Richard Nakka's *Experimental Rocketry* Web Site

Technical Notepad #5 -- KNER Ideal Performance Calculations

Note 1

Potassium Nitrate - Erythritol (KNER) propellant
65/35 O/F ratio @ 1000 psia chamber pressure

From PROPEP results, for 100 grams mixture:

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 KNER            Run using June 1988 Version of PEP,
 Case   1 of   1     29 Nov 2006 at   8:48: 8.54 pm

  CODE                                     WEIGHT    D-H  DENS      COMPOSITION
   821 POTASSIUM NITRATE                   65.000  -1169  0.07620    1N   3O   1K
  1091 ERYTHRITOL                          35.000  -1731  0.05240    4C  10H   4O

THE PROPELLANT DENSITY IS 0.06575 LB/CU-IN OR  1.8199 GM/CC
THE TOTAL PROPELLANT WEIGHT IS  100.0000 GRAMS

NUMBER OF GRAM ATOMS OF EACH ELEMENT PRESENT IN INGREDIENTS

   2.865940 H     1.146376 C     0.642877 N     3.075006 O
   0.642877 K

****************************CHAMBER RESULTS FOLLOW    *****************************

 T(K)  T(F)  P(ATM)   P(PSI) ENTHALPY  ENTROPY  CP/CV     GAS   RT/V
1608. 2435.   68.02  1000.00  -136.57   172.02  1.1392  2.593   26.237

SPECIFIC HEAT (MOLAR) OF GAS AND TOTAL=   10.214   14.503
NUMBER MOLS GAS AND CONDENSED=   2.5927   0.3147

  0.95381 H2O       0.49905 CO        0.47220 H2        0.33254 CO2
  0.32130 N2        0.31467 K2CO3*    0.01285 KHO       0.00052 K
 2.24E-04 NH3      7.55E-05 K2H2O2   4.71E-05 CH4      7.96E-06 H
 7.66E-06 KCN      4.78E-06 CH2O     4.57E-06 KH       4.48E-06 CNH

THE MOLECULAR WEIGHT OF THE MIXTURE IS   34.395

****************************EXHAUST RESULTS FOLLOW    *****************************

 T(K)  T(F)  P(ATM)   P(PSI) ENTHALPY  ENTROPY  CP/CV     GAS   RT/V
1030. 1394.    1.00    14.70  -164.52   172.02  1.1518  2.579    0.388

SPECIFIC HEAT (MOLAR) OF GAS AND TOTAL=    9.367   13.407
NUMBER MOLS GAS AND CONDENSED=   2.5787   0.3214

  0.78506 H2O       0.64720 H2        0.50100 CO2       0.32362 CO
  0.32141 K2CO3&    0.32139 N2        0.00029 CH4       0.00006 NH3
 3.55E-05 KHO

THE MOLECULAR WEIGHT OF THE MIXTURE IS   34.481

**********PERFORMANCE:  FROZEN ON FIRST LINE, SHIFTING ON SECOND LINE**********

IMPULSE   IS EX      T*      P*      C*     ISP*   OPT-EX  D-ISP     A*M   EX-T
  153.8  1.1451   1499.   39.14  3024.7            9.94  279.9  0.09403   942.
  156.0  1.1145   1523.   39.57  3089.1    116.9   10.43  283.8  0.09603  1030.
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The effective Molecular Weight is given by dividing the number GAS moles into the system mass. Since the system mass is 100 grams:

$$MW(effective) = \frac{100}{2.5787} = 38.78 \text{ g/mole}$$

Note that this is the proper molecular weight to use in the thermodynamic equations.

The mass fraction of condensed phase is given by the mass of the condensed phase (K_2CO_3) divided by the system mass

The MW of K_2CO_3 = 138.21 g/mole, thus

$$X = \frac{0.3214\,(138.21)}{100} = 0.444$$

Note 2

KNER 65/35 O/F ratio @ 1000 psia chamber pressure

Mole fractions and mass fractions for each combustion product are calculated in the table below:

	MW (g/mol)	Number of moles	Mole fraction	System mass (g)	Mass fraction
CO	28.01	0.4991	0.1717	13.978	0.1398
H2	2.02	0.4722	0.1624	0.954	0.0095
KH	40.11	0.0000	0.0000	0.000	0.0000
N2	28.02	0.3213	0.1105	9.003	0.0900
CO2	44.01	0.3325	0.1144	14.635	0.1464
H2O	18.02	0.9538	0.3281	17.188	0.1719
KOH	56.11	0.0129	0.0044	0.721	0.0072
OH	17.01	0.0000	0.0000	0.000	0.0000
H	1.01	0.0000	0.0000	0.000	0.0000
K	39.1	0.0005	0.0002	0.020	0.0002
K2O2H2	112.22	0.0001	0.0000	0.008	0.0001
K2CO3(L)	138.21	0.3147	0.1082	43.491	0.4349
total moles:		2.9070	1.000	100.00	1.000
gas moles:		2.5924	0.8918	56.508	0.5651
condensed phase moles:		0.3147	0.1082	43.491	0.4349

The table below shows the computation of ***k***, the ratio of specific heats:

	Specific Heat of solid (Cs) and gas (Cp) at constant pressure											
	Cs	Cp										
Temp	K_2CO_3	KOH	CO	CO_2	H_2	H_2O	N_2	Gas	Mixture	**k**	**k'**	**k**
K	Ref. JANAF	Ref. NIST	Ref. JANAF					only		mixture	gas	2-phase
300	114.70		29.14	37.221	28.849	33.60	29.125	31.62	45.54	1.2233	1.3568	1.0745
400	128.14		29.34	41.325	29.181	34.26	29.249	32.50	48.06	1.2092	1.3437	1.0677
500	140.05		29.75	44.627	29.26	35.23	29.58	33.42	50.42	1.1975	1.3312	1.0626
600	150.67		30.44	47.321	29.327	36.33	30.11	34.38	52.67	1.1874	1.3190	1.0585
700	160.48		31.17	49.564	29.441	37.50	30.754	35.34	54.82	1.1788	1.3077	1.0552
800	170.04		31.90	51.434	29.624	38.72	31.433	36.29	56.93	1.1710	1.2972	1.0523
900	179.52		32.58	52.999	29.881	39.99	32.09	37.21	59.01	1.1640	1.2877	1.0498
1000	188.95		33.18	54.308	30.205	41.27	32.697	38.10	61.04	1.1577	1.2791	1.0474
1100	198.32		33.71	55.409	30.581	42.54	33.241	38.95	63.03	1.1520	1.2714	1.0454
1200	205.26		34.18	56.342	30.992	43.77	33.723	39.74	64.67	1.1475	1.2645	1.0439
1300	209.20		34.57	57.137	31.423	44.95	34.147	40.49	65.89	1.1444	1.2584	1.0430
1400	209.20		34.92	57.802	31.861	46.05	34.518	41.17	66.57	1.1427	1.2530	1.0429
1500	209.20		35.22	58.379	32.298	47.09	34.843	41.81	67.20	1.1412	1.2483	1.0427
1600	209.20	57.5	35.48	58.886	32.725	48.05	35.128	42.67	68.07	1.1391	1.2420	1.0426
1700	209.20	57.8	35.71	59.317	32.139	48.94	35.378	43.02	68.42	1.1383	1.2395	1.0425
1800	209.20	58.1	35.91	59.701	33.537	49.75	35.6	43.69	69.09	1.1368	1.2350	1.0423
1900	209.20	58.4	36.09	60.049	33.917	50.50	35.796	44.14	69.54	1.1358	1.2321	1.0422
2000	209.20	58.7	36.25	60.35	34.28	51.18	35.971	44.55	69.95	1.1349	1.2294	1.0421
2100	209.20	58.9	36.39	60.622	34.624	51.82	36.126	44.94	70.34	1.1341	1.2270	1.0421
2200	209.20	59.1	36.52	60.865	34.952	52.41	36.268	45.29	70.69	1.1333	1.2249	1.0420
2300	209.20		36.64	61.086	35.263	52.95	36.395	45.31	70.71	1.1332	1.2247	1.0420
2400	209.20		36.32	61.287	35.559	53.44	36.511	45.53	70.93	1.1328	1.2234	1.0419
2500	209.20		36.84	61.471	35.842	53.90	36.616	45.89	71.29	1.1320	1.2213	1.0419
	Note: Units of Cp and Cs are J/mol-K											

The values for Cp and Cs are taken from the JANAF Thermochemical Tables and NIST Chemistry WebBook.

Note that the highlighted range (yellow) is applicable for interpolation of the values at 1608 K, the chamber combustion temperature under consideration.

The Cp for the gas only products and mixture (gas+condensed) is given by

$$Cp_{gas} = \frac{1}{n} \sum_i n_i \, Cp_i$$

$$Cp_{mix} = \frac{1}{n} \sum_i \left(n_i \, Cp_i + n_s \, C_s \right)$$

where n_i is the number of moles of gas component i , n_s the number of moles of condensed component, n the total number of gas moles. The ratio of specific heats for the mixture, for the gas-only, and for two-phase flow is given by

$$k_{mix} = \frac{Cp_{mix}}{Cp_{mix} - \bar{R}}$$

where $\bar{R}$ = 8.314 J/mol-K (universal gas constant).

$$k'_{(gas)} = \frac{Cp_{gas}}{Cp_{gas} - \bar{R}}$$

$$k_{2ph} = k' \left[\frac{1 + \psi \dfrac{Cs}{Cp_{gas}}}{1 + k' \psi \dfrac{Cs}{Cp_{gas}}} \right]$$

where $\psi = X/(1-X)$.

Note that *k* for two-phase (gas+condensed) flow is a modified form of the gas-only *k'*. This is the correct form of k to use in the thermodynamic equations involving products with a significant fraction of condensed-phase particles. The value of *k* given in the PROPEP output (Cp/Cv) is for the mixture.

Note 3

Characteristic exhaust velocity is given by

$$c^* = \sqrt{\frac{\bar{R} T_o}{M\,k}\left(\frac{k+1}{2}\right)^{\frac{k+1}{k-1}}}$$

with
To = 1608 K
M = 38.78 kg/kmol
k = 1.1390 Note: k for the *mixture* is the proper value to use, as c* represents a static condition
$\bar{R}$ = 8314 J/kmol-K

this gives c* = 923 m/s (3027 ft/s).

Note 4

The propellant specific impulse is given by the effective exhaust velocity divided by g.

$$I_{sp} = \frac{c}{g} = \frac{1}{g}\sqrt{\frac{2k}{(k-1)}\frac{\bar{R} T_o}{M}\left[1-\left(\frac{P_e}{P_o}\right)^{\frac{k-1}{k}}\right]}$$

with
To = 1608 K
M = 38.78 kg/kmol
k = 1.0426 Note: k for *2-phase flow* is the proper value to use, as *Isp* involves two-phase flow.

Thus, *Isp* = 167 sec.
for standard conditions of Po = 68 atm. (1000 psia) and Pe = 1 atm., and g = 9.806 m/s
(maximum theoretical, assumes frozen equilibrium, and no particle velocity lag or thermal lag).

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