927 84.470 84.999 85.515 86.017 86.507 86.985 87.452 87.908 88.354 88.791	BF 54.147 54.876 55.549 56.173 56.756 57.302 57.816 58.302 58.762 59.199 59.616 60.014 60.395 60.761 61.111 61.449 61.774 62.088 62.391 62.684 62.968 63.243 63.2510 63.768 64.020 64.265 64.503 64.735 64.961 65.182 65.397 65.607 65.813	BH 42.515 43.203 43.836 44.428 44.971 45.485 45.969 46.427 46.861 47.275 47.669 48.046 48.408 48.755 49.088 49.409 49.719 50.019 50.313 50.589 50.860 51.134 51.379 51.628 51.870 52.105 52.335 52.558 52.776 52.989 53.197 53.400 53.599	$\begin{array}{r} B\\ 37.665\\ 38.115\\ 38.544\\ 38.949\\ 39.329\\ 39.329\\ 39.689\\ 40.021\\ 40.331\\ 40.619\\ 40.881\\ 41.123\\ 41.358\\ 41.592\\ 41.814\\ 42.026\\ 42.234\\ 42.431\\ 42.621\\ 42.802\\ 42.977\\ 43.142\\ 43.297\\ 43.142\\ 43.297\\ 43.454\\ 43.606\\ 43.753\\ 43.606\\ 43.753\\ 43.606\\ 43.753\\ 43.606\\ 43.753\\ 43.899\\ 44.038\\ 44.178\\ 44.314\\ 44.446\\ 44.574\\ 44.574\\ 44.700\\ 44.920\\ \end{array}$
4200 4300 4400 4500 4600 4700 4800 5000 5100 5200 5300 5200 5300 5400 5500 5600 5700 5800 5900 6000	88.791 89.218 89.636 90.046 90.839 91.224 91.603 91.974 92.339 92.697 93.048 93.393 93.733 94.067 94.395 94.718 95.036 95.349	65.813 66.013 66.210 66.402 66.590 66.774 66.954 67.131 67.305 67.475 67.642 67.806 67.967 68.125 68.280 68.433 68.583 68.730 68.876	53.598 53.792 53.982 54.166 54.350 54.529 54.704 55.044 55.210 55.372 55.531 55.688 55.842 55.842 55.993 56.142 56.288 56.432 56.574	$\begin{array}{r} 44.820\\ 44.941\\ 45.056\\ 45.169\\ 45.278\\ 45.384\\ 45.487\\ 45.587\\ 45.683\\ 45.782\\ 45.683\\ 45.782\\ 45.879\\ 45.973\\ 46.066\\ 46.158\\ 46.247\\ 43.335\\ 46.422\\ 46.507\\ 46.590\end{array}$

# TABLE III - FREE-ENERGY FUNCTION OF GASES

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		TABI	LE IV - PHYSICA	L-CHEMICAL PR(	OPERTIES	OF PROPE	<b>LLANTS</b>			
		Tempers	atures in super	scripts, <sup>o</sup> C.	Referenc	ses in pe	rentheses.			
Propellants	Mole- cular weight M	Density (gram/cc)	Enthalpy of formation, $\Delta H_{f}$ (k-cal/mole)	Enthalpy of vapor- ization, AH (k-cal/mole)	Boil- ing point (OC)	Freez- ing point (oc)	Vapor pressure (mm)	Refractive index nD	Viscosity (centipoises)	
Diborane	27.688	(11qu1d) 0.4818-129.5 (12)	(gas) -4425 (3)	3.1 <sup>18</sup> (15)	-92.5 (2)	-165.5 (2)	212.23 <b>-</b> 112 (16)			
Fluorine	38.000	(11qu1d) 1.14-200 (16)	(gas) 0 <sup>25</sup>	1.60 <sup>-188</sup> (15)	-188 (15)	-223.0 (2)	760,-187.92 (14)	(gas) 1.00019520		
Fluorine oxide	54.000	(11qu1d) 1.90 <sup>-223</sup> .8 (2)	(gas) 5.5 <sup>25</sup> (14)	2.65-144.9 (14)	-144.9 (14)	-223.8 (2)	760-144.9 (14)			
Oxygen	32.000	(11qu1d) 1.14-183 (2)	(gas ) 0 <sup>25</sup>	1.629 <sup>-</sup> 183 (15)	-183.0 (2)	-218.4 (2)	760-182.97	(liquid) 1.221-181	(11qu1d) 0.189-252.07 (96%)	
Hydrogen peroxide	34.016	(11qu1d) 1.436 <sup>25</sup> 8(13)	(liquid) -45,218 (15)	11.61 <sup>18</sup> (15)	152.1 (2)	-0.89 (2)	2.1 <sup>25</sup> (14)	(11qu1d) (1413922 (13)	(11quid) (11quid) 1.30718 (13)	
<sup>a</sup> Extrapolate	d.								NACA	

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peliant chamber density temperatu (gram/y temperatu (gram/y temperatu (gram/s) (°K) (°K) (°K) (°K) (°K) (°K) (°K) (°K	Tre molecular weight in combustion chamber, Mc (gram/mole) gram/mole) 23.53 22.23 20.80 23.53 20.80 23.53 20.80 23.53 20.80 23.53 20.80 23.53 20.80 23.53 20.80 19.72 19.82 19.82	Specific 1 1 b = sec/1 b) 1 b = sec/1 b) 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	Volume specific impulse, Id [mpulse, Id [b-sec [cu ft (62.43] 291.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 290.8 249.5 249.5 249.5	Tempor- a ture at nozzle exit, Te (°K) (°K) 2655 2655 2655 2655 2655 2655 2655 265	Specific impulse, I (lb-sec/lb) 315.5 317.9 318.4 318.4 318.9 307.1	Volume specific impulse, Id 1mpulse, Id 317.0 315.2 309.8 295.6 293.7 281.6 265.6 265.6	Temper- ature at nozzle exit, Te (oK) 4270 4298 4113 3650 3650 3650 3389 3122 3122	Mean molecular weight at nozzie exit, Me (gram) mole) 26.30 24.59 22.55 21.68 22.55 21.68 20.55
1.005         5380           .993         5374           .993         5374           .993         5374           .993         5374           .928         4835           .928         4835           .928         4835           .928         4835           .9265         4940           1.403         4750           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.086         4007           .803         3953	24.00 23.53 22.23.53 20.680 20.680 20.680 20.680 19.682 19.83 19.83 19.83 19.83 19.83		246 + F2 291.2 290.8 286.3 286.3 277.5 277.5 277.5 277.5 249.5 249.5 249.5 249.5 249.5 249.5 249.5 249.5 249.5 26 + F20	2655 2667 2640 2481 2481 2451 2287 2287 2287 2110	315.5 317.4 322.4 318.4 317.9 317.9 307.1	317.0 315.2 309.8 295.6 293.7 281.6 265.6	4270 4298 4113 3600 3122 3122	26.87 26.87 24.59 22.73 22.56 21.668 20.568 20.568 20.568
1.005         5380           .993         5374           .961         5240           .928         5374           .928         5374           .928         5374           .928         5374           .928         5374           .928         5374           .928         5374           .928         4467           .965         4040           1.403         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.187         4701           1.086         4007           1.086         3953	24.00 23.53 23.53 20.68 19.68 19.83 19.83 19.83 19.83 19.83 19.83	m         m           m         m	291.2 290.8 290.8 286.3 277.5 277.5 277.5 277.5 2864.3 2644.3 249.5 249.5 249.5	2655 2667 2640 2481 2451 2451 2287 2287 2287 2287 2287	315.5 317.6 322.4 318.4 317.9 307.1 307.1	317.0 315.2 315.2 309.8 295.6 293.7 285.6 281.6 265.6 265.6	4270 4298 4113 3650 3560 3389 3122 3122	26.87 26.30 24.59 22.73 22.56 22.56 22.56 22.56 21.66 22.66 21.66 20.56
• 993 • 961 • 928 • 928 • 928 • 928 • 928 • 928 • 4835 • 900 • 4467 • 965 • 4040 • 1,403 • 4700 • 1,529 • 4007 • 1,529 • 4701 • 1,143 • 4700 • 1,529 • 4701 • 1,143 • 4701 • 1,143 • 4,709 • 1,086 • 4,007 • 4,709 • 1,086 • 4,007 • 4,709 • 1,086 • 4,007 • 4,007 • 4,007 • 4,007 • 4,000 • 1,086 • 4,007 • 4,000 • 1,086 • 4,007 • 4,000 • 1,086 • 4,000 • 1,086 • 4,000 • 4,000 • 1,087 • 4,000 • 1,086 • 4,000 • 4,000 • 1,087 • 4,000 • 1,000 • 4,000 • 4,000 • 1,000 • 4,000 • 1,000 • 4,000 • 1,000 • 1,0000 • 1,0000 • 1,0000 • 1,0000 • 1,00000 • 1,00000 • 1,0000000 • 1,000000000000000000000000000000000000	23.53 23.53 20.680 23.53	0 0 0 0 0 0 0 0 0 0 0 0 0 0	290.8 286.3 277.5 277.5 277.5 264.3 264.5 264.5 249.5 249.5 249.5	2667 2640 2481 2451 2287 2110 2110	317.4 322.4 318.4 317.9 317.9 307.1	315.2 309.8 293.6 2893.7 2881.6 2881.6 2881.6 2881.6	4298 4113 3650 3589 3122 3122	24.59 24.59 22.56 28.73 28.73 28.73 28.73 28.73 28.73 28.73 29.73 20.75 20.75
•961 5240 •928 4900 •928 4900 •924 4835 •900 4467 •965 4040 •965 4040 •965 1.329 1.086 4750 1.143 4750 1.143 4750 1.143 4750 1.143 4750 1.086 4007 0.890 3953	22.23 20.80 20.80 20.80 23.03 19.83 19.83 19.83 19.83 23.03	0000 000000000000000000000000000000000	286.3 277.5 277.5 277.5 264.3 249.5 249.5 249.5	2640 2481 2451 2287 2110	322.4 318.4 317.9 317.9 307.1	309.08 293.0 293.0 209.0 200.0	4113 3650 3660 3389 3122 3122	24.59 22.73 22.56 21.68 20.55
• 928 • 928 • 924 • 924 • 965 • 965 • 4040 • 467 • 465 • 1.403 • 4750 • 4750 • 1.086 • 4750 • 1.329 • 4701 • 1.87 • 4607 • 1.086 • 4007 • 1.086 • 3953 • 953 • 955	20.680 20.682 19.72 23.03 21.97 19.83 19.83 222 222	0 0 0 0 0 0 0 0 0 0 0 0 0 0	277.5 275.5 264.3 264.5 249.5 249.5 2H6 + P20	2481 2451 2287 2110	318.4 317.9 312.9 307.1	295.6 293.7 281.6 265.6	3650 3600 3389 3122	22-73 22-56 21-68 20-55
• 924 4835 • 900 4467 • 965 4040 • 4467 • 4667 1.403 4750 1.187 4701 1.187 4701 1.187 4701 1.187 4701 1.086 1.086 0.890 3953 0.890 3953	20.62 19.72 19.72 19.83 19.83 19.83	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	275.5 264.3 249.5 2H6 + P20	2451 2287 2110	317.9 312.9 307.1	293.7 281.6 265.6	3600 3389 3122	22.55 21.68 20.55 20.55
• 900 4467 • 965 4040 1.403 4750 1.329 4701 1.187 4701 1.187 4701 1.187 4701 1.086 4007 0.890 3953	19.72 18.76 23.03 21.97 19.83 19.83	0000 0000 0000000000000000000000000000	264.3 249.5 249.5 249.5 249.5	2287 2110	512.9 307.1	281.6 265.6	3389 3122	20.55 20.55
1.403 1.329 1.187 1.187 1.187 4701 1.187 4701 1.187 4701 1.086 1.086 1.086 1.086 1.086 1.086 1.086 1.086 1.0890 1.0860 1.0860 1.0800 1.0000 1.0800 1.0000 1.0800 1.0800 1.0800 1.0800 1.0800 1.0000 1.0000 1.0000 1.0000 1.0000 1.00000 1.0000 1.0000 1.00000 1.00000 1.00000 1.00000 1.00000000	23.03 21.97 19.83 19.22	р 2000 2000 2000 2000 2000 2000 2000 20	2H6 + F20					
1.403 4750 1.329 4701 1.187 4701 1.143 4700 1.143 4309 1.086 4007 0.890 3953	23.03 21.97 19.83 19.22	280°0 286°0 286°0	0 002					0 - 30
1.329 1.187 1.143 1.143 4.460 1.143 4.460 1.143 4.007 1.086 4.007 0.890 3.953 3.990	21.97 19.83 19.22	286.0		2432	302.3	424.2	3737	
1.187 1.143 1.143 1.086 4007 4.007 4.007 4.007 4.007 0.890 3.953 3.990	19.83	0 200	380.1	2440	309.2	410.9	3749	23,95
1.143 4309 1.086 4007 0.890 3953 0.873 3990	19.82	20000	350.2	2373	316.2	375.3	3493	21.53
1.086 4007 0.890 3953 .873 3990		295.3	337.4	2315	314.7	359.6	3357	20.93
0.890 3953	18•49	293 <b>.</b> 5	318•7	2216	311.3	338 O	3172	20.14
0.390 3953 .873 3990		Д	<sup>2,4</sup> 6 + 02				•	
•873 3990	23.98	261.3	232.4	2438	270.9	241.0	3139	26.08
	. 23.10	267.5	233 <b>.</b> 6	2462	278.2	242.8	3170	25,16
2207 750	21.50	278.3	234.8	2475	288.2	243.2	3176	23,38
•786 3915	18.42	295.4	232.3	2380	305.3	240.1	2980	19.78
•760 3740	11.11	299 9 299 2	227.9	2240	311.4	236.7	2830	18.21
0095 C41.	10°47	294•7	C+812	2086	303.5	226.1	2481	17.27
		B2	. H <sub>6</sub> + H <sub>2</sub> 02					
1.250 2858	22.48	230.6	288.2	1780	234.9	293.5	1968	22,95
1.161 3218	21.41	251.2	291.7	2042	259.1	300.9	2467	22.56
1.009 3204	17.99	271.7	274.2	1980	277.4	280.0	2197	18.50
.913 3020	15.69	281.2	256.7	1814	284.3	259.6	1931	15,95
. 846 2846	14.16	285.8	241.9	1672	289.3	245.4	1899	14.69
•825 2473	13.60	270.2	223.0	1422	279.2	230 <b>.4</b>	1845	14,80

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Figure 1. - Theoretical performance of diborane with liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide. Isentropic expansion from 20.4 to 1 atmosphere.





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Figure 1. - Continued. Theoretical performance of diborane with liquid fluorine, liquid fluorine oxide, liquid oxygen, and 100percent hydrogen peroxide. Isentropic expansion from 20.4 to 1 atmosphere.





conditions.

Figure 2. - Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide.



exit conditions.

Figure 2. - Continued. Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide.



Figure 2. - Continued. Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide.

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(d) Liquid fluorine oxide  $F_20$ ; equilibrium nozzle-exit conditions.

Figure 2. - Continued. Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100percent hydrogen peroxide. 27



(e) Liquid oxygen 02; combustion-chamber conditions.





conditions.

Figure 2. - Continued. Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100-percent hydrogen peroxide.

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Figure 2. - Concluded. Composition of products of reaction of diborane with liquid fluorine oxide, liquid oxygen, and 100percent hydrogen peroxide.