

FileEditor:junk.out

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

problem

rocket fac ac/at=3.0
 p,bar=100,
 sup,ae/at=100000,
 react
 name=AL(cr) wt=0.10 t,k=298.15
 name=NH4CLO4(I) wt=0.835 t,k=298.15
 name=C6H6(L) wt=0.065 t,k=298.15
 end

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

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

Pc,BAR = 100.000000

Pc/P =

SUBSONIC AREA RATIOS =

SUPERSONIC AREA RATIOS =100000.0000

NFZ= 1 Mdot/Ac= 0.000000E+00 Ac/At= 3.000000E+00

REACTANT	WT.FRAC	(ENERGY/R),K	TEMP,K	DENSITY
EXPLODED FORMULA				
N: AL(cr)	0.100000	0.496279E-05	298.15	0.0000
AL	1.00000			
N: NH4CLO4(I)	0.835000	-0.355724E+05	298.15	0.0000
N	1.00000	H 4.00000	CL 1.00000	O 4.00000
N: C6H6(L)	0.065000	0.590293E+04	298.15	0.0000
C	6.00000	H 6.00000		

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

g12/97 *AL	tpis96 ALC	tpis96 ALC2
tpis96 ALCL	tpis96 ALCL2	tpis96 ALCL3
tpis96 ALH	tpis96 ALHCL	tpis96 ALHCL2
tpis96 ALH2	tpis96 ALH2CL	tpis96 ALH3
tpis96 ALN	tpis96 *ALO	tpis96 ALOCL
tpis96 ALOCL2	tpis96 ALOH	tpis96 ALOHCL
tpis96 ALOHCL2	tpis96 ALO2	tpis96 AL(OH)2
tpis96 AL(OH)2CL	tpis96 AL(OH)3	tpis96 AL2

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tpis96	AL2C2	tpis96	AL2CL6	tpis96	AL2O
tpis96	AL2O2	tpis96	AL2O3	g 7/97	*C
g 8/99	CCL	g 8/99	CCL2	n12/93	CCL3
tpis91	CCL4	tpis79	*CH	g 9/99	CHCL
n12/93	CHCL2	g 7/99	CHCL3	g 4/02	CH2
g12/99	CH2CL	tpis91	CH2CL2	g 4/02	CH3
tpis91	CH3CL	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
tpis91	COCL	tpis91	COCL2	tpis91	COHCL
g 9/99	*CO2	tpis91	COOH	tpis91	*C2
tpis91	C2CL	g 5/02	C2CL2	tpis91	C2CL3
g 5/02	C2CL4	g 5/02	C2CL6	g 6/01	C2H
g 5/02	C2HCL	g 5/02	C2HCL3	g 1/91	C2H2,acetylene
g 5/01	C2H2,vinylidene	tpis91	C2H2CL2	g 4/02	CH2CO,ketene
g 3/02	O(CH)2O	srd 01	HO(CO)2OH	g 7/01	C2H3,vinyl
g 5/02	C2H3CL	srd 01	CH2CL-COOH	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
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,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 7/97	*CL	g 6/95	CLCN
tpis89	CLO	g 7/93	CLO2	tpis89	CL2
tpis89	CL2O	g 6/97	*H	tpis96	HALO
tpis96	HALO2	g 6/01	HCN	g 1/01	HCO
tpis89	HCCN	g 6/01	HCCO	tpis89	HCL
g 6/01	HNC	g 7/00	HNCO	g10/01	HNO
tpis89	HNO2	g 5/99	HNO3	g 1/01	HOCL
g 4/02	HO2	tpis78	*H2	g 5/01	HCHO,formaldehy
g 6/01	HCOOH	g 8/89	H2O	g 6/99	H2O2

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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 NOCL
g 4/99 NO2	g 4/99 NO2CL	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
coda89 AL(cr)	coda89 AL(L)	tpis96 ALCL3(cr)
tpis96 ALCL3(L)	tpis96 ALH3(a)	tpis96 ALN(cr)
tpis96 ALN(cr)	tpis96 ALN(L)	tpis96 ALN(L)
tpis96 AL(OH)3(a)	tpis96 AL2O3(a)	tpis96 AL2O3(a)
tpis96 AL2O3(a)	tpis96 AL2O3(L)	tpis96 AL4C3(cr)
tpis96 AL4C3(cr)	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)	j 9/65 NH4CL(II)	j 9/65 NH4CL(III)
j 9/65 NH4CL(III)		

O/F = 0.000000

ENTHALPY	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
(KG-MOL)(K)/KG	h(2)/R	h(1)/R	h0/R
	-0.24790250E+03	0.00000000E+00	-0.24790250E+03
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*AL	0.37062379E-02	0.00000000E+00	0.37062379E-02
*N	0.71070447E-02	0.00000000E+00	0.71070447E-02
*H	0.33421020E-01	0.00000000E+00	0.33421020E-01
*CL	0.71070447E-02	0.00000000E+00	0.71070447E-02
*O	0.28428179E-01	0.00000000E+00	0.28428179E-01
*C	0.49928410E-02	0.00000000E+00	0.49928410E-02

POINT	ITN	T	AL	N	H	CL
		O	C			
1	23	3352.544	-18.241	-13.185	-10.132	-18.906
		-14.841	-16.856			
ADD	AL2O3(L)					
1	5	3507.682	-21.206	-13.302	-9.988	-18.588
		-14.957	-16.536			
2	2	3502.473	-21.208	-13.322	-10.005	-18.617
		-14.974	-16.562			
Pinf/Pt = 1.724306						
3	3	3334.020	-21.879	-13.491	-10.236	-18.874
		-15.180	-16.980			
Pinf/Pt = 1.723291						
3	2	3334.197	-21.878	-13.491	-10.236	-18.874
		-15.180	-16.979			
4	2	3496.148	-21.232	-13.328	-10.013	-18.626
		-14.982	-16.577			
4	2	3495.158	-21.235	-13.329	-10.014	-18.628
		-14.983	-16.579			
4	1	3495.073	-21.236	-13.329	-10.014	-18.628
		-14.983	-16.579			
2	2	3505.161	-21.207	-13.311	-9.996	-18.602
		-14.965	-16.548			
Pinf/Pt = 1.724330						

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3	3	3336.399	-21.878	-13.481	-10.227	-18.859
		-15.171	-16.967			
Pinf/Pt = 1.723325						
3	2	3336.574	-21.877	-13.480	-10.227	-18.859
		-15.171	-16.966			
4	2	3498.825	-21.230	-13.318	-10.004	-18.611
		-14.973	-16.563			
4	2	3497.833	-21.234	-13.319	-10.005	-18.613
		-14.974	-16.566			
4	1	3497.748	-21.234	-13.319	-10.006	-18.613
		-14.974	-16.566			
END OF CHAMBER ITERATIONS						
4	14	316.111	-170.779	-18.899	-17.052	-54.607
		-94.072	-1.711			
PHASE CHANGE, REPLACE AL2O3(L) WITH AL2O3(a)						
4	3	297.457	-193.448	-18.895	-17.507	-56.348
		-98.923	-1.392			
4	7	419.528	-134.782	-18.124	-15.741	-45.711
		-72.499	-6.449			
4	2	418.190	-135.213	-18.130	-15.747	-45.801
		-72.721	-6.379			

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM

COMPOSITION DURING EXPANSION FROM FINITE AREA COMBUSTOR

Pin = 1450.4 PSIA
 Ac/At = 3.0000 Pinj/Pinf = 1.022482
 CASE =

REACTANT	WT FRACTION (SEE NOTE)	ENERGY KJ/KG-MOL	TEMP K
NAME AL(cr)	0.1000000	0.000	298.150
NAME NH4CLO4(I)	0.8350000	-295767.000	298.150
NAME C6H6(L)	0.0650000	49079.999	298.150

O/F= 0.00000 %FUEL= 0.000000 R,EQ.RATIO= 1.008563 PHI,EQ.RATIO= 0.000000

	INJECTOR	COMB END	THROAT	EXIT
Pinj/P	1.0000	1.0465	1.7621	5648019.
P, BAR	100.00	95.556	56.751	0.00002
T, K	3507.68	3497.75	3336.57	418.19
RHO, KG/CU M	1.0832 1	1.0381 1	6.5246 0	1.7674-5
H, KJ/KG	-2061.19	-2082.59	-2548.85	-8706.97
U, KJ/KG	-2984.42	-3003.11	-3418.65	-8807.14
G, KJ/KG	-33445.7	-33398.7	-32421.9	-12451.1
S, KJ/(KG)(K)	8.9474	8.9532	8.9532	8.9532
M, (1/n)	31.590	31.593	31.895	34.710
MW, MOL WT	29.914	29.915	30.160	32.612
(dLV/dLP)t	-1.03191	-1.03184	-1.02845	-1.00000
(dLV/dLT)p	1.5481	1.5489	1.5187	1.0001
Cp, KJ/(KG)(K)	4.4638	4.4728	4.3997	1.1552

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GAMMAS	1.1228	1.1227	1.1213	1.2616
SON VEL,M/SEC	1018.2	1016.6	987.6	355.5
MACH NUMBER	0.000	0.204	1.000	10.255

PERFORMANCE PARAMETERS

Ae/At	3.0001	1.0000	100000.0
CSTAR, M/SEC	1517.8	1517.8	1517.8
CF	0.1363	0.6507	2.4020
Ivac, M/SEC	4655.9	1868.3	3673.2
Isp, M/SEC	206.9	987.6	3645.8

MOLE FRACTIONS

ALCL	0.00023	0.00023	0.00014	0.00000
ALCL2	0.00008	0.00008	0.00005	0.00000
ALCL3	0.00011	0.00011	0.00008	0.00000
*ALO	0.00004	0.00004	0.00002	0.00000
ALOCL	0.00037	0.00036	0.00025	0.00000
ALOCL2	0.00001	0.00001	0.00001	0.00000
ALOH	0.00043	0.00042	0.00025	0.00000
ALOHCL	0.00028	0.00028	0.00016	0.00000
ALOHCL2	0.00129	0.00126	0.00088	0.00000
ALO2	0.00001	0.00001	0.00001	0.00000
AL(OH)2	0.00019	0.00019	0.00010	0.00000
AL(OH)2CL	0.00100	0.00097	0.00065	0.00000
AL(OH)3	0.00066	0.00064	0.00042	0.00000
*CO	0.07362	0.07349	0.06819	0.00000
*CO2	0.07572	0.07586	0.08239	0.16282
COOH	0.00001	0.00001	0.00000	0.00000
*CL	0.03340	0.03346	0.03216	0.00000
CLO	0.00043	0.00042	0.00031	0.00000
CL2	0.00029	0.00029	0.00024	0.00000
*H	0.01169	0.01168	0.00984	0.00000
HALO2	0.00003	0.00003	0.00002	0.00000
HCL	0.17299	0.17309	0.17793	0.23178
HNO	0.00001	0.00001	0.00001	0.00000
HOCL	0.00019	0.00019	0.00014	0.00000
HO2	0.00012	0.00011	0.00008	0.00000
*H2	0.03983	0.03978	0.03613	0.00892
H2O	0.33964	0.33986	0.35033	0.42015
H2O2	0.00002	0.00002	0.00001	0.00000
*N	0.00001	0.00001	0.00000	0.00000
*NO	0.01013	0.01004	0.00843	0.00000
NOCL	0.00001	0.00001	0.00000	0.00000
NO2	0.00002	0.00002	0.00001	0.00000
*N2	0.10121	0.10126	0.10294	0.11589
*O	0.00784	0.00782	0.00640	0.00000
*OH	0.04933	0.04914	0.04293	0.00000
*O2	0.02569	0.02568	0.02407	0.00000
AL2O3(a)	0.00000	0.00000	0.00000	0.06043
AL2O3(L)	0.05305	0.05312	0.05437	0.00000

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS

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WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*AL	ALC	ALC2	ALH	ALHCL
ALHCL2	ALH2	ALH2CL	ALH3	ALN
AL2	AL2C2	AL2CL6	AL2O	AL2O2
AL2O3	*C	CCL	CCL2	CCL3
CCL4	*CH	CHCL	CHCL2	CHCL3
CH2	CH2CL	CH2CL2	CH3	CH3CL
CH2OH	CH3O	CH4	CH3OH	CH3OOH
*CN	CNN	COCL	COCL2	COHCL
*C2	C2CL	C2CL2	C2CL3	C2CL4
C2CL6	C2H	C2HCL	C2HCL3	C2H2,acetylene
C2H2,vinylidene	C2H2CL2	CH2CO,ketene	O(CH)2O	HO(CO)2OH
C2H3,vinyl	C2H3CL	CH2CL-COOH	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,isoctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	CLCN	CLO2
CL2O	HALO	HCN	HCO	HCCN
HCCO	HNC	HNCO	HNO2	HNO3
HCHO,formaldehy	HCOOH	(HCOOH)2	NCO	*NH
NH2	NH3	NH2OH	NO2CL	NO3
NCN	N2H2	NH2NO2	N2H4	N2O
N2O3	N2O4	N2O5	N3	N3H
O3	AL(cr)	AL(L)	ALCL3(cr)	ALCL3(L)
ALH3(a)	ALN(cr)	ALN(L)	AL(OH)3(a)	AL4C3(cr)
C(gr)	H2O(cr)	H2O(L)	NH4CL(II)	NH4CL(III)

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