Engineering Notes

Correlations for Theoretical Rocket Thrust with Shifting Expansion

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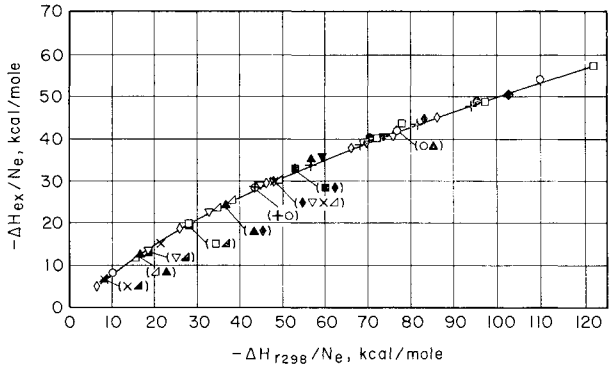
THE theoretical thrust of a chemical rocket with isentropic and shifting-equilibrium expansion after adiabatic combustion is not so adaptable to simplifying relations as when the expansion is frozen. However, empirical correlations between the theoretical enthalpy drop on equilibrium expansion at 1000 psia/1 atm ratio and the propellant heat of reaction at 298°K have been found which apply to diverse systems.[1] They provide an improved insight into the energy-to-thrust conversion process with equilibrium expansion and often permit simple computation of theoretical specific impulse to a good accuracy.

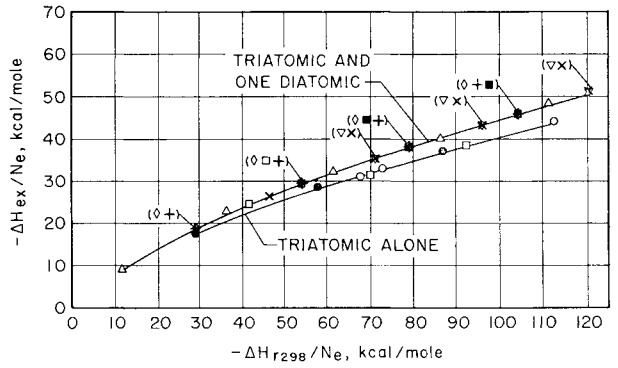
The correlations hold for propellants grouped with respect to the number of atoms per molecule of their major, or "effective," species without regard to dissociation. Then, theoretical heat drops on expansion per mole of the effective species, $-\Delta H_{ex}/N_e$, plotted vs heats of reaction per mole to the same species at 298°K, $-\Delta H_{r298}/N_e$, describe coincident curves for each group.

Figures 1 and 2 were constructed in this manner for an expansion ratio of 1000 psia/1 atm with shifting equilibrium



System	Symbol
$(HF)(H_2)_{0.5}$	○
(HF)(CO)	●
(LiF)(HF)	□
(LiF)(CO)	■
$(HF)(CO)(N_2)_{0.5}$	▲
$(HF)(H_2)_{1.5}$	◇
$(LiF)(HF)_2$	◆
$(HF)(H_2)_{2.5}$	▽
$(HF)_2(CO)(N_2)_{0.5}$	▼
$(LiF)(HF)_3$	+
$(HF)(H_2)_{4.5}$	×
$(HF)(H_2)_{6.5}$	◿
$(HCl)(N_2)$	◮

Fig. 1 Energy conversion of unambiguous diatomic species (1000 psia/1 atm, shifting expansion).



System	Symbol
(BOF)	○
(H_2O)	●
$(BOF)(MgF_2)$	□
(BOF)(HF)	■
$(H_2O)(HF)$	△
$(MgF_2)(HF)$	▽
$(BOF)(N_2)$	×
$(H_2O)(N_2)$	+
$(H_2O)(H_2)$	◇

Fig. 2 Energy conversion of unambiguous triatomic species, alone and with one diatomic (1000 psia/1 atm, shifting expansion).

from results obtained on a large electronic computer with all possible exhaust species considered and their accepted thermodynamic data[2] used, and with "propellant" formulations that comprised selected elemental combinations and associated heats of formation, as needed to define the curves. The results are applicable to actual systems whose elemental compositions and heats of formation fit the curves.

Figure 1 is the relation obtained for formulations that produce only diatomic-gas effective species. Figure 2 applies to systems that produce only triatomic gases and one triatomic plus one diatomic gas as effective species. Results for other combinations of effective species fit their media curves as well as do those of Figs. 1 and 2, leading to construction of loci curves exemplified in Fig. 3 for various ratios of diatomic-to-triatomic effective species, and similar curves are applicable to systems with other atoms/mole ratios of their effective species.

The foregoing energy input values (i.e., $-\Delta H_{r298}/N_e$) of about 25 kcal/mole, the loci curves coincide whenever the average number of atoms per molecule of all the effective species, N_A/N_e, are the same, which permits construction of the more general curves of Fig. 4 from a large proportion of almost 2000 computations.† Figure 4 applies to within a few percent to systems whose products are all gases, with the exception of the noble gases, and whose effective species are predictable. The last often requires that the oxidizer and fuel elements of the formulation be balanced to their (relatively) stable products, i.e., without excess of fuel or oxidizer elements to compete for deficient oxidizer or fuel.

The result leads to the postulate that the major species effectively act similarly with respect to shifting-equilibrium rocket thrust, regardless of differing degrees of dissociation; only the atoms/molecule of the effective species is critical.

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† An 8½- × 11-in. copy of Fig. 4, from which data can be accurately read, is available on written request to the author.

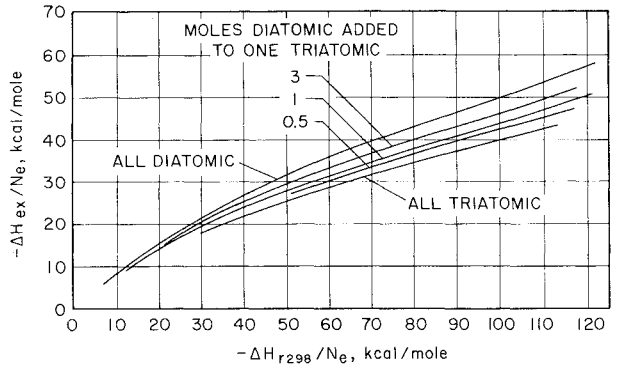

Fig. 3 Loci of energy conversion of unambiguous triatomic species with added diatomics (1000 psia/1 atm, shifting expansion).

For example, nitrogen and hydrogen (both diatomic) can be interchanged in the curves, although the latter dissociates much more than the former. The practical corollary is that the expansion energy of rocket formulations whose effective species are gaseous and predictable (as explained) can be estimated from the curves.

Theoretical specific impulse I_s is equal to 295 $(-\Delta H_{ex}/W)^{1/2}$ where $-\Delta H_{ex}$ is the theoretical expansion energy in kcal for W grams of propellant, and the constant 295 is the value of $(2J/g)^{1/2}$ for these units, J being the mechanical equivalent of heat and g the gravity constant. In using Fig. 4 to estimate I_s, the propellant is designated by its effective species through the applicable chemical equation and its $-\Delta H_{r298}$ to these species then determined by customary means. Dividing the latter by N_e, the moles of effective species, provides a value for direct entry into Fig. 4 on the proper N_A/N_e curve to obtain $-\Delta H_{ex}/N_e$. The latter, multiplied by N_e and divided by W, provides the necessary parameter for computing I_s.

An example for the nitrogen tetroxide-hydrazine system, formulated with 43 parts by weight of oxidizer (0.62 moles/100 g of propellant) and 57 parts by weight of fuel (1.34 moles), is given below for expansion from 1000 psia to 1 atm with shifting equilibrium:

$$0.62\ N_2O_4(l) + 1.34\ N_2H_4\ (l) = 2.48\ H_2O(g) + 1.96\ N_2(g) + 0.20\ H_2(g)$$

$$-\Delta H_{r298} = -[0.62\ (-5.4) + 1.34\ (12.0)] + [2.48\ (-57.8) + 0 + 0] = 156.1 \text{ kcal}$$

$$N_e = 2.48 + 1.96 + 0.20 = 4.64 \text{ moles effective species}$$

$$-\Delta H_{r298}/N_e = 33.7 \text{ kcal/mole}$$

$$N_A/N_e = [3\ (2.48) + 2\ (1.96) + 2\ (0.20)]/4.64 = 2.51 \text{ atoms/mole}$$

From Fig. 4, at this $-\Delta H_{r298}/N_e$ value and N_A/N_e curve (interpolating for the latter),

$$-\Delta H_{ex}/N_e = 20.7 \text{ kcal/mole}$$

$$-\Delta H_{ex} = 20.7\ (4.64) = 102.0 \text{ kcal}$$

Then, $I_s = 295\ (-\Delta H_{ex}/W)^{1/2} = 295\ [(102.0)/100.0]^{1/2} = 290$ sec, compared to I_s by machine computation = 291 sec.

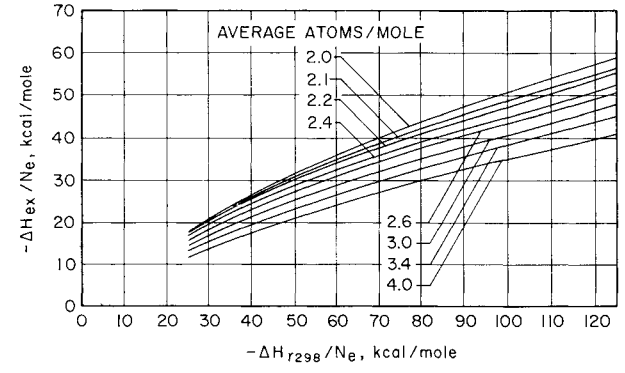

Fig. 4 Loci of energy conversion of unambiguous gaseous species of various average atoms/mole (1000 psia/1 atm, shifting expansion).

Good agreement between theoretical specific impulses estimated by Fig. 4 and computed directly are typical, so the empirical method can be used with confidence to an accuracy better than 2% whenever the effective species can be unambiguously predicted. An example of a formulation which, however, cannot be handled by Fig. 4 is $B_5H_9 + 7.5\ F_2$, since its effective species are not the readily predictable $5\ BF_3 + 4.5\ H_2$, because interaction between these species will occur with the formation of some HF and partial dissociation of BF_3 to other effective species—i.e., there is insufficient oxidizer to combine with all the fuel, so that the effective species cannot be unambiguously predicted. On the other hand, the effective species of the formulation $B_5H_9 + 12\ F_2$ are $5\ BF_3 + 9$ HF, as can be readily predicted, and the system fits the atoms/mole curve that applies to this assumption, i.e., sufficient oxidizer is now present, so that the effective species can be unambiguously predicted.

References

[1] Muenger, J. R. and Greiner, L., "Estimation of performance factors for rocket propellants," Texaco Inc. (1962).

[2] Stull, D. R., *JANAF Interim Thermochemical Tables* (The Dow Chemical Co., Midland, Mich. (December 31, 1960), Vol. 1.

Storability Design Criteria for Space Propulsion

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THE storability of propellants in space is of great current interest because the higher-performing liquid propellants are cryogenic in nature and are thus inherently more difficult to store in space. The recent development of novel insulations that perform well in a hard vacuum makes the storage in space of cryogenic propellants attractive for periods up to two years. It will be shown that efficiently stored cryogenic propellants offer performance superior to that of many conventionally storable propellants.

Analysis

An analytical technique has been developed to permit evaluation of a wide variety of propellant combinations stored in space for time periods of up to two years. The rating criterion is the maximum velocity increment that each combination is able to impart, after space storage, to a "standard" upper-stage vehicle that is assumed to have constant gross and payload weights. A computer program has also been developed to determine tradeoffs between the weight penalties

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