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Computational Determination of the Specific Impulse of Solid Rocket Propellant Compositions of closo-Dodecaborate ([B12H12]2–) Salts with HTPB Binder and Ammonium Perchlorate as an Oxidizer.

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RESULTS OF THERMOCHEMICAL CALCULATION:

Job title : Test calculation
Comment :

Combustion condition:

Isobaric combustion (p=const.)
Chamber pressure = 7.000 MPa
Ambient pressure = 0.100 MPa
Expansion conditions: Equilibrium expansion

Reactant information:
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1. BAM-H-1, 6 %
2. Ammonium perchlorate (AP), 80 %
3. Polybutadiene hydroxyl terminated (HTPB), 14 %

C(1.462) H(5.619) N(0.893) O(3.265) Cl(0.813) B(0.240)

Molecular weight = 119.38
Oxygen balance = -32.46548 %
Enthalpy of formation = -2192.98 kJ/kg
Internal energy of formation = -2099.92 kJ/kg

Parameters in combustion chamber:

- Heat of isobaric combustion	= -3647.12	kJ/kg
- Total enthalpy of combustion prod.	= -2193.92	kJ/kg
- Entropy of combustion products	= 10.41	kJ/K kg
- Isobaric combustion temperature	= 2477.1	K
- Mole number of gaseous products	= 43.931	mol/kg expl.
- Total mole number of products	= 43.931	mol/kg expl.
- Volume of gaseous products (at SATP)	= 1089.00	L/kg expl.
- Mass of gaseous products	= 999.9	g/kg expl.
- Mass of condensed products	= 0.0	g/kg expl.
- Mean molecular mass of gaseous prod.	= 22.762	g
- Mean molecular mass of all products	= 22.762	g
- Specific gas constant	= 365.242	J/kg K
- Specific heat capacity at p=const. (Cp)	= 1885.26	J/kgK
- Specific heat capacity at V=const. (Cv)	= 1520.02	J/molK
- Specific heat ratio (Cp/Cv)	= 1.2403	

Composition of combustion products in chamber:

Products	mol/mol	mol/kg	Mol %
CO =	1.270858 E00	1.064585 E01	24.2331
H2 =	1.149538 E00	9.629558 E00	21.9198
H2O =	1.133296 E00	9.493502 E00	21.6101
HCl =	8.094033 E-01	6.780288 E00	15.4340
N2 =	4.463018 E-01	3.738624 E00	8.5102
BHO2 =	2.204950 E-01	1.847064 E00	4.2045
CO2 =	1.911895 E-01	1.601575 E00	3.6457
H =	6.987292 E-03	5.853182 E-02	0.1332
B2O3 =	6.919831 E-03	5.796671 E-02	0.1319
B(OH)3 =	5.169168 E-03	4.330159 E-02	0.0986
Cl =	3.374071 E-03	2.826425 E-02	0.0643
BO2 =	2.873672 E-04	2.407246 E-03	0.0055
BO =	2.257148 E-04	1.890790 E-03	0.0043
NH3 =	1.406752 E-04	1.178421 E-03	0.0027
NO =	5.288438 E-05	4.430070 E-04	0.0010
HCN =	2.483975 E-05	2.080800 E-04	0.0005
Cl2 =	1.280116 E-05	1.072340 E-04	0.0002
CClO =	1.007722 E-05	8.441583 E-05	0.0002
CHNO =	3.604383 E-06	3.019354 E-05	0.0001
NH2 =	2.413288 E-06	2.021586 E-05	0.0000
BCl3 =	2.232127 E-06	1.869830 E-05	0.0000
CH4 =	1.232861 E-06	1.032755 E-05	0.0000
B =	1.123565 E-06	9.411988 E-06	0.0000
BCl =	9.293137 E-07	7.784765 E-06	0.0000
ClO =	1.683941 E-07	1.410620 E-06	0.0000
BH2 =	8.295492 E-08	6.949048 E-07	0.0000
N =	3.154457 E-08	2.642456 E-07	0.0000
CH3OH =	9.193176 E-09	7.701028 E-08	0.0000
CNO =	7.738001 E-09	6.482044 E-08	0.0000
CH2Cl2 =	9.727513 E-11	8.148637 E-10	0.0000
BN =	8.563519 E-11	7.173571 E-10	0.0000

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      C2H4 =    5.905273 E-11          4.946787 E-10   0.0000
      N2H4 =    2.340671 E-12          1.960756 E-11   0.0000
      B2O3(l) =         1.630237 E-12          1.365632 E-11   0.0000
      C2H6 =    1.337863 E-13          1.120714 E-12   0.0000
      CHCl3 =   1.239273 E-13          1.038126 E-12   0.0000
      B2O3(s) =         9.373642 E-14          7.852203 E-13   0.0000
      B(l) =    1.706907 E-15          1.429859 E-14   0.0000

Parameters at the nozzle throat:
---------------------------------
    - Total enthalpy of combustion prod.       = -2697.96   kJ/kg
    - Temperature at nozzle throat             = 2219.2   K
    - Pressure at nozzle throat                = 3.9   MPa
    - Mole number of gaseous products          = 43.880   mol/kg expl.
    - Total mole number of  products           = 43.880   mol/kg expl.
    - Volume of gaseous products (at SATP)     = 1087.74   L/kg expl.
    - Mass of gaseous products                 = 999.9   g/kg expl.
    - Mass of condensed products               = 0.0   g/kg expl.
    - Mean molecular mass of gaseous prod.     = 22.788   g
    - Mean molecular mass of all products      = 22.788   g
    - Specific gas constant                    = 364.816   J/kg K
    - Specific heat capacity at p=const. (Cp)  = 1852.33   J/kgK
    - Specific heat capacity at V=const. (Cv)  = 1487.52   J/molK
    - Specific heat ratio (Cp/Cv)              = 1.2453

 Characteristic parameters at the nozzle throat:
.................................................
    - Flow velocity at nozzle throat           = 1004.0   m/s
    - Sound velocity at throat )               = 1004.1   m/s
    - Mach number at nozzle throat             = 1.000
    - Critical pressure ratio (pt/pc)          = 0.555
    - Pressure ratio (pc/pt)                   = 1.802

Composition of combustion products at nozzle throat:
----------------------------------------------------------------------
       Products mol/mol         mol/kg          Mol %
----------------------------------------------------------------------
      CO =      1.253207 E00           1.049799 E01    23.9244
      H2 =      1.168340 E00           9.787063 E00    22.3043
      H2O =     1.111129 E00           9.307810 E00    21.2121
      HCl =     8.115299 E-01          6.798102 E00    15.4926
      N2 =      4.463465 E-01          3.738998 E00    8.5210
      BHO2 =    2.214716 E-01          1.855245 E00    4.2280
      CO2 =     2.088596 E-01          1.749595 E00    3.9872
      B(OH)3 =  7.874920 E-03          6.596740 E-02   0.1503
      B2O3 =    5.271303 E-03          4.415717 E-02   0.1006
      H =       2.608604 E-03          2.185201 E-02   0.0498
      Cl =      1.273866 E-03          1.067104 E-02   0.0243
      NH3 =     1.084958 E-04          9.088580 E-04   0.0021
      BO2 =     7.545909 E-05          6.321131 E-04   0.0014
      BO =      5.476563 E-05          4.587660 E-04   0.0010
      HCN =     1.423462 E-05          1.192419 E-04   0.0003
      NO =      9.780126 E-06          8.192711 E-05   0.0002
      Cl2 =     4.292990 E-06          3.596193 E-05   0.0001
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      CClO =    3.216073 E-06           2.694071 E-05   0.0001
      CHNO =    1.840842 E-06           1.542054 E-05   0.0000
      BCl3 =    1.696402 E-06           1.421058 E-05   0.0000
      CH4 =     1.418348 E-06           1.188136 E-05   0.0000
      NH2 =     6.477880 E-07           5.426453 E-06   0.0000
      BCl =     1.855318 E-07           1.554181 E-06   0.0000
      B =       7.883756 E-08           6.604141 E-07   0.0000
      ClO =     1.708526 E-08           1.431215 E-07   0.0000
      BH2 =     1.523741 E-08           1.276422 E-07   0.0000
      CH3OH =   4.885697 E-09           4.092698 E-08   0.0000
      N =       2.818243 E-09           2.360813 E-08   0.0000
      CNO =     1.165625 E-09           9.764319 E-09   0.0000
      C2H4 =    3.957689 E-11           3.315315 E-10   0.0000
      CH2Cl2 =  3.859059 E-11           3.232694 E-10   0.0000
      B2O3(l) =         5.603831 E-12           4.694272 E-11   0.0000
      BN =      4.412840 E-12           3.696591 E-11   0.0000
      N2H4 =    4.320737 E-13           3.619437 E-12   0.0000
      B2O3(s) =         3.260262 E-13           2.731088 E-12   0.0000
      C2H6 =    1.099387 E-13           9.209451 E-13   0.0000
      CHCl3 =   2.797765 E-14           2.343659 E-13   0.0000
      B(l) =    6.777494 E-16           5.677437 E-15   0.0000

Parameters at the nozzle exit:
---------------------------------
    - Total enthalpy of combustion prod.       = -4885.76   kJ/kg
    - Temperature at nozzle exit               = 1208.4   K
    - Pressure at nozzle throat                 = 0.1   MPa
    - Mole number of gaseous products          = 42.894   mol/kg expl.
    - Total mole number of  products           = 43.845   mol/kg expl.
    - Volume of gaseous products (at SATP)     = 1063.29   L/kg expl.
    - Mass of gaseous products                 = 933.7   g/kg expl.
    - Mass of condensed products               = 66.2   g/kg expl.
    - Mean molecular mass of gaseous prod.     = 21.769   g
    - Mean molecular mass of all products      = 22.807   g
    - Specific gas constant                    = 356.618   J/kg K
    - Specific heat capacity at p=const. (Cp)  = 1704.58   J/kgK
    - Specific heat capacity at V=const. (Cv)  = 1347.96   J/molK
    - Specific heat ratio (Cp/Cv)              = 1.2646

 Characteristic parameters at the nozzle exit:
.................................................
    - Specific impulse                         = 236.52   s
    - Exhaust (or nozzle exit) velocity        = 2320.3   m/s
    - Characteristic exhaust velocity (c*)     = 1422.4   m/s
    - Thrust coefficient (Cf)                  = 1.631
    - Nozzle area expansion ratio (Ae/At)      = 8.02
    - Pressure ratio (pc/pe)                   = 70.000
    - Sound velocity at nozzle exit            = 732.55   m/s
    - Mach number at nozzle exit               = 3.167
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Composition of combustion products at the nozzle exit:

Products	mol/mol	mol/kg	Mol %
H2 =	1.415946 E00	1.186123 E01	27.0525
CO =	1.006197 E00	8.428810 E00	19.2240
H2O =	9.703504 E-01	8.128526 E00	18.5391
HCl =	8.128206 E-01	6.808914 E00	15.5294
CO2 =	4.558440 E-01	3.818558 E00	8.7092
N2 =	4.463899 E-01	3.739362 E00	8.5285
B2O3(l) =	1.135973 E-01	9.515925 E-01	2.1703
B(OH)3 =	9.976436 E-03	8.357158 E-02	0.1906
BHO2 =	2.850191 E-03	2.387576 E-02	0.0545
NH3 =	4.769030 E-05	3.994967 E-04	0.0009
CH4 =	4.586749 E-05	3.842273 E-04	0.0009
H =	6.434651 E-07	5.390241 E-06	0.0000
HCN =	5.127113 E-07	4.294930 E-06	0.0000
Cl =	2.837466 E-07	2.376916 E-06	0.0000
B2O3 =	9.583006 E-08	8.027585 E-07	0.0000
CHNO =	2.447344 E-08	2.050115 E-07	0.0000
BCl3 =	6.385183 E-09	5.348802 E-08	0.0000
Cl2 =	5.996682 E-10	5.023359 E-09	0.0000
CClO =	4.716512 E-10	3.950974 E-09	0.0000
BN =	3.051069 E-10	2.555849 E-09	0.0000
CH3OH =	2.888374 E-10	2.419561 E-09	0.0000
B(l) =	2.139786 E-10	1.792477 E-09	0.0000
B2O3(s) =	1.841085 E-10	1.542258 E-09	0.0000
B =	1.822359 E-10	1.526572 E-09	0.0000
CHCl3 =	1.674091 E-10	1.402369 E-09	0.0000
N =	1.553676 E-10	1.301498 E-09	0.0000
N2H4 =	1.550260 E-10	1.298637 E-09	0.0000
ClO =	1.273701 E-10	1.066966 E-09	0.0000
BH2 =	1.142917 E-10	9.574098 E-10	0.0000
CNO =	1.108650 E-10	9.287043 E-10	0.0000
BCl =	9.033762 E-11	7.567489 E-10	0.0000
CH2Cl2 =	4.989008 E-11	4.179240 E-10	0.0000
C2H4 =	3.779707 E-11	3.166222 E-10	0.0000
C2H6 =	2.488754 E-11	2.084804 E-10	0.0000
BO =	2.294051 E-11	1.921703 E-10	0.0000
NO =	1.546689 E-11	1.295645 E-10	0.0000
BO2 =	1.092416 E-11	9.151055 E-11	0.0000
NH2 =	1.901836 E-12	1.593148 E-11	0.0000

Notes:
- DataBase: E:\Copy of MHR-2.xlsx
- Activity : Model 1: Condensed products form pure phase (Default)

********** NEW RUN **********

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