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

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problem  case=coal2008
  hp      p,atm=1,10,  t,k=1500
react
  fuel=H2O wt=60.  t,k=298
  oxid=O2  wt=30.  t,k=298
  fuel=H2O2(L) wt=42.82 t,k=298
  fuel=SiO2(a-qz) wt=9.62 t,k=298
  fuel=coal wt=100.  t,k=298
  h,kj/mol=-245.47 C 6.251 H 5.35 O 1.114 N 0.081 S 0.022
end

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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 = 1500.0000

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

P,BAR = 1.013250 10.132500

REACTANT	WT.FRAC	(ENERGY/R),K	TEMP,K	DENSITY
EXPLODED FORMULA				
F: H2O	0.282433	-0.290854E+05	298.00	0.0000
H 2.00000	O 1.00000			
O: O2	1.000000	-0.530002E+00	298.00	0.0000
O 2.00000				
F: H2O2(L)	0.201563	-0.225862E+05	298.00	0.0000
H 2.00000	O 2.00000			
F: SiO2(a-qz)	0.045283	-0.109532E+06	298.00	0.0000
SI 1.00000	O 2.00000			
F: coal	0.470721	-0.295231E+05	298.00	0.0000
C 6.25100	H 5.35000	O 1.11400	N 0.08100	S 0.02200

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

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 5/01 COS	g 9/99 *CO2	tpis91 COOH
g11/01 CS	g 6/95 CS2	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

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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	n 6/01 C2S2	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
g 2/00 C3H8O,2propanol	srd 01 CNCOCN	n 6/01 C3OS
g 7/88 C3O2	n 6/01 C3S2	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,isoctane	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 4/01 H2S	tpis89 H2SO4
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	g 5/97 *S	g10/01 SH
tpis89 SN	tpis89 SO	tpis89 SO2
tpis89 SO3	tpis89 S2	tpis89 S2O
tpis89 S3	tpis89 S4	tpis89 S5
tpis89 S6	tpis89 S7	tpis89 S8
g 8/97 *Si	tpis91 SiC	tpis91 SiC2
tpis91 SiH	g 3/01 SiH2	g 3/99 SiH3
tpis91 SiH4	g 5/99 SiN	tpis91 SiO
tpis91 SiO2	tpis91 SiS	tpis91 SiS2
tpis91 Si2	tpis91 Si2C	j 3/67 Si2N
g 7/95 Si3	n 4/83 C(gr)	n 4/83 C(gr)

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n 4/83	C(gr)	g11/99	H2O(cr)	g 8/01	H2O(L)
g 8/01	H2O(L)	j 9/77	H2SO4(L)	tpis89	S(a)
tpis89	S(b)	tpis89	S(L)	tpis89	S(L)
tpis89	S(L)	tpis89	S(L)	tpis89	S(L)
tpis91	Si(cr)	tpis91	Si(cr)	tpis91	Si(L)
tpis91	SiC(b)	tpis91	SiC(b)	tpis91	SiC(L)
tpis91	SiO2(a-qz)	tpis91	SiO2(b-qz)	tpis91	SiO2(b-crt)
tpis91	SiO2(L)	tpis91	SiS(cr)	tpis91	SiS(L)
tpis91	SiS2(cr)	tpis91	SiS2(cr)	tpis91	SiS2(L)
g 7/95	Si2N2O(cr)	g 7/95	Si2N2O(cr)	tpis91	Si3N4(cr)
tpis91	Si3N4(cr)				

O/F = 0.141216

ENTHALPY	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
(KG-MOL) (K) /KG	h(2)/R	h(1)/R	h0/R
	-0.81115923E+03	-0.16563198E-01	-0.71078685E+03
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*H	0.68356023E-01	0.00000000E+00	0.59897515E-01
*O	0.34273024E-01	0.62502344E-01	0.37766175E-01
*Si	0.75366400E-03	0.00000000E+00	0.66040415E-03
*C	0.29385206E-01	0.00000000E+00	0.25749023E-01
*N	0.38077135E-03	0.00000000E+00	0.33365395E-03
*S	0.10341938E-03	0.00000000E+00	0.90622062E-04

POINT	ITN	T	H	O	SI	C
		N	S			
1	21	888.278	-9.155	-41.077	-3.718	-0.602
		-15.110	-18.302			
ADD	SiO2(b-qz)					
1	7	917.559	-9.135	-40.263	-46.894	-0.847
		-15.166	-17.505			
ADD	C(gr)					
1	3	934.762	-9.121	-39.542	-46.235	-1.429
		-15.191	-17.542			
2	4	1048.038	-8.209	-35.814	-41.648	-1.590
		-14.165	-17.120			

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = coal2008

	REACTANT	WT FRACTION	ENERGY	TEMP
		(SEE NOTE)	KJ/KG-MOL	K
FUEL	H2O	0.2824327	-241831.038	298.000
OXIDANT	O2	1.0000000	-4.407	298.000
FUEL	H2O2(L)	0.2015628	-187793.400	298.000
FUEL	SiO2(a-qz)	0.0452834	-910706.689	298.000
FUEL	coal	0.4707211	-245470.000	298.000

O/F= 0.14122 %FUEL= 87.625804 R,EQ.RATIO= 2.196380 PHI,EQ.RATIO= 6.841962

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THERMODYNAMIC PROPERTIES

P, BAR	1.0132	10.133
T, K	934.76	1048.04
RHO, KG/CU M	2.6085-1	2.4386 0
H, KJ/KG	-5909.84	-5909.84
U, KJ/KG	-6298.28	-6325.35
G, KJ/KG	-16427.7	-16721.8
S, KJ/(KG) (K)	11.2520	10.3164

M, (1/n)	20.009	20.972
MW, MOL WT	18.780	19.850
(dLV/dLP)t	-1.10783	-1.11692
(dLV/dLT)p	2.9077	2.8052
Cp, KJ/(KG) (K)	16.8116	13.7550
GAMMAS	1.1125	1.1235
SON VEL,M/SEC	657.4	683.2

MOLE FRACTIONS

CH4	0.03076	0.06097
*CO	0.24694	0.25513
COS	0.00005	0.00006
*CO2	0.15681	0.15453
*H2	0.37542	0.31154
H2O	0.12383	0.15918
H2S	0.00165	0.00173
NH3	0.00001	0.00005
*N2	0.00313	0.00329
C(gr)	0.04900	0.04041
SiO2(b-qz)	0.01240	0.01311

* 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	CH3OH	CH3OOH	*CN	CNN
COOH	CS	CS2	*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	C2S2
*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	C3OS	C3O2
C3S2	*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

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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	*H
HCN	HCO	HCCN	HCCO	HNC
HNCO	HNO	HNO2	HNO3	HO2
HCHO, formaldehy	HCOOH	H2O2	H2SO4	(HCOOH) 2
*N	NCO	*NH	NH2	NH2OH
*NO	NO2	NO3	NCN	N2H2
NH2NO2	N2H4	N2O	N2O3	N2O4
N2O5	N3	N3H	*O	*OH
*O2	O3	*S	SH	SN
SO	SO2	SO3	S2	S2O
S3	S4	S5	S6	S7
S8	*Si	SiC	SiC2	SiH
SiH2	SiH3	SiH4	SiN	SiO
SiO2	SiS	SiS2	Si2	Si2C
Si2N	Si3	H2O (cr)	H2O (L)	H2SO4 (L)
S (a)	S (b)	S (L)	Si (cr)	Si (L)
SiC (b)	SiC (L)	SiO2 (a-qz)	SiO2 (b-crt)	SiO2 (L)
SiS (cr)	SiS (L)	SiS2 (cr)	SiS2 (L)	Si2N2O (cr)
Si3N4 (cr)				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS