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         NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA2, MAY 21, 2004
                   BY  BONNIE MCBRIDE AND SANFORD GORDON
      REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

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 problem   case=Prob5 phi,eq.ratio=.909091,
       hp   p,atm=1,  t,k=2000
 react
   fuel=CH4 moles=1  t,k=298
   oxid=Air moles=1  t,k=298
 end

 OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
 RKT=F  FROZ=F  EQL=F  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

 T,K =  2000.0000

 TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

 P,BAR =     1.013250

    REACTANT           MOLES    (ENERGY/R),K   TEMP,K  DENSITY
        EXPLODED FORMULA
 F: CH4              1.000000  -0.897291E+04   298.00  0.0000
          C  1.00000  H  4.00000
 O: Air              1.000000  -0.156227E+02   298.00  0.0000
          N  1.56168  O  0.41959  AR 0.00937  C  0.00032

  SPECIES BEING CONSIDERED IN THIS SYSTEM
 (CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
  LAST thermo.inp UPDATE:    9/09/04

  g 3/98  *Ar              g 7/97  *C               tpis79  *CH
  g 4/02  CH2              g 4/02  CH3             g11/00  CH2OH
  g 7/00  CH3O             g 8/99  CH4             g 7/00  CH3OH
  srd 01  CH3OOH           g 8/99  *CN             g12/99  CNN
  tpis79  *CO              g 9/99  *CO2            tpis91  COOH
  tpis91  *C2              g 6/01  C2H             g 1/91  C2H2,acetylene
  g 5/01  C2H2,vinylidene  g 4/02  CH2CO,ketene    g 3/02  O(CH)2O
  srd 01  HO(CO)2OH        g 7/01  C2H3,vinyl      g 9/00  CH3CN
  g 6/96  CH3CO,acetyl     g 1/00  C2H4            g 8/88  C2H4O,ethylen-o
  g 8/88  CH3CHO,ethanal   g 6/00  CH3COOH         srd 01  OHCH2COOH
  g 7/00  C2H5             g 7/00  C2H6            g 8/88  CH3N2CH3
  g 8/88  C2H5OH           g 7/00  CH3OCH3         srd 01  CH3O2CH3
  g 7/00  CCN              tpis91  CNC             srd 01  OCCN
  tpis79  C2N2             g 8/00  C2O             tpis79  *C3
  n 4/98  C3H3,1-propynl   n 4/98  C3H3,2-propynl  g 2/00  C3H4,allene
  g 1/00  C3H4,propyne     g 5/90  C3H4,cyclo-     g 3/01  C3H5,allyl
  g 2/00  C3H6,propylene   g 1/00  C3H6,cyclo-     g 6/01  C3H6O,propylox
  g 6/97  C3H6O,acetone    g 1/02  C3H6O,propanal  g 7/01  C3H7,n-propyl
  g 9/85  C3H7,i-propyl    g 2/00  C3H8            g 2/00  C3H8O,1propanol
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| | | | | | |
|---|---|---|---|---|---|
| g 2/00 | C3H8O,2propanol | srd 01 | CNCOCN | g 7/88 | C3O2 |
| g tpis | *C4 | g 7/01 | C4H2,butadiyne | g 8/00 | C4H4,1,3-cyclo- |
| n10/92 | C4H6,butadiene | n10/93 | C4H6,1butyne | n10/93 | C4H6,2butyne |
| g 8/00 | C4H6,cyclo- | n 4/88 | C4H8,1-butene | n 4/88 | C4H8,cis2-buten |
| n 4/88 | C4H8,tr2-butene | n 4/88 | C4H8,isobutene | g 8/00 | C4H8,cyclo- |
| g10/00 | (CH3COOH)2 | n10/84 | C4H9,n-butyl | n10/84 | C4H9,i-butyl |
| g 1/93 | C4H9,s-butyl | g 1/93 | C4H9,t-butyl | g12/00 | C4H10,n-butane |
| g 8/00 | C4H10,isobutane | g 6/01 | C4N2 | g 8/00 | *C5 |
| g 5/90 | C5H6,1,3cyclo- | g 1/93 | C5H8,cyclo- | n 4/87 | C5H10,1-pentene |
| g 2/01 | C5H10,cyclo- | n10/84 | C5H11,pentyl | g 1/93 | C5H11,t-pentyl |
| n10/85 | C5H12,n-pentane | n10/85 | C5H12,i-pentane | n10/85 | CH3C(CH3)2CH3 |
| g 2/93 | C6H2 | g11/00 | C6H5,phenyl | g 8/00 | C6H5O,phenoxy |
| g 8/00 | C6H6 | g 8/00 | C6H5OH,phenol | g 1/93 | C6H10,cyclo- |
| n 4/87 | C6H12,1-hexene | g 6/90 | C6H12,cyclo- | n10/83 | C6H13,n-hexyl |
| g 6/01 | C6H14,n-hexane | g 7/01 | C7H7,benzyl | g 1/93 | C7H8 |
| g12/00 | C7H8O,cresol-mx | n 4/87 | C7H14,1-heptene | n10/83 | C7H15,n-heptyl |
| n10/85 | C7H16,n-heptane | n10/85 | C7H16,2-methylh | n 4/89 | C8H8,styrene |
| n10/86 | C8H10,ethylbenz | n 4/87 | C8H16,1-octene | n10/83 | C8H17,n-octyl |
| n 4/85 | C8H18,n-octane | n 4/85 | C8H18,isooctane | n10/83 | C9H19,n-nonyl |
| g 3/01 | C10H8,naphthale | n10/83 | C10H21,n-decyl | g 8/00 | C12H9,o-bipheny |
| g 8/00 | C12H10,biphenyl | g 6/97 | *H | g 6/01 | HCN |
| g 1/01 | HCO | tpis89 | HCCN | g 6/01 | HCCO |
| g 6/01 | HNC | g 7/00 | HNCO | g10/01 | HNO |
| tpis89 | HNO2 | g 5/99 | HNO3 | g 4/02 | HO2 |
| tpis78 | *H2 | g 5/01 | HCHO,formaldehy | g 6/01 | HCOOH |
| g 8/89 | H2O | g 6/99 | H2O2 | g 6/01 | (HCOOH)2 |
| g 5/97 | *N | g 6/01 | NCO | g 4/99 | *NH |
| g 3/01 | NH2 | tpis89 | NH3 | tpis89 | NH2OH |
| tpis89 | *NO | g 4/99 | NO2 | j12/64 | NO3 |
| tpis78 | *N2 | g 6/01 | NCN | g 5/99 | N2H2 |
| tpis89 | NH2NO2 | g 4/99 | N2H4 | g 4/99 | N2O |
| g 4/99 | N2O3 | tpis89 | N2O4 | g 4/99 | N2O5 |
| tpis89 | N3 | g 4/99 | N3H | g 5/97 | *O |
| g 4/02 | *OH | tpis89 | *O2 | g 8/01 | O3 |
| n 4/83 | C(gr) | n 4/83 | C(gr) | n 4/83 | C(gr) |
| g11/99 | H2O(cr) | g 8/01 | H2O(L) | g 8/01 | H2O(L) |

O/F =  18.962372

| | EFFECTIVE FUEL | EFFECTIVE OXIDANT | MIXTURE |
|---|---|---|---|
| ENTHALPY | h(2)/R | h(1)/R | h0/R |
| (KG-MOL)(K)/KG | -0.55932260E+03 | -0.53936211E+00 | -0.28531187E+02 |

| KG-FORM.WT./KG | bi(2) | bi(1) | b0i |
|---|---|---|---|
| *C | 0.62334580E-01 | 0.11013248E-04 | 0.31330653E-02 |
| *H | 0.24933832E+00 | 0.00000000E+00 | 0.12490415E-01 |
| *N | 0.00000000E+00 | 0.53915890E-01 | 0.51215014E-01 |
| *O | 0.00000000E+00 | 0.14486046E-01 | 0.13760378E-01 |
| *Ar | 0.00000000E+00 | 0.32331996E-03 | 0.30712349E-03 |

| POINT | ITN | T | C | H | N | O | AR |
|---|---|---|---|---|---|---|---|
| 1 | 27 | 2143.585 | -23.537 | -13.279 | -13.754 | -16.543 | -26.154 |

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = Prob5

| | REACTANT | MOLES | ENERGY KJ/KG-MOL | TEMP K |
|---|---|---|---|---|
| FUEL | CH4 | 1.0000000 | -74605.353 | 298.000 |
| OXIDANT | Air | 1.0000000 | -129.895 | 298.000 |

O/F=  18.96237  %FUEL=  5.009425  R,EQ.RATIO= 0.909229  PHI,EQ.RATIO= 0.909091

THERMODYNAMIC PROPERTIES

| | |
|---|---|
| P, BAR | 1.0132 |
| T, K | 2143.58 |
| RHO, KG/CU M | 1.5784-1 |
| H, KJ/KG | -237.22 |
| U, KJ/KG | -879.18 |
| G, KJ/KG | -21025.5 |
| S, KJ/(KG)(K) | 9.6979 |
| M, (1/n) | 27.763 |
| (dLV/dLP)t | -1.00119 |
| (dLV/dLT)p | 1.0370 |
| Cp, KJ/(KG)(K) | 1.8461 |
| GAMMAs | 1.2096 |
| SON VEL,M/SEC | 881.2 |

MOLE FRACTIONS

| | |
|---|---|
| *Ar | 0.00853 |
| *CO | 0.00261 |
| *CO2 | 0.08438 |
| *H | 0.00013 |
| *H2 | 0.00104 |
| H2O | 0.17075 |
| *NO | 0.00297 |
| *N2 | 0.70947 |
| *O | 0.00024 |
| *OH | 0.00307 |
| *O2 | 0.01682 |

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

| | | | | |
|---|---|---|---|---|
| *C | *CH | CH2 | CH3 | CH2OH |
| CH3O | CH4 | CH3OH | CH3OOH | *CN |
| CNN | COOH | *C2 | C2H | C2H2,acetylene |
| C2H2,vinylidene | CH2CO,ketene | O(CH)2O | HO(CO)2OH | C2H3,vinyl |
| CH3CN | CH3CO,acetyl | C2H4 | C2H4O,ethylen-o | CH3CHO,ethanal |
| CH3COOH | OHCH2COOH | C2H5 | C2H6 | CH3N2CH3 |
| C2H5OH | CH3OCH3 | CH3O2CH3 | CCN | CNC |

| | | | | |
|---|---|---|---|---|
| OCCN | C2N2 | C2O | *C3 | C3H3,1-propynl |
| C3H3,2-propynl | C3H4,allene | C3H4,propyne | C3H4,cyclo- | C3H5,allyl |
| C3H6,propylene | C3H6,cyclo- | C3H6O,propylox | C3H6O,acetone | C3H6O,propanal |
| C3H7,n-propyl | C3H7,i-propyl | C3H8 | C3H8O,1propanol | C3H8O,2propanol |
| CNCOCN | C3O2 | *C4 | C4H2,butadiyne | C4H4,1,3-cyclo- |
| C4H6,butadiene | C4H6,1butyne | C4H6,2butyne | C4H6,cyclo- | C4H8,1-butene |
| C4H8,cis2-buten | C4H8,tr2-butene | C4H8,isobutene | C4H8,cyclo- | (CH3COOH)2 |
| C4H9,n-butyl | C4H9,i-butyl | C4H9,s-butyl | C4H9,t-butyl | C4H10,n-butane |
| C4H10,isobutane | C4N2 | *C5 | C5H6,1,3cyclo- | C5H8,cyclo- |
| C5H10,1-pentene | C5H10,cyclo- | C5H11,pentyl | C5H11,t-pentyl | C5H12,n-pentane |
| C5H12,i-pentane | CH3C(CH3)2CH3 | C6H2 | C6H5,phenyl | C6H5O,phenoxy |
| C6H6 | C6H5OH,phenol | C6H10,cyclo- | C6H12,1-hexene | C6H12,cyclo- |
| C6H13,n-hexyl | C6H14,n-hexane | C7H7,benzyl | C7H8 | C7H8O,cresol-mx |
| C7H14,1-heptene | C7H15,n-heptyl | C7H16,n-heptane | C7H16,2-methylh | C8H8,styrene |
| C8H10,ethylbenz | C8H16,1-octene | C8H17,n-octyl | C8H18,n-octane | C8H18,isooctane |
| C9H19,n-nonyl | C10H8,naphthale | C10H21,n-decyl | C12H9,o-bipheny | C12H10,biphenyl |
| HCN | HCO | HCCN | HCCO | HNC |
| HNCO | HNO | HNO2 | HNO3 | HO2 |
| HCHO,formaldehy | HCOOH | H2O2 | (HCOOH)2 | *N |
| NCO | *NH | NH2 | NH3 | NH2OH |
| NO2 | NO3 | NCN | N2H2 | NH2NO2 |
| N2H4 | N2O | N2O3 | N2O4 | N2O5 |
| N3 | N3H | O3 | C(gr) | H2O(cr) |
| H2O(L) | | | | |