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COMPARISON OF EXPERIMENTAL AND KINETICALLY LIMITED THEORETICAL PERFORMANCE OF THE HYDROGEN-FLUORINE PROPELLANT SYSTEM

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SUMMARY

Theoretical calculations of the performance of a hydrogen-fluorine (H - F) rocket engine were performed, and the results were compared with experimental data for three nozzles, each with an area ratio of 100. The chamber pressure was 60 pounds per square inch absolute, and oxidant-fuel ratios from 7 to 19 were used. A one-dimensional theoretical model, used with an assumed reaction mechanism and rates, gave results in good agreement with experiment for the contoured and 25°-angle conical nozzles. Results for the longer 15°-angle conical nozzle agreed qualitatively but not quantitatively with experiment. The theoretical results agreed with the experimentally observed trend of performance with change in nozzle configuration. Variation of the H + H recombination rate had about the same absolute effect on performance over the entire oxidant-fuel ratio range, whereas variation of the H + F recombination rate had a much larger absolute effect at high oxidant-fuel ratio values than at low values. The assumed rate for the H + F recombination, which gave reasonable agreement between theory and experiment, was consistent with the recently published theoretical and experimental rate information on this reaction.

Also, the kinetically calculated gas temperature profile through the contoured nozzle was not highly sensitive to increase in the oxidant-fuel ratio.

INTRODUCTION

A considerable amount of interest has been shown during the last few years in the calculation of nonequilibrium performance of liquid rocket propellant systems. In particular, the hydrogen-fluorine (H - F) system has received recent attention in references 1 and 2. These workers integrated the exact equations of one-dimensional, chemically reacting flow and studied the effect of various reaction rates on the specific impulse of this propellant combination. Most of the rate variation was done at a chamber pressure of 300 pounds per square inch absolute, a rather high value for the study of nonequilibrium effects, which are less important at this pressure than at lower values.

Reference 1 assumes the following reaction mechanism, which considers the hydrogen recombination as three separate three-body reactions:

$$H + H + H_2 \rightleftarrows 2H_2 \qquad \text{(I)}$$

$$H + H + H \rightleftarrows H_2 + H \qquad \text{(II)}$$

$$H + H + HF \rightleftarrows H_2 + HF \qquad \text{(III)}$$

$$H + F + M \rightleftarrows HF + M \qquad \text{(IV)}$$

$$F + H_2 \rightleftarrows HF + H \qquad \text{(V)}$$

where M is the generalized third body. In reference 1, performance is given as a function of initial mixture composition for one set of rate constants. The main conclusion is that an increase in the rate of reaction III increases the calculated performance to the level of the higher observed experimental performance. No other rates were changed to determine their effect.

The work of reference 2 assumes the following mechanism:

$$H + F + M \rightleftarrows HF + M \qquad (\Delta H^{o}_{298} = -136 \text{ kcal/mole}) \qquad \text{(IV)}$$

$$F + H_2 \rightleftarrows HF + H \qquad (\Delta H^{o}_{298} = -32 \text{ kcal/mole}) \qquad \text{(V)}$$

$$H + H + M \rightleftarrows H_2 + M \qquad (\Delta H^{o}_{298} = -104 \text{ kcal/mole}) \qquad \text{(VI)}$$

$$F + F + M \rightleftarrows F_2 + M \qquad (\Delta H^{o}_{298} = -38 \text{ kcal/mole}) \qquad \text{(VII)}$$

$$H + F_2 \rightleftarrows HF + F \qquad (\Delta H^{o}_{298} = -98 \text{ kcal/mole}) \qquad \text{(VIII)}$$

where ΔH^{o}_{298} is the heat of reaction. Reference 2 presents a sensitivity study to determine the relative effect of reactions IV and VI on overall performance. The rate constant for each of these reactions was individually changed, while all other rates were held constant. In this way, the individual effects of reactions IV and VI on performance were calculated at a chamber pressure of 300 pounds per square inch absolute for two oxidant-fuel ratios (o/f) of 8 and 19. Results show that performance is quite sensitive to the rate of reaction VI (the H atom recombination) at the fuel-rich o/f = 8 and rather insensitive to the rate of reaction IV (the H + F atom recombination). For o/f = 19 (close to the stoichiometric value of 18.85), performance is more sensitive to the rate of reaction IV, although reaction VI still plays a very significant role. This trend is the expected one, since F atom concentration is low during the entire expansion at o/f = 8 and high at o/f = 19.

Because experimental hydrogen-fluorine reaction rate data are scarce, there has not yet been any satisfactory comparison between experimental performance data and theoretical kinetically limited calculations. This type of comparison is desirable in evaluating the ability of a one-dimensional idealized model to approximate the performance of a real three-dimensional process. By comparison of experimental and theoretical results it may be possible, in some cases, to determine which of several proposed rate constant expressions is most reasonable for a given chemical reaction.

Inasmuch as additional rate data have become available recently, a program was undertaken to perform one-dimensional theoretical performance calculations which could be directly compared with experimental data. The purpose of this work is twofold: (1) to determine how well both the trends and the magnitudes of the experimental data can be theoretically predicted and (2) to find out which set of several proposed rate constant expressions comes closest to predicting experimental results for the particular experimental engine and nozzles under consideration. Therefore, theoretical performance of hydrogen-fluorine mixtures was calculated for the test conditions used by Aukerman and Church (ref. 3). A chamber pressure of 60 pounds per square inch absolute was used for all calculations, and the oxidant-fuel ratio was varied from 7 to 19. The engine thrust was approximately 1400 pounds. Reaction rate constants were systematically changed to determine the effect on performance of both the hydrogen and the hydrogen fluoride recombination rates. Several recently proposed rate equations for the latter reaction are compared to determine which one gives theoretical results in best agreement with experiment.

THEORY AND INPUT DATA

Computer Program

The computer program used in these calculations is one developed under NASA contract and described in references 2 and 4. The assumptions involved are as follows:

(1) One-dimensional inviscid flow
(2) Thermally perfect gases
(3) Negligible transport properties
(4) All internal energies in thermal equilibrium

The assumption of microscopic reversibility is used to calculate the backward rate constant for any reaction from the ratio of the forward rate constant to the equilibrium constant. The equations of mass, momentum, and energy conservation plus the equation of state are solved simultaneously with the equations for the rates of change of species concentrations due to chemical reaction. The detailed equations are given in references 2 and 4.

Kinetic Mechanism and Species

Only four species (H, F, H_2, and HF) were used to set up the chemical reaction mechanism. For all oxidant-fuel ratios used herein, the concentration of molecular fluorine (F_2) is negligible in the combustion chamber and the convergent nozzle section. The chemical reaction in this nozzle section essentially controls the final performance, since the species concentrations effectively "freeze" to constant values soon after the gas enters the divergent nozzle section. The F_2 species was therefore dropped from consideration, and the complete mechanism used in all calculations consists of reactions IV, V, and VI. This mechanism does not include the effect of different third bodies in the recombination reactions.

The primary problem in using this mechanism is obtaining rate constant data for the chemical reactions. Only the hydrogen atom recombination (reaction VI) has been extensively studied experimentally. Rate constants for reactions IV and V generally have to be estimated theoretically or by analogy to reactions between similar species. The technique used herein was to choose a set of rates which were considered reasonable. Then, calculations are performed with these rates and with moderate variations of them to find the rates which best predict the available experimental data. The set of assumed rates used in this investigation was taken, essentially, from reference 1 and is listed in table I. The rate constant k_{VI} for reaction VI is an experimental value from reference 5. The value of k_{IV} was assumed equal to k_{VI}, and k_V was obtained from an analogy to the O + H_2 reaction.

During the course of this investigation, some new rate information concerning the value of k_{IV} was published. A theoretical expression for k_{IV}, calculated by using the recent cascade deactivation theory, was presented in reference 2. The relation is

$$k_{IV}(\text{argon}) = 4.91\times10^{15}\, e^{3050/RT} \qquad (\text{cm}^6/(\text{mole}^2)(\text{sec})) \tag{1}$$

TABLE I. - HYDROGEN-FLUORINE REACTION RATE PARAMETERS IN THE EXPRESSION

$k = DT^e \exp(-E_A/RT)$†

Reaction	D, cm, mole, sec	e	E_A, cal/mole
IV	7.5×10^{18}	-1	0
V	5×10^{12}	0	5700
VI	7.5×10^{18}	-1	0

†Where k is rate constant, D is preexponential constant, T is temperature in °K, e is temperature exponent, E_A is activation energy, and R is universal gas constant.

where the expression in the first parentheses is the third body, R is the universal gas constant (cal/(mole)(°K)), and T is the temperature (°K).

Until very recently there were no experimental data available for either the HF recombination or dissociation reactions. However, the latter reaction has recently been studied by Jacobs, Giedt, and Cohen in a shock tube in the temperature range of 3800° to 5400° K. Their rate expression for the dissociation of HF in an argon atmosphere is given in reference 6. By use of this rate expression along with a curve-fitted equation for the equilibrium constant of reaction IV, rate constants were calculated for k_{IV} and fitted to the equation k_{IV} = Constant/T over the temperature range 2000° to 5000° K. The resulting expression, obtained by a least-squares procedure, is

$$k_{IV}(\text{argon}) = \frac{3.0\times10^{18}}{T} \qquad (\text{cm}^6/(\text{mole}^2)(\text{sec})) \tag{2}$$

This relation was adjusted for the presence of mainly HF as the third body for the reaction, since this situation is the one existing in the rocket nozzle. In order to estimate the correction for using the polar HF molecule, the known third body effects on the recombination of H atoms were used as a guide. For the reaction $H + H + M \rightarrow H_2 + M$ the data in reference 7 indicate that H_2O is 15 times as efficient a third body as argon. The molecules HF and H_2O are both polar and have about the same molecular weight. Since HF has fewer vibrational degrees of freedom than H_2O, it should be less efficient. It was therefore assumed that HF should be about 10 times as efficient as argon for both recombination reactions. Hence, for the reaction $H + F + HF \rightarrow HF + HF$, the following rate expression can be written:

$$k_{IV}(\text{HF}) = \frac{3.0\times10^{19}}{T} \qquad (\text{cm}^6/(\text{mole}^2)(\text{sec})) \tag{3}$$

A graphic comparison of equations (1), (2), and (3) is shown in figure 1 along with the assumed rate of table I. Plotted also in this figure is k_{IV}(argon) calculated by ordinary collision theory (ref. 8). The rate of table I falls approximately halfway between the recently reported theoretical and experimental rates for argon as the third body. Excluding the collision theory rate, which is presented only for the sake of completeness,

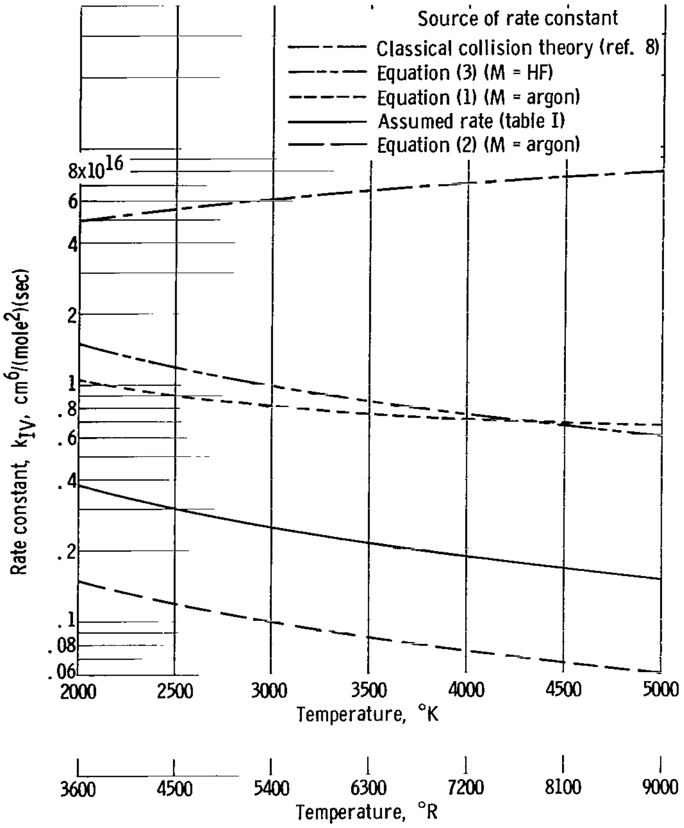


Figure 1. - Rate constant expressions for reaction $H + F + M \rightarrow HF + M$.

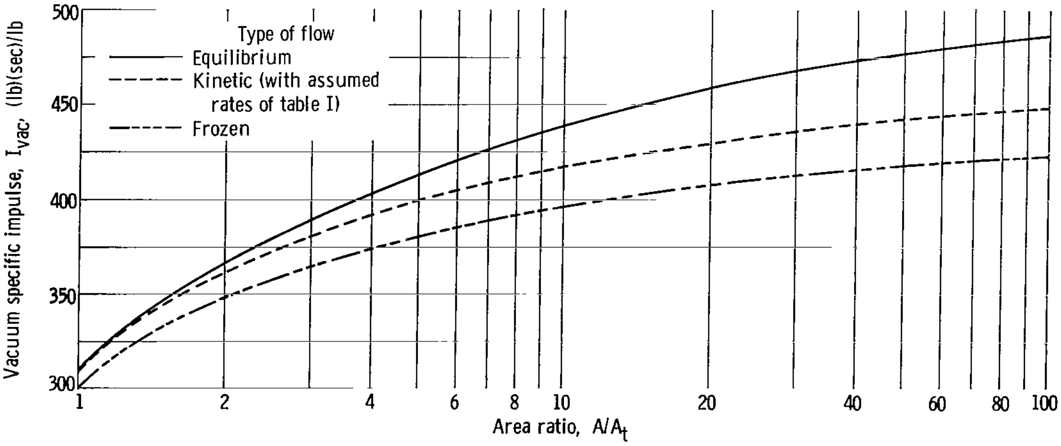


Figure 2. - Performance as function of area ratio for contoured nozzle. Chamber pressure, 60 pounds per square inch absolute; oxidant-fuel ratio, 9.

the remaining four rate expressions shown in figure 1 all agree within a factor of 10.

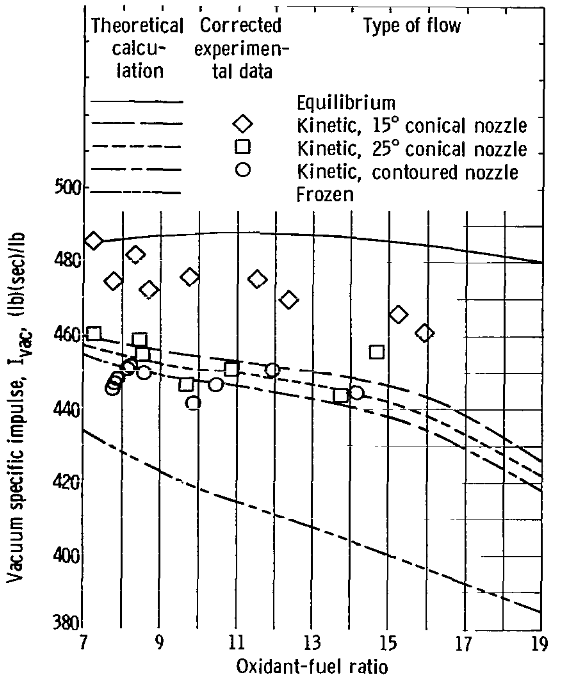


Figure 3. - Theoretical and experimental performance for three different nozzles. Chamber pressure, 60 pounds per square inch absolute; assumed reaction rates of table I used for all kinetic calculations.

Typical Results

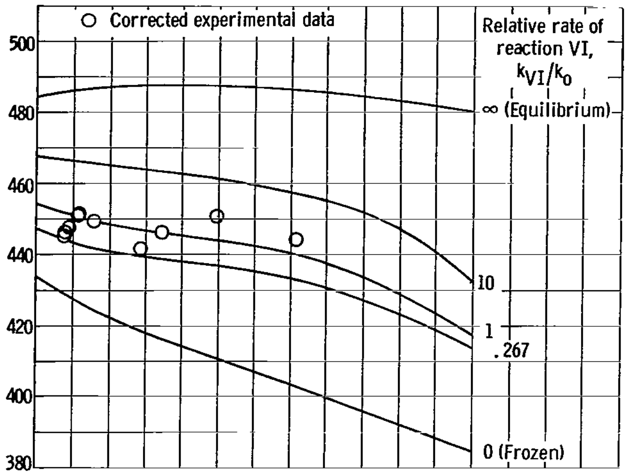
A sample kinetic calculation is shown in figure 2, where vacuum specific impulse I_{vac} is plotted against nozzle area ratio. Shown also are the performance curves for the limiting assumptions of infinite chemical reaction rates (chemical equilibrium flow) and zero chemical reaction rates (frozen flow). These limiting curves were calculated by using the performance program of Zeleznik and Gordon (ref. 9). The kinetic curve was calculated with the assumed rates of table I. Any changes in the various reaction rates move the kinetic curve between these two limits. The heats of reaction listed in the INTRODUCTION for reactions IV, V, and VI indicate that the recombination reactions IV and VI should be responsible for the majority of the heat release in the expanding gas. These reactions are, therefore, the ones to be varied first in attempting to obtain agreement between theoretical and experimental results.

RESULTS AND DISCUSSION

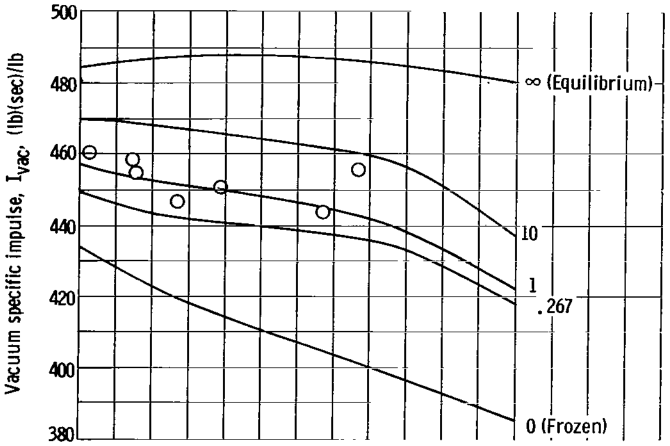
Comparison of Performance for Three Nozzle Configurations

Figure 3 presents theoretical and experimental performance data for three nozzle configurations, each having an exit area ratio A/A_t of 100. Nozzle 1 is a contoured nozzle, nozzle 2 is conical with an expansion half-angle of 25^{o}, and nozzle 3 is a longer conical nozzle with a half-angle of 15^{o}. For each nozzle, the vacuum specific impulse I_{vac} is shown as a function of o/f. The theoretical calculations employ the assumed rates of table I.

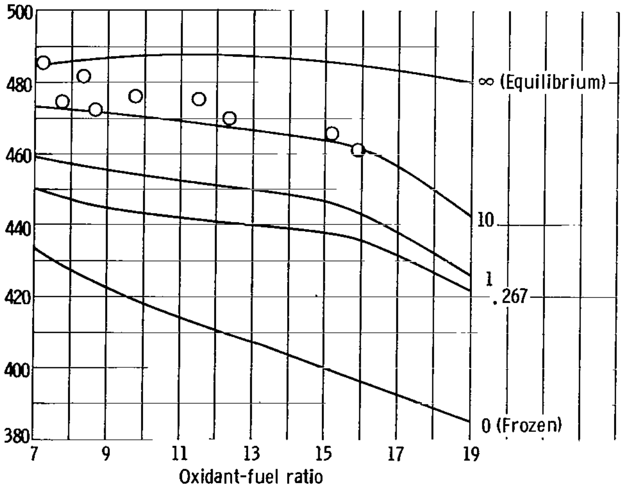
Experimental data are reported in reference 3. They have been corrected for nozzle divergence losses and combustion inefficiency by dividing the experimental value by the



(a) Contoured nozzle.



(b) 25° Conical nozzle.



(c) 15° Conical nozzle.

Figure 4. - Experimental and theoretical performance comparison with variation of k_{VI}. Chamber pressure, 60 pounds per square inch absolute; area ratio, 100; assumed rate of table I used for reaction IV in all kinetic calculations.

product of two correction factors, λ and η_{c*}. The nozzle divergence factor λ is calculated geometrically; the experimental characteristic velocities $c*$ used to calculate the efficiency factor η_{c*} were read from the average curve obtained by plotting the $c*$ data against o/f for all three nozzles.

The comparison in figure 3 shows that the theoretical curve is in reasonably good agreement with the experimental data for the contoured and the 25°-angle conical nozzles. For the longer conical nozzle, the theoretical line has the correct slope but lies considerably below all the experimental points. The theory gives the correct qualitative trend of performance with change in nozzle configuration. It does not, however, predict the magnitude of the experimentally observed increase in performance level in changing from the short to the long conical nozzle.

Effect of Recombination Rates on Performance

In order to determine the effect of individual reaction rate variations on the results just presented, the rates of each of the recombination reactions IV and VI were separately varied, while the other was held constant at its assumed rate. Figure 4 shows the effect on theoretical performance of varying the hydrogen atom recombination rate k_{VI}. Three different values of k_{VI} were used for all three nozzles. It is convenient to describe the rate variation in terms of the relative rate k_j/k_o, where k_j is the rate constant actually used for reaction j, and k_o is the assumed rate of table I for this same reaction. The three values of k_{VI}/k_o used for reaction VI are 0.267, 1.0, and 10. The rates found in the literature lie within this range (refs. 6 to 8). The value of k_{IV}/k_o was held at 1.0 for all cases.

The separate performance curves of figure 4 for the three nozzles show more clearly the result observed in figure 3. The assumed rate $k_{VI}/k_o = 1$ gives good agreement with experimental data for the first two nozzles, but k_{VI}/k_o has to be increased to 10 in order to get good quantitative agreement for the 15°-angle conical nozzle. A significant point shown in figure 4 is that a change in k_{VI} causes about the same absolute change in performance over the entire o/f range for all nozzle configurations. The theoretical slopes are in close agreement with the experimental trend of performance with o/f for all nozzles. This result shows that any other k_{VI} value within the limits previously stated would change all three theoretical lines in figure 3 by about the same amount and not affect their separation. If the assumed rates are used for all other reactions, there is apparently no single expression for k_{VI} which accurately predicts experimental results for all three nozzles.

Figure 5 shows the results of varying the H + F recombination rate constant k_{IV} while k_{VI}/k_o was maintained at the value 1.0. Results are shown for the contoured

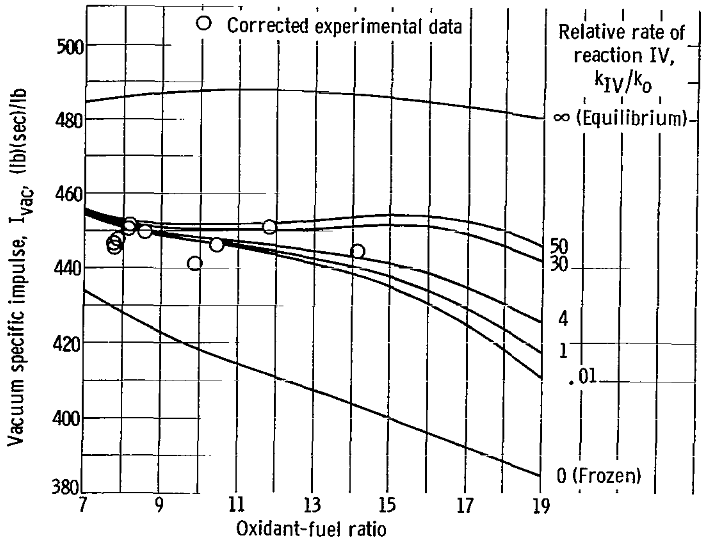
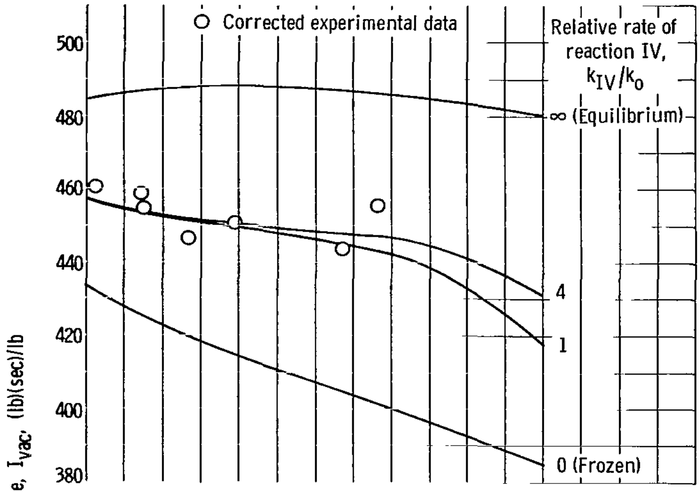


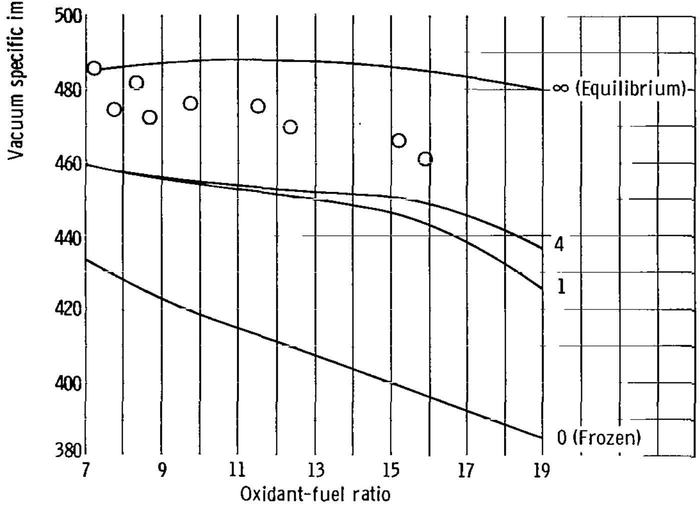
Figure 5. - Theoretical and experimental performance comparison for contoured nozzle with variation of k_{IV}. Chamber pressure, 60 pounds per square inch absolute; area ratio, 100; assumed rate of table I used for reaction VI in all kinetic calculations.

nozzle only. Inasmuch as k_{IV} is more uncertain than k_{VI}, the value of k_{IV}/k_o was varied from 0.01 to 50. The curves of figure 5 show that changing k_{IV} has no significant effect on performance in the low o/f (fuel-rich) range. This result is expected, since F atom concentration in the combustion chamber is low under these conditions. The effect of k_{IV} on performance increases, however, with increasing o/f, and the result is a change in the trend of I_{vac} with o/f. The theoretical curve for $k_{IV}/k_o = 4$ predicts the experimental data about as well as the curve for $k_{IV}/k_o = 1$. When k_{IV}/k_o is increased to 30 and 50, however, the theoretical performance trend seems to deviate from that observed experimentally. Therefore, increasing k_{IV} will not improve the agreement between theory and experiment. Decreasing k_{IV} by a factor of 100 has either a negligible or a small effect on performance over the entire o/f range.

Figure 1 shows that the recent theoretical and experimental work on the rate of the $H + F + M \rightarrow HF + M$ reaction gives rates ranging from 0.4 to 4 times the assumed rate constants calculated from the equation of table I. The results of figure 5 show that the newer rate expressions and the present assumed k_{IV} rate all give theoretical performance results consistent with the experimental data for the contoured nozzle. (Results for $k_{IV}/k_o = 0.4$ would be essentially the same as those for $k_{IV}/k_o = 1$.) In figure 6, theoretical results are shown for the two conical nozzles with $k_{IV}/k_o = 1$ and 4, while k_{VI}/k_o is maintained at 1.0. For each nozzle, both theoretical lines give trends consistent with the theoretical data and with the corresponding theoretical trends for the contoured nozzle.



(a) 25° Conical nozzle.



(b) 15° Conical nozzle.

Figure 6. - Experimental and theoretical performance comparison for conical nozzles with variation of k_{IV}. Chamber pressure, 60 pounds per square inch absolute; area ratio, 100; assumed rate of table I used for reaction VI in all kinetic calculations.

Effect of $F + H_2 \rightleftarrows HF + H$ Reaction on Performance

On the basis of energy considerations, it was stated previously that the three-body recombination reactions IV and VI should be more important in determining performance than the two-body shuffle reaction V. Obviously, the importance of a reaction depends on additional factors, for example, rate constant value and concentrations of reactants. A significant increase in k_V at any given temperature would have several effects on species concentrations. Some effects would tend to decrease the net heat release into the flowing gases, while others would tend to increase this heat release. The actual effect of a given

TABLE II. - EFFECT OF REACTIONS IV AND V

ON PERFORMANCE

[Contoured nozzle; chamber pressure, 60 psia; area ratio, 100; vacuum specific impulse $(I_{vac})_0$ calculated with all relative reaction rates equal to 1.0; vacuum specific impulse $(I_{vac})_{IV}$ calculated with only k_{IV}/k_o increased to 100; vacuum specific impulse $(I_{vac})_V$ calculated with only k_V/k_o increased to 100.]

Oxidant-fuel ratio, o/f	$(I_{vac})_{IV}/(I_{vac})_0$	$(I_{vac})_V/(I_{vac})_0$
9	1.009	1.002
13	1.029	1.004
15	1.049	1.010
19	1.089	1.003

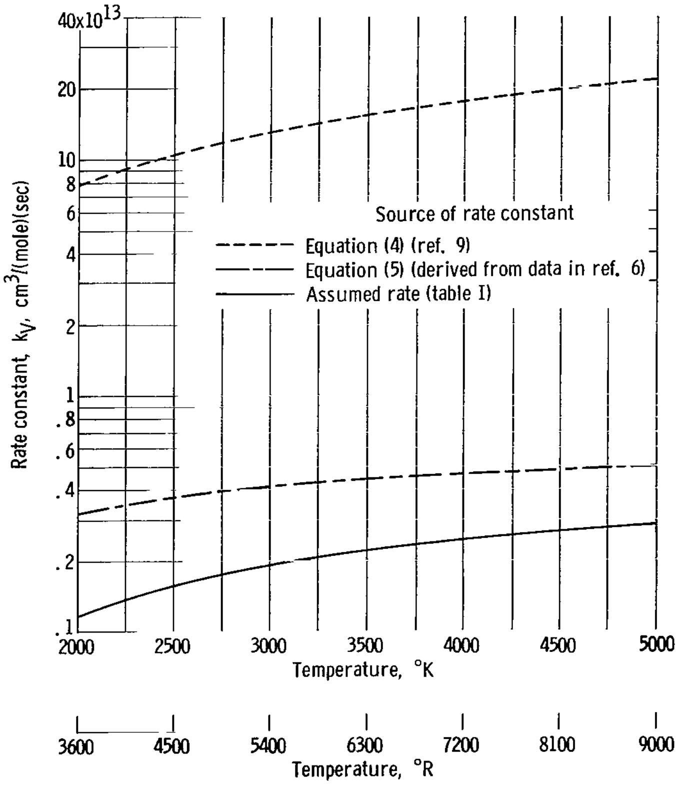


Figure 7. - Rate constant expressions for reaction F + $H_2 \rightarrow$ HF + H.

change in k_V on performance can be shown only by detailed calculations, and these calculations were performed at four o/f values. The results are shown in table II, in which the separate effects of reactions IV and V on performance are compared. In this table two dimensionless performance ratios are defined, and their values are listed at four o/f values. The ratio $\left(I_{vac}\right)_{IV}/\left(I_{vac}\right)_0$ shows the effect of increasing k_{IV}/k_o alone to 100, while $\left(I_{vac}\right)_V/\left(I_{vac}\right)_0$ shows the effect of increasing k_V/k_o alone to 100. All relative rates except the one changed are maintained at 1.0 in these calculations. At all o/f values used, the results show that the effect of increasing k_V alone is much less important than the effect of increasing k_{IV}. Moreover, the various effects of increasing k_V alone just about balance each other over the entire o/f range. The performance of the hydrogen-fluorine system is thus not sensitive to a two-order-of-magnitude increase in k_V. Nevertheless, because the assumed k_V (table I) was obtained by an analogy technique, it is germane to compare it with other published equations to ensure that the assumed k_V is not grossly in error. A theoretical expression for k_V and an experimental expression for k_{-V}, the reverse of reaction V, have recently been published. A graphic comparison of these two equations with the assumed k_V is shown in figure 7, in which the lowest line shows the assumed equation of this investigation, and the top line shows the theoretically calculated equation of reference 10, which is

$$k_V = 7.8\times10^{11}T^{0.69}e^{-2500/RT} \qquad (\text{cm}^3/(\text{mole})(\text{sec})) \tag{4}$$

The middle line of figure 7 shows the experimentally derived rate k_V obtained from the experimental rate given in reference 6 for k_{-V}. Equilibrium constants were used to convert the reverse rates to values of k_V at several temperatures between 2000° and 5000° K. These values were then curve-fitted by a least-squares technique which gave the following expression for k_V:

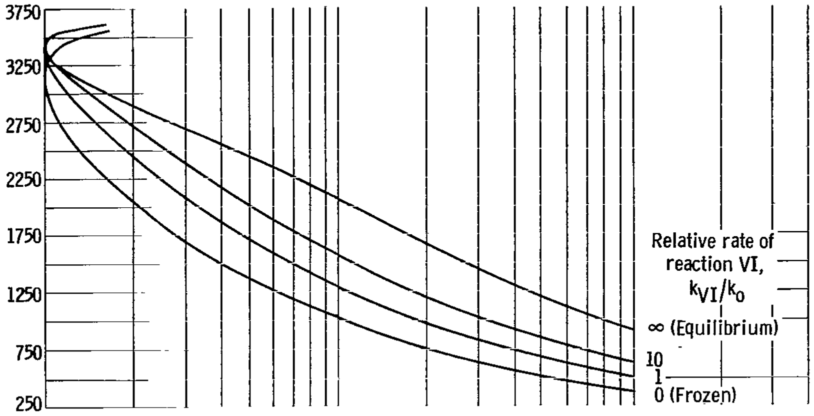
$$k_V = 2.04\times10^{13}T^{-0.12}e^{-3750/RT} \qquad (\text{cm}^3/(\text{mole})(\text{sec})) \tag{5}$$

It is apparent that the assumed rate agrees within a factor of 2 to 3 with the experimentally derived rate (eq. (5)), while it is lower than the rate of equation (4) by a factor of about 70. The results of table II show that the calculated results of the present investigation would be essentially unchanged if either equation (4) or (5) were used in place of the expression in table I.

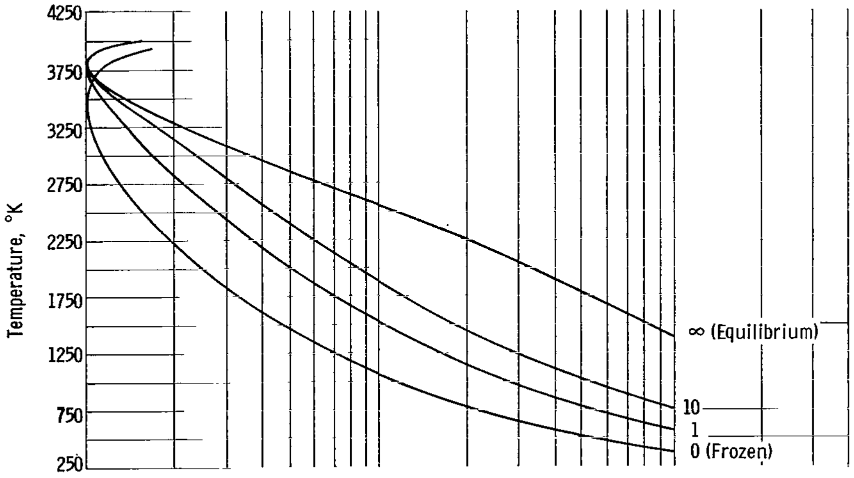
Nozzle Temperature Profiles

For nozzle cooling problems it will be of interest to compare kinetically calculated nozzle temperature profiles with the equilibrium and frozen profiles. This comparison is shown in figure 8, for the contoured nozzle with two different values of k_{VI} at three o/f values. Equilibrium temperatures exist up to the nozzle throat, after which the kinetic temperature drops much more rapidly than the equilibrium temperature. The profiles of figure 8 show that the kinetically calculated exit temperature is not very sensitive to change in o/f, whereas the equilibrium exit temperature increases significantly as o/f increases from 9 to 15.

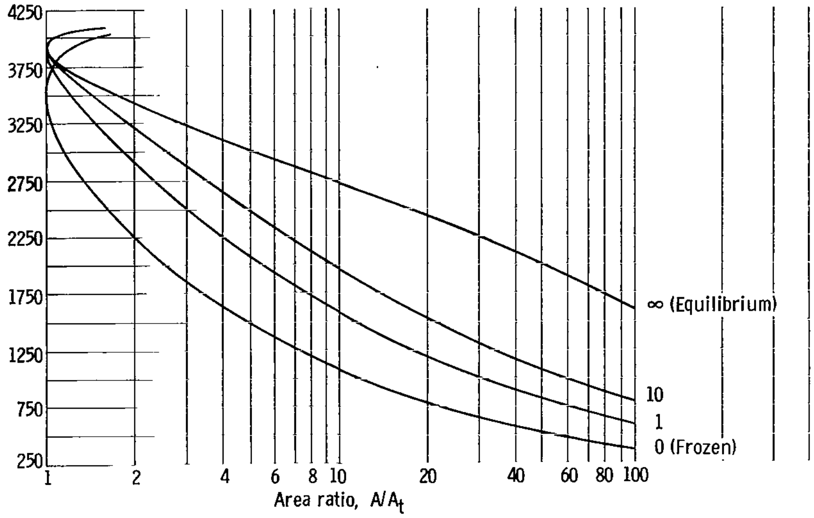
In figure 9 the temperature factor $(T_{kin} - T_{fr})/(T_{eq} - T_{fr})$ is plotted against oxidant-fuel ratio for the nozzle-exit area ratio. In this factor, T_{kin}, T_{fr}, and T_{eq} are the kinetic, frozen, and equilibrium gas temperatures, respectively. For any kinetic performance calculation, this temperature factor gives the fractional recovery of the maximum temperature difference $T_{eq} - T_{fr}$. Figure 9 shows that this fractional recovery decreases with increasing o/f for the entire range of o/f values from 7 to 19. The temperature factor plotted for any other fixed area ratio in the nozzle shows the same



(a) Oxidant-fuel ratio, 9.



(b) Oxidant-fuel ratio, 13.



(c) Oxidant-fuel ratio, 15.

Figure 8. - Temperature profile through contoured nozzle. Chamber pressure, 60 pounds per square inch absolute; assumed rates of table I used for reactions IV and V in all kinetic calculations.

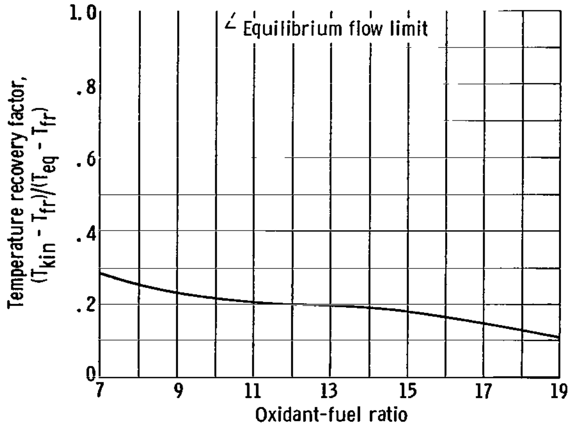


Figure 9. - Temperature recovery factor as function of oxidant-fuel ratio. Contoured nozzle; chamber pressure, 60 pounds per square inch absolute; area ratio, 100; assumed reaction rates of table I used for all kinetic calculations.

behavior. It can be concluded from figures 8 and 9 that the kinetically calculated free-stream gas temperature profile is rather insensitive to a change in the oxidant-fuel ratio at a chamber pressure of 60 pounds per square inch absolute.

GENERAL REMARKS

The fact that the theoretical calculations reported herein do not fully agree with experimental results has more than one interpretation. A one-dimensional idealized model was used to simulate a process which is at least two-dimensional in nature. However, it is doubtful that merely extending the idealized model to two dimensions will effect a great improvement in the agreement between theory and experiment. Additional changes in the model may help. These changes might include the addition of new chemical reactions and accounting for nonuniform mixing. An equally important factor that should be critically examined is the correction of the raw experimental performance data for various inefficiencies not considered in the model. The method used herein places all combustion losses together in the experimental c* efficiency η_{c*}. Although this technique has certain limitations, the three nozzles compared in the present investigation were all used with the same injector and combustion chamber during the experimental measurements. Therefore, no amount of manipulation of the c* data can alter the relative positions of the experimental performance curves for the three nozzles. Thus, the method of c* correction does not alter the conclusions from the comparison of the three nozzles. More work is needed, however, on the proper method of correcting experimental data to ideal conditions before a complete evaluation of any theoretical performance model can be given.

The present investigation has, nevertheless, given support to the use of a one-dimensional theoretical model. The theoretical results obtained with this model, by employing reaction rates which are consistent with experimental and theoretical rates, agree with the experimental trend of I_{vac} with o/f. The theoretical results also agree with the experimentally observed trend of performance in changing from one nozzle to another. These conclusions are strictly valid only for the nozzles and thrust level used. Evidence presented in reference 2, however, indicates that vacuum specific impulse is only slightly sensitive to thrust level up to a value of 100 000 pounds at a chamber pressure of 60 pounds per square inch absolute.

SUMMARY OF RESULTS

Theoretical calculations of the performance of a small-scale hydrogen-fluorine (H - F) engine with three different nozzles were performed for a chamber pressure of 60 pounds per square inch absolute and oxidant-fuel ratios from 7 to 19. Rates for the two important recombination reactions were varied from assumed values used herein, and results are compared with experimental data for the same nozzles and operating conditions. Temperature profiles through one nozzle are also presented. The results of this investigation are as follows:

1. The one-dimensional theoretical model, used with the assumed reaction mechanism and rates, gave results in good agreement with experiment for the contoured and the shorter conical nozzles. Results for the longer conical nozzle agreed qualitatively but not quantitatively with experiment. The theory agreed qualitatively with the observed trend of performance with change in nozzle configuration.

2. Changing only the hydrogen recombination rate caused approximately the same absolute change in performance for all oxidant-fuel ratios from 7 to 19. The slope of the performance curve remained essentially unchanged.

3. Changing only the H + F recombination rate had a much larger absolute effect on performance at high oxidant-fuel ratios than at low values. The slope of the performance curve was changed, and only a limited range of H + F recombination rates gave agreement with the experimental performance trend with oxidant-fuel ratio. The assumed rate constant k_{IV} for the reaction $H + F + M \rightleftarrows HF + M$ (where M is the third body) which gave good agreement with experiment, is consistent with the recently published theoretical and experimental information on this reaction.

4. The kinetically calculated gas temperature profile through the contoured nozzle was not highly sensitive to an increase in the oxidant-fuel ratio from 9 to 15.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, June 3, 1966,
129-01-02-01-22.

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