# 23 Boron–Oxidizer Systems

# 23.1 OVERVIEW

**TARIE 23 1** 

This chapter concerns the adiabatic properties of the boron-oxygen system and another thirty boron-oxidizer combinations. Equation 23.1 is a general description of the chemical reactions in question, and Table 23.1 provides a broad overview of the most basic results. The thermochemical descriptions within this chapter were derived from the *FactPS* and *FToxid* databases of

Boron–Oxidizer Systems			
Section	Pages	Oxidizer	Maximum T <sub>ad</sub> (K)
23.2	762	$O_2$	3687
23.3	764	TiO <sub>2</sub>	1429
23.4	765	$V_2O_5$	2323
23.5	767	Nb <sub>2</sub> O <sub>5</sub>	2120
23.6	768	Ta <sub>2</sub> O <sub>5</sub>	1622
23.7	769	$Cr_2O_3$	1662
23.8	770	MoO <sub>3</sub>	2323
23.9	772	WO <sub>3</sub>	2323
23.10	773	MnO	1459
23.11	774	$Mn_3O_4$	1855
23.12	775	$Mn_2O_3$	2216
23.13	777	$MnO_2$	2316
23.14	779	FeO	2274
23.15	781	$Fe_3O_4$	2274
23.16	783	$Fe_2O_3$	2274
23.17	785	CoO	2322
23.18	787	$Co_3O_4$	2323
23.19	789	NiO	2323
23.20	790	Cu <sub>2</sub> O	2314
23.21	791	CuO	2317
23.22	792	$Ag_2O$	2262
23.23	793	ZnO	1177
23.24	794	CdO	1094
23.25	795	HgO	2551
-	-	$B_2O_3$	-
-	-	$SiO_2$	-
23.26	796	SnO	2103
23.27	797	$SnO_2$	2303
23.28	798	PbO	2006
23.29	799	$Pb_3O_4$	2008
23.30	800	$PbO_2$	2189
23.31	801	$Sb_2O_3$	2018
23.32	802	Bi <sub>2</sub> O <sub>3</sub>	2039

*FactSage* 7.0.\* Only pure substances were considered in the condensed phases. Gases were treated ideally, and ideal gas mixing was assumed. Charged species were not considered in any phase.

boron + oxidizer 
$$\rightarrow$$
 adiabatic equilibrium products  
(*P* = 1 atm, *T*<sub>i</sub> = 298.15 K, *T*<sub>ad</sub> = adiabatic equilibrium temperature) (23.1)

Within each of the following sections, you will find one or two general figures as well as written descriptions of certain fuel-to-oxidizer ratios. Temperature points (T1, T2, and so on) describe features and points of interest along adiabatic temperature profiles. Similarly, gas points (G1, G2, and so on) refer to adiabatic gas production profiles. Some adiabatic temperature charts contain flat regions where the adiabatic temperature remains constant despite variations in the stoichiometry of the system. Some of these plateaus are described and explained (see Chapter 2 and Tables 2.10–2.15 for additional information).

# 23.2 BORON + $O_2$



FIGURE 23.1 Adiabatic equilibrium temperature profile, B (fuel) + O<sub>2</sub> (oxidizer).

T1. 23% fuel, 3540.55 K

solids: none liquids: none gases: 34.48% BO<sub>2</sub>, 29.52% B<sub>2</sub>O<sub>3</sub>, 13.87% O<sub>2</sub>, 12.46% BO, 9.42% O, 0.25% (BO)<sub>2</sub> a combination of reactions with excess oxidizer remaining:  $(25.3\% \text{ fuel}) \text{ B} + \text{O}_2 \rightarrow \text{BO}_2$  $(31.1\% \text{ fuel}) 4\text{B} + 3\text{O}_2 \rightarrow 2\text{B}_2\text{O}_3$  $(40.3\% \text{ fuel}) 2\text{B} + \text{O}_2 \rightarrow 2\text{BO}$ 

<sup>\*</sup> Bale, C. W.; Pelton, A. D.; Thompson, W. T.; Eriksson, G.; Hack, K.; Chartrand, P.; Decterov, S.; Jung, I.-H.; Melançon, J.; Petersen, S. *FactSage*, version 7.0; CRCT ThermFact, Inc. and GTT-Technologies, 2015; www.factsage.com (accessed September, 2019).

**T2.** 31% fuel, 3686.99 K—peak temperature solids: none liquids: none gases: 36.49% BO, 30.29% B<sub>2</sub>O<sub>3</sub>, 25.32% BO<sub>2</sub>, 4.88% O, 1.82% O<sub>2</sub>, 1.20% (BO)<sub>2</sub> a combination of reactions with excess oxidizer remaining:  $(25.3\% \text{ fuel}) \text{ B} + \text{O}_2 \rightarrow \text{BO}_2$  $(31.1\% \text{ fuel}) 4\text{B} + 3\text{O}_2 \rightarrow 2\text{B}_2\text{O}_3$ (40.3% fuel)  $2B + O_2 \rightarrow 2BO$ **T3.** 38% fuel, 3304.37 K solids: none liquids: none gases: 60.14% BO, 22.71% B<sub>2</sub>O<sub>3</sub>, 15.41% (BO)<sub>2</sub>, 1.59% BO<sub>2</sub>, 0.10% B<sub>2</sub>O a combination of reactions:  $(31.1\% \text{ fuel}) 4\text{B} + 3\text{O}_2 \rightarrow 2\text{B}_2\text{O}_3$  $(40.3\% \text{ fuel}) 2B + O_2 \rightarrow (BO)_2$ (40.3% fuel)  $2B + O_2 \rightarrow 2BO$ **T4.** 41% fuel, 3040.51 K solids: none liquids: 0.68% B gases: 50.00% BO, 42.46% (BO)<sub>2</sub>, 3.65% B<sub>2</sub>O<sub>3</sub>, 2.97% B<sub>2</sub>O, 0.18% B a combination of reactions:  $(31.1\% \text{ fuel}) 4\text{B} + 3\text{O}_2 \rightarrow 2\text{B}_2\text{O}_3$  $(40.3\% \text{ fuel}) 2B + O_2 \rightarrow (BO)_2$ (40.3% fuel)  $2B + O_2 \rightarrow 2BO$  $(57.5\% \text{ fuel}) 4\text{B} + \text{O}_2 \rightarrow 2\text{B}_2\text{O}$ **T5.** 54% fuel, 2746.30 K solids: none liquids: 23.99% B gases: 49.56% (BO)<sub>2</sub>, 16.91% BO, 8.60% B<sub>2</sub>O<sub>3</sub>, 0.91% B<sub>2</sub>O a combination of reactions with excess fuel remaining:  $(31.1\% \text{ fuel}) 4\text{B} + 3\text{O}_2 \rightarrow 2\text{B}_2\text{O}_3$  $(40.3\% \text{ fuel}) 2B + O_2 \rightarrow (BO)_2$ (40.3% fuel)  $2B + O_2 \rightarrow 2BO$ 

- Points 1–5 correspond to the maximum amounts of BO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>, BO, B<sub>2</sub>O, and (BO)<sub>2</sub>, respectively.
- From 76% to 84% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K. Alone, B<sub>2</sub>O<sub>3</sub>(l) vaporizes with slight decomposition at about 2323 K.
- From 63% to 72% fuel, the temperature is limited to 2350 K by the B(s-l) transition.
- B(l) is present from 41% to 72% fuel with the maximum amount (38.76%) occurring at 62% fuel. B(g) is present from 40% to 45% fuel with the maximum amount (0.18%) occurring at 41% fuel. Pure B(l) vaporizes at 4141 K.

# 23.3 BORON + $TiO_2$



**FIGURE 23.2** Adiabatic equilibrium temperature profile, B (fuel) + TiO<sub>2</sub> (oxidizer).

- **T1.** 4.4% fuel, 656.18 K solids: 85.83% Ti<sub>2</sub>O<sub>3</sub>, 13.98% B<sub>2</sub>O<sub>3</sub>, 0.19% TiB<sub>2</sub> liquids: none gases: none
- T2. 31.1% fuel, 1428.86 K—peak temperature solids: 59.95% TiB<sub>2</sub> liquids: 40.04% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 31.1% fuel: 10B + 3TiO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3TiB<sub>2</sub>
  - Elemental titanium is not predicted to occur at any point.

### 23.4 BORON + $V_2O_5$



**FIGURE 23.3** Adiabatic equilibrium temperature profile, B (fuel)  $+ V_2O_5$  (oxidizer).



 $B + V_2O_5$ 

Adiabatic Equilibrium Gas Products

100

90

80

70

60 50 40

**FIGURE 23.4** Adiabatic equilibrium gas production profile, B (fuel) +  $V_2O_5$  (oxidizer).

- **T1.** 3.8% fuel, 1633.00 K solids: 63.94% VO<sub>2</sub> liquids: 23.52% VO<sub>2</sub>, 12.24% B<sub>2</sub>O<sub>3</sub>, 0.31% V<sub>2</sub>O<sub>5</sub> gases: none simplified equation at 3.8% fuel: 2B +  $3V_2O_5 \rightarrow B_2O_3 + 6VO_2$
- T2. 7.3% fuel, 3.47% gas produced, 2323.01 K—peak temperature solids: 75.43% V<sub>2</sub>O<sub>3</sub>
  liquids: 20.06% B<sub>2</sub>O<sub>3</sub>, 1.04% VO<sub>2</sub>
  gases: 3.42% B<sub>2</sub>O<sub>3</sub>
  simplified equation at 7.3% fuel: 4B + 3V<sub>2</sub>O<sub>5</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3V<sub>2</sub>O<sub>3</sub>
- **T3.** 10.6% fuel, 2146.71 K solids: 0.58% V<sub>2</sub>O<sub>3</sub> liquids: 65.29% VO, 34.13% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 10.6% fuel: 2B + V<sub>2</sub>O<sub>5</sub> → B<sub>2</sub>O<sub>3</sub> + 2VO
- **T4.** 26.5% fuel, 12.76% gas produced, 2294.55 K solids: 52.82%  $V_3B_4$  liquids: 34.42%  $B_2O_3$  gases: 10.61%  $B_2O_3$ , 1.97% (BO)<sub>2</sub>, 0.18% BO simplified equation at 26.3% fuel: 18B + 3V<sub>2</sub>O<sub>5</sub> → 5B<sub>2</sub>O<sub>3</sub> + 2V<sub>3</sub>B<sub>4</sub>

- **T5.** 27.6% fuel, 13.05% gas produced, 2288.93 K solids:  $53.33\% V_2B_3$ , 0.14%  $V_3B_4$  liquids:  $33.49\% B_2O_3$  gases: 10.45%  $B_2O_3$ , 2.40% (BO)<sub>2</sub>, 0.19% BO simplified equation at 27.3% fuel:  $19B + 3V_2O_5 \rightarrow 5B_2O_3 + 3V_2B_3$
- **T6.** 30.6% fuel, 13.43% gas produced, 2286.03 K solids: 54.84% VB<sub>2</sub>, 0.50% V<sub>2</sub>B<sub>3</sub> liquids: 31.23% B<sub>2</sub>O<sub>3</sub> gases: 10.55% B<sub>2</sub>O<sub>3</sub>, 2.68% (BO)<sub>2</sub>, 0.20% BO simplified equation at 30.4% fuel: 22B +  $3V_2O_5 \rightarrow 5B_2O_3 + 6VB_2$ 
  - Elemental vanadium is not predicted to occur at any point.
  - From 3.5% to 4.8% fuel, the temperature is limited to 1633 K by the VO<sub>2</sub>(s-1) transition.
  - From 31.2% to 42.4% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
  - From 27.7% to 30.6% fuel, the temperature appears to be limited to 2286 K by the reaction
    of B<sub>2</sub>O<sub>3</sub>(l) and VB<sub>2</sub>(s) which forms V<sub>2</sub>B<sub>3</sub>(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also
    vaporized.
  - From 26.6% to 27.6% fuel, the temperature appears to be limited to 2289 K by the reaction of  $B_2O_3(l)$  and  $V_2B_3(s)$  which forms  $V_3B_4(s)$ ,  $(BO)_2(g)$ , and BO(g). Some  $B_2O_3$  is also vaporized.
  - From 14.0% to 26.4% fuel, the temperature appears to be limited to 2297 K by the reaction of  $B_2O_3(l)$  and  $V_3B_4(s)$  which forms VO(l), (BO)<sub>2</sub>(g), and BO(g). Some  $B_2O_3$  is also vaporized.
  - From 7.4% to 8.9% fuel, the temperature appears to be limited to 2321 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and VO(l) which forms V<sub>2</sub>O<sub>3</sub>(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
  - From 6.9% to 7.3% fuel, the temperature is limited to about 2323 K by the vaporization of  $B_2O_3(l)$ .
- G1. 31.2% fuel, 14.17% gas produced, 2191.63 K—peak gas solids: 54.90% VB<sub>2</sub>
  liquids: 30.91% B<sub>2</sub>O<sub>3</sub>
  gases: 8.51% (BO)<sub>2</sub>, 5.41% B<sub>2</sub>O<sub>3</sub>, 0.24% BO a combination of two reactions:
  (30.4% fuel) 22B + 3V<sub>2</sub>O<sub>5</sub> → 5B<sub>2</sub>O<sub>3</sub> + 6VB<sub>2</sub>
  (34.9% fuel) 18B + 2V<sub>2</sub>O<sub>5</sub> → 5(BO)<sub>2</sub> + 4VB<sub>2</sub>

# 23.5 BORON + $Nb_2O_5$



FIGURE 23.5 Adiabatic equilibrium temperature profile, B (fuel) + Nb<sub>2</sub>O<sub>5</sub> (oxidizer).

- **T1.** 2.7% fuel, 906.13 K solids: 91.23% NbO<sub>2</sub>, 0.20% NbB<sub>2</sub> liquids: 8.57% B<sub>2</sub>O<sub>3</sub> gases: none
- T2. 23.0% fuel, 2120.49 K—peak temperature solids: 66.35% NbB<sub>2</sub> liquids: 33.61% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 23.0% fuel: 22B + 3Nb<sub>2</sub>O<sub>5</sub> → 5B<sub>2</sub>O<sub>3</sub> + 6NbB<sub>2</sub>
  - Elemental niobium is not predicted to occur at any point.

# 23.6 BORON + $Ta_2O_5$



FIGURE 23.6 Adiabatic equilibrium temperature profile, B (fuel) + Ta<sub>2</sub>O<sub>5</sub> (oxidizer).

**T1.** 15.2% fuel, 1622.00 K—*peak temperature* solids: 77.68% TaB<sub>2</sub> liquids: 22.25% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 15.2% fuel: 22B +  $3Ta_2O_5 \rightarrow 5B_2O_3 + 6TaB_2$ 

• Elemental tantalum is not predicted to occur at any point.

# 23.7 BORON + $Cr_2O_3$



**FIGURE 23.7** Adiabatic equilibrium temperature profile, B (fuel) +  $Cr_2O_3$  (oxidizer).

- **T1.** 17.2% fuel, 1375.76 K solids: 31.78% CrB, 30.11% Cr, 0.34% Cr<sub>2</sub>O<sub>3</sub> liquids: 37.77% B<sub>2</sub>O<sub>3</sub> gases: none a combination of two reactions:  $(12.5\% \text{ fuel}) 2B + Cr_2O_3 \rightarrow B_2O_3 + 2Cr$  $(22.1\% \text{ fuel}) 4B + Cr_2O_3 \rightarrow B_2O_3 + 2CrB$
- **T2.** 22.2% fuel, 1661.90 K—*peak temperature* solids: 63.92% CrB, 0.44% CrB<sub>2</sub> liquids: 35.64% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 22.1% fuel: 4B + Cr<sub>2</sub>O<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 2CrB
- **T3.** 29.9% fuel, 1581.53 K solids: 67.77% CrB<sub>2</sub>, 0.12% CrB liquids: 32.11% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 29.9% fuel: 6B + Cr<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2CrB<sub>2</sub>
  - T1 corresponds to the maximum amount of Cr.
  - From 15.4% to 17.2% fuel, the temperature appears to be limited by the 2CrB(s) +  $Cr_2O_3(s) \rightarrow 4Cr(s) + B_2O_3(l)$  reaction, which occurs at 1376 K.

#### 23.8 BORON + $MoO_3$



**FIGURE 23.8** Adiabatic equilibrium temperature profile, B (fuel) +  $MoO_3$  (oxidizer).



**FIGURE 23.9** Adiabatic equilibrium gas production profile, B (fuel) + MoO<sub>3</sub> (oxidizer).

- **T1.** 4.7% fuel, 1.70% gas produced, 2250.61 K solids: 83.44% MoO<sub>2</sub> liquids: 14.86% B<sub>2</sub>O<sub>3</sub> gases: 1.18% (MoO<sub>3</sub>)<sub>3</sub>, 0.28% B<sub>2</sub>O<sub>3</sub>, 0.14% (MoO<sub>3</sub>)<sub>4</sub> simplified equation at 4.8% fuel: 2B + 3MoO<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3MoO<sub>2</sub>
- T2. 13.0% fuel, 22.50% gas produced, 2322.95 K—peak temperature solids: 57.68% Mo liquids: 19.81% B<sub>2</sub>O<sub>3</sub> gases: 21.90% B<sub>2</sub>O<sub>3</sub>, 0.18% (MoO<sub>3</sub>)<sub>3</sub>, 0.12% MoO<sub>3</sub>, 0.11% (MoO<sub>3</sub>)<sub>2</sub> simplified equation at 13.1% fuel: 2B + MoO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + Mo
- T3. 15.8% fuel, 26.22% gas produced, 2316.69 K solids: 56.33% Mo<sub>2</sub>B, 2.79% Mo liquids: 14.65% B<sub>2</sub>O<sub>3</sub> gases: 25.05% B<sub>2</sub>O<sub>3</sub>, 0.96% (BO)<sub>2</sub>, 0.19% BO simplified equation at 15.8% fuel: 5B + 2MoO<sub>3</sub> → 2B<sub>2</sub>O<sub>3</sub> + Mo<sub>2</sub>B
- **T4.** 18.6% fuel, 27.49% gas produced, 2310.90 K solids: 59.93% MoB, 0.42% Mo<sub>2</sub>B liquids: 12.16% B<sub>2</sub>O<sub>3</sub> gases: 25.36% B<sub>2</sub>O<sub>3</sub>, 1.85% (BO)<sub>2</sub>, 0.27% BO simplified equation at 18.4% fuel: 3B + MoO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + MoB

- **T5.** 26.2% fuel, 24.69% gas produced, 2250.71 K solids: 62.81% Mo<sub>2</sub>B<sub>5</sub>, 0.21% MoB liquids: 12.30% B<sub>2</sub>O<sub>3</sub> gases: 15.08% B<sub>2</sub>O<sub>3</sub>, 9.17% (BO)<sub>2</sub>, 0.43% BO a combination of two reactions: (25.3% fuel) 9B + 2MoO<sub>3</sub>  $\rightarrow$  2B<sub>2</sub>O<sub>3</sub> + Mo<sub>2</sub>B<sub>5</sub> (29.2% fuel) 11B + 2MoO<sub>3</sub>  $\rightarrow$  3(BO)<sub>2</sub> + Mo<sub>2</sub>B<sub>5</sub>
- The maximum amount of molybdenum, 57.93% Mo(s), occurs at 13.1% fuel and 2321.52 K.
- From 26.8% to 45.0% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
- From 19.5% to 26.2% fuel, the temperature appears to be limited to 2251 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and Mo<sub>2</sub>B<sub>5</sub>(s) which forms MoB(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- The plateau from 4.8% to 9.3% fuel (2252 K) could not be attributed to a simple transition or reaction; species in this region include (MoO<sub>3</sub>)<sub>n</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), B<sub>2</sub>O<sub>3</sub>(l), MoO<sub>2</sub>(s), and Mo(s).
- From 16.1% to 18.6% fuel, the temperature appears to be limited to 2311 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and MoB(s) which forms Mo<sub>2</sub>B(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- From 13.2% to 15.9% fuel, the temperature appears to be limited to 2317 K by the reaction of  $B_2O_3(l)$  and  $Mo_2B(s)$  which forms Mo(s),  $(BO)_2(g)$ , and BO(g). Some  $B_2O_3$  is also vaporized.
- G1. 2.9% fuel, 39.18% gas produced, 1359.59 K—peak gas solids: 51.49% MoO<sub>2</sub> liquids: 9.34% B<sub>2</sub>O<sub>3</sub> gases: 22.05% (MoO<sub>3</sub>)<sub>4</sub>, 12.75% (MoO<sub>3</sub>)<sub>3</sub>, 4.36% (MoO<sub>3</sub>)<sub>5</sub> one reaction with excess oxidizer remaining: (4.8% fuel) 2B + 3MoO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 3MoO<sub>2</sub>
- **G2.** 9.3% fuel, 33.96% gas produced, 2251.82 K solids: 41.12% Mo, 0.62% MoO<sub>2</sub> liquids: 24.30% B<sub>2</sub>O<sub>3</sub> gases: 23.43% (MoO<sub>3</sub>)<sub>3</sub>, 5.61% B<sub>2</sub>O<sub>3</sub>, 2.72% (MoO<sub>3</sub>)<sub>4</sub>, 1.81% (MoO<sub>3</sub>)<sub>2</sub>, 0.25% MoO<sub>3</sub> one reaction with excess oxidizer remaining: (13.1% fuel) 2B + MoO<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + Mo
- **G3.** 18.6% fuel, 27.49% gas produced, 2310.90 K see T4 for details

#### 23.9 BORON + WO<sub>3</sub>



**FIGURE 23.10** Adiabatic equilibrium temperature profile, B (fuel) + WO<sub>3</sub> (oxidizer).

- **T1.** 3.0% fuel, 1699.34 K solids: 89.66% WO<sub>2</sub>, 0.68% W<sub>18</sub>O<sub>49</sub> liquids: 9.66% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 3.0% fuel: 2B + 3WO<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3WO<sub>2</sub>
- **T2.** 8.5% fuel, 7.94% gas produced, 2322.83 K—*peak temperature* solids: 72.25% W liquids: 19.80% B<sub>2</sub>O<sub>3</sub> gases: 7.51% B<sub>2</sub>O<sub>3</sub>, 0.29% (WO<sub>3</sub>)<sub>2</sub> simplified equation at 8.5% fuel: 2B + WO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + W
  - The maximum amount of tungsten, 72.48% W(s), occurs at 8.6% fuel and 2311.44 K.
  - From 4.6% to 5.4% fuel, the temperature appears to be limited by the  $3W_{18}O_{49}(s) \rightarrow 5W(s) + 49WO_3(1)$  decomposition, which occurs at 2011 K.
  - The plateau from 5.7% to 6.2% fuel (2071 K) could not be attributed to a simple transition or reaction; species in this region include (WO<sub>3</sub>)<sub>n</sub>(g), W<sub>3</sub>O<sub>8</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), WO<sub>3</sub>(l), B<sub>2</sub>O<sub>3</sub>(l), and W(s). The vaporization of WO<sub>3</sub> and W<sub>3</sub>O<sub>8</sub> from W(s)/WO<sub>3</sub>(l) mixtures is expected to occur at 2087 K.
  - From 9.2% to 17.7% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
- G1. 6.2% fuel, 27.21% gas produced, 2071.06 K—peak gas solids: 52.33% W
  liquids: 19.67% B<sub>2</sub>O<sub>3</sub>, 0.79% WO<sub>3</sub>
  gases: 13.74% (WO<sub>3</sub>)<sub>3</sub>, 5.65% (WO<sub>3</sub>)<sub>4</sub>, 4.23% W<sub>3</sub>O<sub>8</sub>, 3.30% (WO<sub>3</sub>)<sub>2</sub>, 0.30% B<sub>2</sub>O<sub>3</sub>
  a combination of two reactions with excess oxidizer remaining:
  (1.0% fuel) 2B + 9WO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 3W<sub>3</sub>O<sub>8</sub>
  (8.5% fuel) 2B + WO<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + W



**FIGURE 23.11** Adiabatic equilibrium gas production profile, B (fuel) + WO<sub>3</sub> (oxidizer).

### 23.10 BORON + MnO



FIGURE 23.12 Adiabatic equilibrium temperature profile, B (fuel) + MnO (oxidizer).

- **T1.** 20.3% fuel, 1458.92 K—peak temperature solids: 73.53% MnB, 0.40% MnB<sub>2</sub> liquids: 26.07% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 20.3% fuel: 5B + 3MnO  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3MnB
- **T2.** 28.9% fuel, 1386.83 K solids: 76.74% MnB<sub>2</sub> liquids: 23.26% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 28.9% fuel: 8B + 3MnO  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3MnB<sub>2</sub>
  - Elemental manganese is not predicted to occur at any point.

# 23.11 BORON + $Mn_3O_4$



**FIGURE 23.13** Adiabatic equilibrium temperature profile, B (fuel) +  $Mn_3O_4$  (oxidizer).

- T1. 3.1% fuel, 1257.51 K solids: 89.94% MnO, 0.17% MnB liquids: 9.89% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 3.1% fuel: 2B + 3Mn<sub>3</sub>O<sub>4</sub> → B<sub>2</sub>O<sub>3</sub> + 9MnO
  T2. 20.9% fuel, 1842.97 K solids: 66.55% MnB liquids: 32.06% B<sub>2</sub>O<sub>3</sub>, 1.30% Mn gases: none simplified equation at 21.1% fuel: 17B + 3Mn<sub>3</sub>O<sub>4</sub> → 4B<sub>2</sub>O<sub>3</sub> + 9MnB
  T3. 21.1% fuel, 1855.08 K—*peak temperature* solids: 67.87% MnB
- solids: 67.87% MnB liquids: 32.01%  $B_2O_3$ , 0.13% Mn gases: none simplified equation at 21.1% fuel: 17B +  $3Mn_3O_4 \rightarrow 4B_2O_3 + 9MnB$
- **T4.** 29.1% fuel, 1701.78 K solids: 71.17% MnB<sub>2</sub> liquids: 28.77% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 29.1% fuel: 26B + 3Mn<sub>3</sub>O<sub>4</sub> → 4B<sub>2</sub>O<sub>3</sub> + 9MnB<sub>2</sub>
  - T2 corresponds to the maximum amount of Mn.

### 23.12 BORON + $Mn_2O_3$



FIGURE 23.14 Adiabatic equilibrium temperature profile, B (fuel) +  $Mn_2O_3$  (oxidizer).

FIGURE 23.15 Adiabatic equilibrium gas production profile, B (fuel) +  $Mn_2O_3$  (oxidizer).

- **T1.** 1.5% fuel, 1157.89 K solids: 95.14%  $Mn_3O_4$ liquids: 4.83%  $B_2O_3$ gases: none simplified equation at 1.5% fuel:  $2B + 9Mn_2O_3 \rightarrow B_2O_3 + 6Mn_3O_4$
- **T2.** 4.4% fuel, 1870.66 K solids: 85.56% MnO liquids: 14.17% B<sub>2</sub>O<sub>3</sub>, 0.27% Mn gases: none simplified equation at 4.4% fuel: 2B +  $3Mn_2O_3 \rightarrow B_2O_3 + 6MnO$
- **T3.** 15.1% fuel, 1844.13 K solids: 21.12% MnB liquids: 41.44% Mn, 37.44%  $B_2O_3$ gases: none a combination of two reactions: (12.0% fuel) 2B + Mn<sub>2</sub>O<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 2Mn (21.5% fuel) 4B + Mn<sub>2</sub>O<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 2MnB
- **T4.** 21.5% fuel, 2216.10 K—*peak temperature* solids: 65.36% MnB liquids: 34.58% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 21.5% fuel: 4B + Mn<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2MnB



- **T5.** 29.1% fuel, 1997.08 K solids: 68.55% MnB<sub>2</sub>, 0.19% MnB liquids: 31.27% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 29.1% fuel:  $6B + Mn_2O_3 \rightarrow B_2O_3 + 2MnB_2$ 
  - T3 corresponds to the maximum amount of Mn.
  - From 5.3% to 15.0% fuel, the temperature appears to be limited by the  $2MnB(s) + 3MnO(s) \rightarrow 5Mn(l) + B_2O_3(l)$  reaction, which occurs at 1843 K.
- G1. 21.4% fuel, 0.28% gas produced, 2201.28 K—peak gas solids: 64.65% MnB liquids: 34.51% B<sub>2</sub>O<sub>3</sub>, 0.56% Mn gases: 0.13% Mn, 0.11% B<sub>2</sub>O<sub>3</sub> simplified equation at 21.5% fuel: 4B + Mn<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2MnB

## 23.13 BORON + $MnO_2$



**FIGURE 23.16** Adiabatic equilibrium temperature profile, B (fuel) +  $MnO_2$  (oxidizer).

- **T1.** 3.8% fuel, 3.45% gas produced, 1878.85 K solids: 84.40%  $Mn_3O_4$  liquids: 12.15%  $B_2O_3$  gases: 3.37%  $O_2$  a combination of two reactions: (5.2% fuel) 4B + 9Mn $O_2 \rightarrow 2B_2O_3 + 3Mn_3O_4$  (decomposition)  $3MnO_2 \rightarrow Mn_3O_4 + O_2$
- T2. 7.7% fuel, 6.98% gas produced, 2315.81 K—peak temperature solids: none liquids: 74.96% MnO, 18.06% B<sub>2</sub>O<sub>3</sub> gases: 6.60% B<sub>2</sub>O<sub>3</sub>, 0.27% Mn simplified equation at 7.7% fuel: 2B + 3MnO<sub>2</sub> → B<sub>2</sub>O<sub>3</sub> + 3MnO
- T3. 14.2% fuel, 13.37% gas produced, 2211.55 K solids: none liquids: 46.51% Mn, 38.35% B<sub>2</sub>O<sub>3</sub>, 1.77% MnO gases: 6.34% Mn, 5.89% B<sub>2</sub>O<sub>3</sub>, 1.05% (BO)<sub>2</sub> simplified equation at 14.2% fuel: 4B + 3MnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Mn
- **T4.** 23.0% fuel, 18.59% gas produced, 2214.88 K solids: 55.74% MnB liquids: 25.68% B<sub>2</sub>O<sub>3</sub> gases: 8.56% B<sub>2</sub>O<sub>3</sub>, 7.65% (BO)<sub>2</sub>, 2.09% Mn, 0.29% BO a combination of two reactions: (22.5% fuel) 7B + 3MnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3MnB (27.2% fuel) 3B + MnO<sub>2</sub> → (BO)<sub>2</sub> + MnB



**FIGURE 23.17** Adiabatic equilibrium gas production profile, B (fuel) + MnO<sub>2</sub> (oxidizer).

- T5. 29.9% fuel, 12.27% gas produced, 2193.99 K solids: 61.29% MnB<sub>2</sub> liquids: 26.43% B<sub>2</sub>O<sub>3</sub> gases: 6.97% (BO)<sub>2</sub>, 4.78% B<sub>2</sub>O<sub>3</sub>, 0.32% Mn, 0.20% BO a combination of two reactions:
  (29.3% fuel) 10B + 3MnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3MnB<sub>2</sub> (33.2% fuel) 4B + MnO<sub>2</sub> → (BO)<sub>2</sub> + MnB<sub>2</sub>
- The maximum amount of manganese, 47.89% Mn(1) and 6.20% Mn(g), occurs at 14.4% fuel and 2206.25 K.
- The plateau from 3.9% to 5.2% fuel (1923 K) could not be attributed to a simple transition or reaction; species in this region include  $O_2(g)$ ,  $B_2O_3(g)$ ,  $B_2O_3(l)$ ,  $Mn_3O_4(s)$ , and MnO(s). The  $2Mn_3O_4(s) \rightarrow 6MnO(s) + O_2(g)$  decomposition is expected to occur at 1925 K.
- From 5.8% to 6.7% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
- The plateau from 30.0% to 40.1% fuel (2189 K) could not be attributed to a simple transition or reaction; species in this region include (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), BO(g), Mn(g), B<sub>2</sub>O<sub>3</sub>(l), MnB<sub>2</sub>(s), and B(s).
- The plateau from 14.5% to 21.3% fuel (2201 K) could not be attributed to a simple transition or reaction; species in this region include Mn(g),  $B_2O_3(g)$ ,  $(BO)_2(g)$ , BO(g), Mn(l),  $B_2O_3(l)$ , and MnB(s).
- From 8.4% to 14.3% fuel, the temperature appears to be limited to 2212 K by the reaction of  $B_2O_3(l)$  and Mn(l) which forms MnO(l) and (BO)<sub>2</sub>(g). Additionally, Mn and  $B_2O_3$  are partly vaporized.
- From 23.1% to 29.5% fuel, the temperature appears to be limited to 2212 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and MnB<sub>2</sub>(s) which forms MnB(s), (BO)<sub>2</sub>(g), and Mn(g). Some of the B<sub>2</sub>O<sub>3</sub> is also vaporized.

G1. 21.3% fuel, 21.06% gas produced, 2201.28 K—peak gas solids: 47.74% MnB liquids: 30.88% B<sub>2</sub>O<sub>3</sub>, 0.33% Mn gases: 9.52% Mn, 8.55% B<sub>2</sub>O<sub>3</sub>, 2.81% (BO)<sub>2</sub>, 0.17% BO a combination of two reactions:
(14.2% fuel) 4B + 3MnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Mn (22.5% fuel) 7B + 3MnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3MnB

#### 23.14 BORON + FeO



**FIGURE 23.18** Adiabatic equilibrium temperature profile, B (fuel) + FeO (oxidizer).

fuel (wt-%)
FIGURE 23.19 Adiabatic equilibrium gas produc-

tion profile, B (fuel) + FeO (oxidizer).

- **T1.** 9.1% fuel, 2017.85 K solids: none liquids: 70.51% Fe, 29.30%  $B_2O_3$ , 0.19% FeO gases: none simplified equation at 9.1% fuel: 2B + 3FeO  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3Fe
  - T2. 14.9% fuel, 0.62% gas produced, 2273.75 K—*peak temperature* solids: 71.94% Fe<sub>2</sub>B liquids: 26.89% B<sub>2</sub>O<sub>3</sub>, 0.55% Fe gases: 0.45% B<sub>2</sub>O<sub>3</sub>, 0.16% (BO)<sub>2</sub> simplified equation at 14.9% fuel: 7B + 6FeO → 2B<sub>2</sub>O<sub>3</sub> + 3Fe<sub>2</sub>B
  - **T3.** 20.1% fuel, 1.92% gas produced, 2252.47 K solids: 73.69% FeB, 0.40% Fe<sub>2</sub>B liquids: 24.00% B<sub>2</sub>O<sub>3</sub> gases: 1.19% B<sub>2</sub>O<sub>3</sub>, 0.69% (BO)<sub>2</sub> simplified equation at 20.1% fuel: 5B + 3FeO → B<sub>2</sub>O<sub>3</sub> + 3FeB
    - T1 corresponds to the maximum amount of Fe.
    - From 6.0% to 6.5% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
    - From 7.4% to 8.0% fuel, the temperature is limited to 1811 K by the Fe(s-l) transition.
    - From 20.3% to 23.4% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.





- From 15.0% to 20.1% fuel, the temperature appears to be limited to 2252 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and FeB(s) which forms Fe<sub>2</sub>B(s) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- From 14.3% to 14.9% fuel, the temperature appears to be limited to 2274 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and Fe<sub>2</sub>B(s) which forms Fe(l) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- G1. 20.3% fuel, 2.99% gas produced, 2191.59 K—*peak gas* solids: 73.94% FeB liquids: 23.01% B<sub>2</sub>O<sub>3</sub> gases: 1.79% (BO)<sub>2</sub>, 1.14% B<sub>2</sub>O<sub>3</sub> simplified equation at 20.1% fuel: 5B + 3FeO → B<sub>2</sub>O<sub>3</sub> + 3FeB

## 23.15 BORON + $Fe_3O_4$



**FIGURE 23.20** Adiabatic equilibrium temperature profile, B (fuel) +  $Fe_3O_4$  (oxidizer).

- **T1.** 11.1% fuel, 2113.36 K solids: 0.35% Fe<sub>2</sub>B liquids: 64.01% Fe, 35.64% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 11.1% fuel: 8B + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4B<sub>2</sub>O<sub>3</sub> + 9Fe
- T2. 16.3% fuel, 1.65% gas produced, 2273.75 K—peak temperature solids: 66.01% Fe<sub>2</sub>B liquids: 31.98% B<sub>2</sub>O<sub>3</sub>, 0.37% Fe gases: 1.19% B<sub>2</sub>O<sub>3</sub>, 0.42% (BO)<sub>2</sub> simplified equation at 16.3% fuel: 25B + 6Fe<sub>3</sub>O<sub>4</sub> → 8B<sub>2</sub>O<sub>3</sub> + 9Fe<sub>2</sub>B
- **T3.** 21.0% fuel, 2.79% gas produced, 2252.47 K solids: 67.69% FeB, 0.49% Fe<sub>2</sub>B liquids: 29.03%  $B_2O_3$  gases: 1.73%  $B_2O_3$ , 1.01% (BO)<sub>2</sub> simplified equation at 20.9% fuel: 17B + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4B<sub>2</sub>O<sub>3</sub> + 9FeB
  - T1 corresponds to the maximum amount of Fe.
  - From 7.3% to 8.0% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
  - From 8.9% to 9.4% fuel, the temperature is limited to 1811 K by the Fe(s-l) transition.
  - From 21.2% to 25.2% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
  - From 16.4% to 21.0% fuel, the temperature appears to be limited to 2252 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and FeB(s) which forms Fe<sub>2</sub>B(s) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
  - From 14.6% to 16.3% fuel, the temperature appears to be limited to 2274 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and Fe<sub>2</sub>B(s) which forms Fe(l) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.



**FIGURE 23.21** Adiabatic equilibrium gas production profile, B (fuel) +  $Fe_3O_4$  (oxidizer).

**G1.** 21.2% fuel, 3.87% gas produced, 2191.59 K—*peak gas* solids: 68.06% FeB liquids: 28.05% B<sub>2</sub>O<sub>3</sub> gases: 2.32% (BO)<sub>2</sub>, 1.48% B<sub>2</sub>O<sub>3</sub> a combination of two reactions: (20.9% fuel) 17B + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4B<sub>2</sub>O<sub>3</sub> + 9FeB (24.6% fuel) 7B + Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  2(BO)<sub>2</sub> + 3FeB

# 23.16 BORON + $Fe_2O_3$



**FIGURE 23.22** Adiabatic equilibrium temperature profile, B (fuel) +  $Fe_2O_3$  (oxidizer).

**FIGURE 23.23** Adiabatic equilibrium gas production profile, B (fuel) +  $Fe_2O_3$  (oxidizer).

- **T1.** 4.3% fuel, 1125.79 K solids: 85.53% FeO (wüstite), 0.62% Fe<sub>3</sub>O<sub>4</sub> (magnetite) liquids: 13.85% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 4.3% fuel:  $2B + 3Fe_2O_3 \rightarrow B_2O_3 + 6FeO$
- **T2.** 11.9% fuel, 2261.69 K solids: none liquids: 61.40% Fe, 38.32%  $B_2O_3$ , 0.29% FeO gases: none simplified equation at 11.9% fuel:  $2B + Fe_2O_3 \rightarrow B_2O_3 + 2Fe$
- **T3.** 16.9% fuel, 4.31% gas produced, 2273.75 K—*peak temperature* solids: 62.29% Fe<sub>2</sub>B liquids: 32.10% B<sub>2</sub>O<sub>3</sub> gases: 3.11% B<sub>2</sub>O<sub>3</sub>, 1.11% (BO)<sub>2</sub> simplified equation at 16.9% fuel:  $3B + Fe_2O_3 \rightarrow B_2O_3 + Fe_2B$
- **T4.** 21.5% fuel, 5.27% gas produced, 2252.47 K solids: 65.23% FeB, 0.27% Fe<sub>2</sub>B liquids: 29.23%  $B_2O_3$  gases: 3.26%  $B_2O_3$ , 1.90% (BO)<sub>2</sub> simplified equation at 21.3% fuel: 4B + Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 2FeB



- T2 corresponds to the maximum amount of Fe.
- From 7.2% to 8.1% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
- From 9.0% to 9.3% fuel, the temperature is limited to 1811 K by the Fe(s-l) transition.
- From 21.8% to 27.9% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
- From 17.1% to 21.5% fuel, the temperature appears to be limited to 2252 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and FeB(s) which forms Fe<sub>2</sub>B(s) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- From 12.1% to 17.0% fuel, the temperature appears to be limited to 2274 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and Fe<sub>2</sub>B(s) which forms Fe(l) and (BO)<sub>2</sub>(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- G1. 21.7% fuel, 6.14% gas produced, 2196.70 K—peak gas solids: 65.36% FeB liquids: 28.50% B<sub>2</sub>O<sub>3</sub> gases: 3.58% (BO)<sub>2</sub>, 2.45% B<sub>2</sub>O<sub>3</sub>, 0.10% BO a combination of two reactions:
  (21.3% fuel) 4B + Fe<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2FeB (25.3% fuel) 10B + 2Fe<sub>2</sub>O<sub>3</sub> → 3(BO)<sub>2</sub> + 4FeB



**FIGURE 23.24** Adiabatic equilibrium temperature profile, B (fuel) + CoO (oxidizer).

**FIGURE 23.25** Adiabatic equilibrium gas production profile, B (fuel) + CoO (oxidizer).

- **T1.** 8.7% fuel, 0.61% gas produced, 2322.23 K—*peak temperature* solids: none liquids: 71.14% Co, 27.41%  $B_2O_3$ , 0.84% CoO gases: 0.60%  $B_2O_3$  simplified equation at 8.8% fuel: 2B + 3CoO  $\rightarrow$   $B_2O_3$  + 3Co
- **T2.** 14.5% fuel, 14.23% gas produced, 2309.75 K solids: 72.87% Co<sub>2</sub>B liquids: 12.45% B<sub>2</sub>O<sub>3</sub>, 0.45% Co gases: 13.03% B<sub>2</sub>O<sub>3</sub>, 1.01% (BO)<sub>2</sub>, 0.14% BO simplified equation at 14.4% fuel: 7B + 6CoO → 2B<sub>2</sub>O<sub>3</sub> + 3Co<sub>2</sub>B
- **T3.** 19.7% fuel, 15.08% gas produced, 2283.40 K solids: 73.86% CoB, 0.80% Co<sub>2</sub>B liquids: 10.27% B<sub>2</sub>O<sub>3</sub> gases: 11.63% B<sub>2</sub>O<sub>3</sub>, 3.20% (BO)<sub>2</sub>, 0.23% BO a combination of two reactions: (19.4% fuel) 5B + 3CoO  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 3CoB (22.4% fuel) 4B + 2CoO  $\rightarrow$  (BO)<sub>2</sub> + 2CoB
  - The maximum amount of cobalt, 71.56% Co(l), occurs at 8.8% fuel and 2309.75 K.
  - From 5.2% to 5.6% fuel, the temperature is limited to 1768 K by the Co(s-l) transition.
  - From 7.4% to 7.7% fuel, the temperature is limited to 2103 K by the CoO(s-l) transition.
  - From 20.4% to 34.0% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.



- From 14.8% to 19.7% fuel, the temperature appears to be limited to 2283 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and CoB(s) which forms Co<sub>2</sub>B(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- From 8.8% to 14.5% fuel, the temperature appears to be limited to 2310 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and Co<sub>2</sub>B(s) which forms Co(l), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- **G1.** 14.5% fuel, 14.23% gas produced, 2309.75 K see T2 for details
- **G2.** 19.7% fuel, 15.08% gas produced, 2283.40 K—*peak gas* see T3 for details

### 23.18 BORON + $Co_3O_4$



**FIGURE 23.26** Adiabatic equilibrium temperature profile, B (fuel) +  $Co_3O_4$  (oxidizer).

B + Co<sub>3</sub>O<sub>4</sub>

Adiabatic Equilibrium Gas Products

100

90

80

70

20

gas products (wt-%)

**FIGURE 23.27** Adiabatic equilibrium gas production profile, B (fuel) +  $Co_3O_4$  (oxidizer).

- **T1.** 2.9% fuel, 1365.09 K solids: 90.65% CoO liquids: 9.34%  $B_2O_3$ gases: none simplified equation at 2.9% fuel:  $2B + 3Co_3O_4 \rightarrow B_2O_3 + 9CoO$
- **T2.** 10.7% fuel, 10.55% gas produced, 2322.61 K—*peak temperature* solids: none liquids: 65.53% Co, 23.92%  $B_2O_3$  gases: 10.42%  $B_2O_3$  simplified equation at 10.7% fuel: 8B +  $3Co_3O_4 \rightarrow 4B_2O_3 + 9Co$
- **T3.** 15.9% fuel, 21.90% gas produced, 2309.74 K solids: 66.59% Co<sub>2</sub>B liquids: 10.83% B<sub>2</sub>O<sub>3</sub>, 0.68% Co gases: 20.05% B<sub>2</sub>O<sub>3</sub>, 1.55% (BO)<sub>2</sub>, 0.22% BO simplified equation at 15.8% fuel: 25B + 6Co<sub>3</sub>O<sub>4</sub> → 8B<sub>2</sub>O<sub>3</sub> + 9Co<sub>2</sub>B
- **T4.** 20.8% fuel, 21.90% gas produced, 2283.40 K solids: 68.60% CoB, 0.18% Co<sub>2</sub>B liquids: 9.32% B<sub>2</sub>O<sub>3</sub> gases: 16.89% B<sub>2</sub>O<sub>3</sub>, 4.64% (BO)<sub>2</sub>, 0.34% BO a combination of two reactions: (20.3% fuel) 17B + 3Co<sub>3</sub>O<sub>4</sub> → 4B<sub>2</sub>O<sub>3</sub> + 9CoB (23.9% fuel) 7B + Co<sub>3</sub>O<sub>4</sub> → 2(BO)<sub>2</sub> + 3CoB

100

- T2 corresponds to the maximum amount of Co.
- From 6.6% to 7.5% fuel, the temperature is limited to 2103 K by the CoO(s-l) transition.
- From 21.7% to 39.2% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(1) mixtures, which occurs at 2192 K.
- From 16.4% to 20.8% fuel, the temperature appears to be limited to 2283 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and CoB(s) which forms Co<sub>2</sub>B(s), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- From 10.8% to 15.9% fuel, the temperature appears to be limited to 2310 K by the reaction of  $B_2O_3(l)$  and  $Co_2B(s)$  which forms Co(l),  $(BO)_2(g)$ , and BO(g). Some  $B_2O_3$  is also vaporized.
- From 8.5% to 10.7% fuel, the temperature is limited to about 2323 K by the vaporization of  $B_2O_3(l)$ .
- **G1.** 15.9% fuel, 21.90% gas produced, 2309.74 K—*peak gas* see T3 for details
- **G2.** 20.8% fuel, 21.90% gas produced, 2283.40 K—*peak gas* see T4 for details



**FIGURE 23.28** Adiabatic equilibrium temperature profile, B (fuel) + NiO (oxidizer).

**FIGURE 23.29** Adiabatic equilibrium gas production profile, B (fuel) + NiO (oxidizer).

- T1. 8.8% fuel, 0.92% gas produced, 2323.08 K—peak temperature solids: none liquids: 71.66% Ni, 27.42% B<sub>2</sub>O<sub>3</sub> gases: 0.91% B<sub>2</sub>O<sub>3</sub> simplified equation at 8.8% fuel: 2B + 3NiO → B<sub>2</sub>O<sub>3</sub> + 3Ni
- **T2.** 19.6% fuel, 15.85% gas produced, 2306.47 K solids: 74.77% NiB liquids: 9.38% B<sub>2</sub>O<sub>3</sub> gases: 14.22% B<sub>2</sub>O<sub>3</sub>, 1.41% (BO)<sub>2</sub>, 0.17% BO simplified equation at 19.4% fuel: 5B + 3NiO → B<sub>2</sub>O<sub>3</sub> + 3NiB
  - T1 corresponds to the maximum amount of Ni.
  - From 4.9% to 5.4% fuel, the temperature is limited to 1728 K by the Ni(s-l) transition.
  - From 20.5% to 34.4% fuel, the temperature appears to be limited by the vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2192 K.
  - From 8.9% to 19.5% fuel, the temperature appears to be limited to 2310 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and NiB(s) which forms Ni(l), (BO)<sub>2</sub>(g), and BO(g). Some B<sub>2</sub>O<sub>3</sub> is also vaporized.
- **G1.** 19.6% fuel, 15.85% gas produced, 2306.47 K—*peak gas* see T2 for details



#### 23.20 BORON + $Cu_2O$



**FIGURE 23.30** Adiabatic equilibrium temperature profile, B (fuel) +  $Cu_2O$  (oxidizer).

**FIGURE 23.31** Adiabatic equilibrium gas production profile, B (fuel) +  $Cu_2O$  (oxidizer).

- **T1.** 4.8% fuel, 2.06% gas produced, 2314.36 K—*peak temperature* solids: none liquids: 84.45% Cu, 13.49%  $B_2O_3$  gases: 1.92%  $B_2O_3$ , 0.10% Cu simplified equation at 4.8% fuel:  $2B + 3Cu_2O \rightarrow B_2O_3 + 6Cu$ 
  - T1 corresponds to the maximum amount of Cu.
  - From 30.3% to 34.0% fuel, the temperature is limited to 1358 K by the Cu(s-l) transition.
  - From 2.4% to 2.9% fuel, the temperature is limited to 1517 K by the Cu<sub>2</sub>O(s-l) transition.
  - The plateau from 5.1% to 8.9% fuel (2189 K) could not be attributed to a simple transition or reaction; species in this region include (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Cu(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). The vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2192 K.

G1. 5.1% fuel, 3.04% gas produced, 2189.18 K—peak gas solids: none liquids: 84.22% Cu, 12.67% B<sub>2</sub>O<sub>3</sub> gases: 1.79% (BO)<sub>2</sub>, 1.13% B<sub>2</sub>O<sub>3</sub> simplified equation at 4.8% fuel: 2B + 3Cu<sub>2</sub>O → B<sub>2</sub>O<sub>3</sub> + 6Cu



#### 23.21 BORON + CuO



**FIGURE 23.32** Adiabatic equilibrium temperature profile, B (fuel) + CuO (oxidizer).

- **T1.** 4.3% fuel, 1956.58 K solids: none liquids: 86.08% Cu<sub>2</sub>O, 13.84% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 4.3% fuel:  $2B + 6CuO \rightarrow B_2O_3 + 3Cu_2O$
- T2. 8.3% fuel, 23.66% gas produced, 2316.70 K—*peak temperature* solids: none liquids: 72.07% Cu, 4.27% B<sub>2</sub>O<sub>3</sub> gases: 22.31% B<sub>2</sub>O<sub>3</sub>, 1.17% Cu, 0.14% BO<sub>2</sub> simplified equation at 8.3% fuel: 2B + 3CuO → B<sub>2</sub>O<sub>3</sub> + 3Cu
  - The maximum amount of copper, 72.61% Cu(l) and 0.93% Cu(g), occurs at 7.9% fuel and 2299.82 K.
  - From 52.6% to 54.1% fuel, the temperature is limited to 1358 K by the Cu(s-l) transition.
  - From 2.0% to 2.7% fuel, the temperature appears to be limited by the 4CuO(s)  $\rightarrow$  2Cu<sub>2</sub>O(s) + O<sub>2</sub>(g) decomposition, which occurs at 1397 K.
  - From 3.0% to 3.6% fuel, the temperature is limited to 1517 K by the Cu<sub>2</sub>O(s-l) transition.
  - The plateau from 9.9% to 29.5% fuel (2189 K) could not be attributed to a simple transition or reaction; species in this region include (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Cu(g), BO(g), Cu(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). The vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2192 K.
  - The plateau from 5.1% to 7.8% fuel (2300 K) could not be attributed to a simple transition or reaction; species include B<sub>2</sub>O<sub>3</sub>(g), O<sub>2</sub>(g), Cu(g), BO<sub>2</sub>(g), Cu(l), Cu<sub>2</sub>O(l), and B<sub>2</sub>O<sub>3</sub>(l).

**G1.** 8.3% fuel, 23.66% gas produced, 2316.70 K—*peak gas* see T2 for details



**FIGURE 23.33** Adiabatic equilibrium gas production profile, B (fuel) + CuO (oxidizer).

 $B + Ag_2O$ 

Adiabatic Equilibrium Gas Products

#### 23.22 BORON + $Ag_2O$



**FIGURE 23.34** Adiabatic equilibrium temperature profile, B (fuel) + Ag<sub>2</sub>O (oxidizer).

**FIGURE 23.35** Adiabatic equilibrium gas production profile, B (fuel) +  $Ag_2O$  (oxidizer).

fuel (wt-%)

100

- **T1.** 3.0% fuel, 17.78% gas produced, 2261.91 K—*peak temperature* solids: none liquids: 81.27% Ag, 0.95% B<sub>2</sub>O<sub>3</sub> gases: 8.67% Ag, 8.60% B<sub>2</sub>O<sub>3</sub>, 0.37% Ag<sub>2</sub>, 0.13% BO<sub>2</sub> simplified equation at 3.0% fuel: 2B +  $3Ag_2O \rightarrow B_2O_3 + 6Ag$ 
  - Ag<sub>2</sub>O(s) is unstable above 468 K. The maximum amount of silver, 92.72% Ag(s), occurs at just 0.4% fuel and 639.07 K.

100

90

80

70

20

10

0

0

10 20 30 40 50 60 70 80 90

- From 39.8% to 41.5% fuel, the temperature is limited to 1234 K by the Ag(s-l) transition.
- The plateau from 3.8% to 16.9% fuel (2165 K) could not be attributed to a simple transition or reaction; species in this region include (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Ag(g), Ag<sub>2</sub>(g), BO(g), Ag(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). The vaporization of boron oxides from B(s)/B<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2192 K.
- **G1.** 3.0% fuel, 17.78% gas produced, 2261.91 K—*peak gas* see T1 for details

### 23.23 BORON + ZnO



FIGURE 23.36 Adiabatic equilibrium temperature profile, B (fuel) + ZnO (oxidizer).

T1. 8.2% fuel, 1176.98 K—peak temperature solids: none liquids: 73.75% Zn, 26.18% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 8.1% fuel: 2B + 3ZnO → B<sub>2</sub>O<sub>3</sub> + 3Zn

- T1 corresponds to the maximum amount of Zn.
- From 47.7% to 51.1% fuel, the temperature is limited to 693 K by the Zn(s-l) transition.
- From 40.0% to 44.6% fuel, the temperature is limited to 723 K by the  $B_2O_3(s-l)$  transition.

#### 23.24 BORON + CdO



**FIGURE 23.37** Adiabatic equilibrium temperature profile, B (fuel) + CdO (oxidizer).

**FIGURE 23.38** Adiabatic equilibrium gas production profile, B (fuel) + CdO (oxidizer).

- **T1.** 5.3% fuel, 82.66% gas produced, 1094.04 K—*peak temperature* solids: 0.27% CdO liquids: 17.07%  $B_2O_3$  gases: 82.66% Cd simplified equation at 5.3% fuel:  $2B + 3CdO \rightarrow B_2O_3 + 3Cd$ 
  - G1 corresponds to the maximum amount of Cd.
  - From 1.5% to 4.8% and 7.1% to 38.3% fuel, the temperature is limited to 1040K by the Cd(l-g) transition.
- **G1.** 5.4% fuel, 82.81% gas produced, 1092.86 K—*peak gas* solids: none liquids: 17.10%  $B_2O_3$  gases: 82.81% Cd simplified equation at 5.3% fuel: 2B + 3CdO  $\rightarrow B_2O_3$  + 3Cd



### 23.25 BORON + HgO



**FIGURE 23.39** Adiabatic equilibrium temperature profile, B (fuel) + HgO (oxidizer).



**FIGURE 23.40** Adiabatic equilibrium gas production profile, B (fuel) + HgO (oxidizer).

- **T1.** 1.9% fuel, 94.54% gas produced, 1911.26 K solids: none liquids: 5.46%  $B_2O_3$  gases: 89.66% Hg, 2.93%  $O_2$ , 1.16% HgO, 0.62%  $B_2O_3$ , 0.12% Hg<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (3.2% fuel) 2B + 3HgO  $\rightarrow$   $B_2O_3$  + 3Hg (decomposition) 2HgO  $\rightarrow$  2Hg +  $O_2$
- **T2.** 3.2% fuel, 100% gas produced, 2550.78 K—*peak temperature* solids: none liquids: none gases: 89.54% Hg, 9.92%  $B_2O_3$ , 0.33%  $BO_2$  simplified equation at 3.2% fuel:  $2B + 3HgO \rightarrow B_2O_3 + 3Hg$ 
  - HgO(s) is unstable above 716 K.
  - T1 and T2 correspond to the maximum amounts of Hg.
- The system produces 100% gas from 2.9% to 3.9% fuel.
- **G1.** 3.2% fuel, 100% gas produced, 2550.78 K—*peak gas* see T2 for details

#### 23.26 BORON + SnO



**FIGURE 23.41** Adiabatic equilibrium temperature profile, B (fuel) + SnO (oxidizer).

**FIGURE 23.42** Adiabatic equilibrium gas production profile, B (fuel) + SnO (oxidizer).

- T1. 5.1% fuel, 2103.30 K—peak temperature solids: none liquids: 83.63% Sn, 16.35% B<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 5.1% fuel: 2B + 3SnO → B<sub>2</sub>O<sub>3</sub> + 3Sn
  - T1 corresponds to the maximum amount of Sn.
  - From 4.2% to 4.6% fuel, the temperature appears to be limited by the vaporization of SnO from Sn(1)/SnO<sub>2</sub>(s) mixtures, which occurs at about 1820 K.

**G1.** 4.7% fuel, 7.47% gas produced, 1835.18 K—*peak gas* solids: none liquids: 77.41% Sn, 15.12%  $B_2O_3$  gases: 3.40% (SnO)<sub>2</sub>, 1.54% SnO, 1.31% (SnO)<sub>4</sub>, 1.20% (SnO)<sub>3</sub> one reaction with excess oxidizer remaining: (5.1% fuel) 2B + 3SnO  $\rightarrow B_2O_3 + 3Sn$ 


#### 23.27 BORON + $SnO_2$



**FIGURE 23.43** Adiabatic equilibrium temperature profile, B (fuel) + SnO<sub>2</sub> (oxidizer).

**FIGURE 23.44** Adiabatic equilibrium gas production profile, B (fuel) + SnO<sub>2</sub> (oxidizer).

- T1. 8.7% fuel, 3.94% gas produced, 2302.71 K—peak temperature solids: none liquids: 71.02% Sn, 25.04% B<sub>2</sub>O<sub>3</sub> gases: 2.92% B<sub>2</sub>O<sub>3</sub>, 0.68% SnO, 0.27% Sn simplified equation at 8.7% fuel: 4B + 3SnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Sn
- The maximum amount of tin, 71.54% Sn(l) and 0.26% Sn(g), occurs at 8.8% fuel and 2287.07 K.
- From 5.4% to 7.2% fuel, the temperature appears to be limited by the vaporization of SnO from Sn(1)/SnO<sub>2</sub>(s) mixtures, which occurs at about 1820 K.
- The plateau from 9.1% to 13.8% fuel (2189 K) could not be attributed to a simple transition or reaction; species in this region include  $(BO)_2(g)$ ,  $B_2O_3(g)$ , Sn(g), Sn(l),  $B_2O_3(l)$ , and B(s). The vaporization of boron oxides from  $B(s)/B_2O_3(l)$  mixtures is expected to occur at 2192 K.

G1. 7.3% fuel, 29.33% gas produced, 1821.06 K—peak gas solids: none liquids: 47.21% Sn, 23.47% B<sub>2</sub>O<sub>3</sub> gases: 12.97% (SnO)<sub>2</sub>, 5.88% (SnO)<sub>4</sub>, 5.44% SnO, 4.98% (SnO)<sub>3</sub> a combination of two reactions:
(4.6% fuel) 2B + 3SnO<sub>2</sub> → B<sub>2</sub>O<sub>3</sub> + 3SnO (8.7% fuel) 4B + 3SnO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Sn



fuel (wt-%)

#### 23.28 BORON + PbO



**FIGURE 23.45** Adiabatic equilibrium temperature profile, B (fuel) + PbO (oxidizer).

T1. 2.2% fuel, 19.08% gas produced, 1935.98 K solids: 29.47% PbB<sub>2</sub>O<sub>4</sub> liquids: 51.46% Pb gases: 11.71% Pb, 7.20% PbO one reaction with excess oxidizer remaining: (2.4% fuel) 2B + 4PbO → PbB<sub>2</sub>O<sub>4</sub> + 3Pb

**T2.** 3.1% fuel, 33.93% gas produced, 2006.15 K—*peak temperature* solids: none liquids: 56.66% Pb, 9.41% B<sub>2</sub>O<sub>3</sub> gases: 32.17% Pb, 0.90% PbO, 0.57% B<sub>2</sub>O<sub>3</sub>, 0.29% Pb<sub>2</sub> simplified equation at 3.1% fuel: 2B + 3PbO → B<sub>2</sub>O<sub>3</sub> + 3Pb

- The maximum amount of lead, 59.50% Pb(l), 30.10% Pb(g), and 0.26% Pb<sub>2</sub>(g), occurs at 3.2% fuel and 1998.62 K.
- From 1.6% to 2.0% fuel, the temperature appears to be limited by the vaporization of Pb and PbO from Pb(1)/PbO(1) mixtures, which occurs at 1780 K.
- From 2.3% to 2.8% fuel, the temperature appears to be limited by the vaporization of Pb, PbO, and B<sub>2</sub>O<sub>3</sub> from Pb(1)/PbB<sub>2</sub>O<sub>4</sub>(s) mixtures, which occurs at 1960 K.
- The plateau from 3.3% to 10.7% fuel (1991 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Pb(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). Alone, Pb(l) is expected to vaporize at 2020 K.
- G1 3.1% fuel, 33.93% gas produced, 2006.15 K—*peak gas* see T2 for details



**FIGURE 23.46** Adiabatic equilibrium gas production profile, B (fuel) + PbO (oxidizer).

#### 23.29 BORON + $Pb_3O_4$



**FIGURE 23.47** Adiabatic equilibrium temperature profile, B (fuel) +  $Pb_3O_4$  (oxidizer).



**FIGURE 23.48** Adiabatic equilibrium gas production profile, B (fuel) +  $Pb_3O_4$  (oxidizer).

**T1.** 1.0% fuel, 0.34% gas produced, 1663.01 K solids: 13.54%  $PbB_2O_4$ liquids: 86.12% PbO gases: 0.25% PbO simplified equation at 1.0% fuel:  $2B + 3Pb_3O_4 \rightarrow PbB_2O_4 + 8PbO$ 

T2. 4.0% fuel, 75.61% gas produced, 2008.01 K—peak temperature solids: none liquids: 12.82% Pb, 11.58% B<sub>2</sub>O<sub>3</sub> gases: 72.50% Pb, 1.30% B<sub>2</sub>O<sub>3</sub>, 1.14% PbO, 0.65% Pb<sub>2</sub> simplified equation at 4.0% fuel: 8B + 3Pb<sub>3</sub>O<sub>4</sub> → 4B<sub>2</sub>O<sub>3</sub> + 9Pb

- The maximum amount of lead, 15.31% Pb(l), 71.00% Pb(g), and 0.64% Pb<sub>2</sub>(g), occurs at 4.1% fuel and 2005.75 K.
- From 1.1% to 2.2% fuel, the temperature appears to be limited by the vaporization of Pb and PbO from Pb(l)/PbO(l) mixtures, which occurs at 1780 K.
- From 2.8% to 3.5% fuel, the temperature appears to be limited by the vaporization of Pb, PbO, and B<sub>2</sub>O<sub>3</sub> from Pb(l)/PbB<sub>2</sub>O<sub>4</sub>(s) mixtures, which occurs at 1960 K.
- The plateau from 4.3% to 19.2% fuel (1991 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Pb(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). Alone, Pb(l) is expected to vaporize at 2020 K.
- **G1.** 4.0% fuel, 75.61% gas produced, 2008.01 K—*peak gas* see T2 for details

#### 23.30 BORON + $PbO_2$



**FIGURE 23.49** Adiabatic equilibrium temperature profile, B (fuel) + PbO<sub>2</sub> (oxidizer).

- **T1.** 2.4% fuel, 63.30% gas produced, 1795.56 K solids: 32.48% PbB<sub>2</sub>O<sub>4</sub> liquids: 4.23% PbO gases: 61.08% PbO, 1.27% O<sub>2</sub>, 0.94% Pb a combination of two reactions: (2.9% fuel) 2B + 3PbO<sub>2</sub>  $\rightarrow$  PbB<sub>2</sub>O<sub>4</sub> + 2PbO (decomposition) 2PbO<sub>2</sub>  $\rightarrow$  2PbO + O<sub>2</sub>
- T2. 3.1% fuel, 69.82% gas produced, 2084.98 K solids: 30.18% PbB<sub>2</sub>O<sub>4</sub> liquids: none gases: 58.11% PbO, 8.63% Pb, 2.73% B<sub>2</sub>O<sub>3</sub>, 0.25% O<sub>2</sub> a combination of two reactions:
  (2.9% fuel) 2B + 3PbO<sub>2</sub> → PbB<sub>2</sub>O<sub>4</sub> + 2PbO (5.7% fuel) 4B + 3PbO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Pb
- T3. 5.7% fuel, 94.28% gas produced, 2188.92 K—peak temperature solids: none liquids: 5.72% B<sub>2</sub>O<sub>3</sub> gases: 81.07% Pb, 12.38% B<sub>2</sub>O<sub>3</sub>, 0.39% Pb<sub>2</sub>, 0.24% PbO, 0.15% (BO)<sub>2</sub> simplified equation at 5.7% fuel: 4B + 3PbO<sub>2</sub> → 2B<sub>2</sub>O<sub>3</sub> + 3Pb
  - The maximum amount of lead, 81.17% Pb(g) and 0.39% Pb<sub>2</sub>(g), occurs at 5.8% fuel and 2180.12 K.
  - The plateau from 17.1% to 31.6% fuel (1991 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Pb(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). Alone, Pb(l) is expected to vaporize at 2020 K.
- **G1.** 5.7% fuel, 94.28% gas produced, 2188.92 K—*peak gas* see T3 for details



**FIGURE 23.50** Adiabatic equilibrium gas production profile, B (fuel) +  $PbO_2$  (oxidizer).

#### 23.31 BORON + $Sb_2O_3$



 $B + Sb_2O_3$ Adiabatic Equilibrium Gas Products gas products (wt-%) fuel (wt-%)

FIGURE 23.51 Adiabatic equilibrium temperature profile, B (fuel) +  $Sb_2O_3$  (oxidizer).

**FIGURE 23.52** Adiabatic equilibrium gas production profile, B (fuel) + Sb<sub>2</sub>O<sub>3</sub> (oxidizer).

- T1. 6.9% fuel, 79.22% gas produced, 2017.54 K—*peak temperature* solids: none liquids: 20.79% B<sub>2</sub>O<sub>3</sub> gases: 61.16% Sb<sub>2</sub>, 11.95% Sb<sub>4</sub>, 4.32% Sb, 1.29% B<sub>2</sub>O<sub>3</sub>, 0.39% SbO, 0.10% (BO)<sub>2</sub> simplified equation at 6.9% fuel: 2B + Sb<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2Sb
  - The maximum amount of antimony, 3.88% Sb(g), 60.17% Sb<sub>2</sub>(g), and 13.60% Sb<sub>4</sub>(g), occurs at 7.0% fuel and 1995.05 K.
  - The plateau from 12.0% to 21.3% fuel (1890 K) could not be attributed to a simple transition or reaction; species in this region include Sb<sub>n</sub>(g), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Sb(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). Alone, Sb(l) is expected to vaporize at 1899 K.
- **G1.** 2.5% fuel, 64.02% gas produced, 1117.38 K solids: none liquids: 27.93% Sb, 8.05%  $B_2O_3$  gases: 63.74%  $Sb_4O_6$ , 0.19%  $Sb_4$  one reaction with excess oxidizer remaining: (6.9% fuel)  $2B + Sb_2O_3 \rightarrow B_2O_3 + 2Sb$
- G2. 6.2% fuel, 80.16% gas produced, 1825.29 K—peak gas solids: none liquids: 19.84% B<sub>2</sub>O<sub>3</sub> gases: 39.75% Sb<sub>2</sub>, 24.46% Sb<sub>4</sub>, 14.47% SbO, 1.35% Sb, 0.12% B<sub>2</sub>O<sub>3</sub> a combination of two reactions:
  (2.4% fuel) 2B + 3Sb<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 6SbO (6.9% fuel) 2B + Sb<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2Sb

#### 23.32 BORON + $Bi_2O_3$



B + Bi<sub>2</sub>O<sub>3</sub> Adiabatic Equilibrium Gas Products 100 90 80 70 gas products (wt-%) 60 50 40 30 20 10 0 30 60 70 80 0 10 20 40 50 90 100 fuel (wt-%)

**FIGURE 23.53** Adiabatic equilibrium temperature profile, B (fuel) +  $Bi_2O_3$  (oxidizer).

**FIGURE 23.54** Adiabatic equilibrium gas production profile, B (fuel) +  $Bi_2O_3$  (oxidizer).

- **T1.** 4.4% fuel, 87.57% gas produced, 2039.42 K—*peak temperature* solids: none liquids: 12.43% B<sub>2</sub>O<sub>3</sub> gases: 50.71% Bi, 34.07% Bi<sub>2</sub>, 1.73% B<sub>2</sub>O<sub>3</sub>, 1.05% BiO simplified equation at 4.4% fuel: 2B + Bi<sub>2</sub>O<sub>3</sub>  $\rightarrow$  B<sub>2</sub>O<sub>3</sub> + 2Bi
- The maximum amount of bismuth, 50.13% Bi(g) and 35.53% Bi<sub>2</sub>(g), occurs at 4.5% fuel and 2027.49 K.
- From 2.0% to 3.3% fuel, the temperature appears to be limited by the vaporization of BiO and Bi from Bi(l)/Bi<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 1827 K.
- The plateau from 11.1% to 22.1% fuel (1842 K) could not be attributed to a simple transition or reaction; species in this region include Bi(g), Bi<sub>2</sub>(g), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), Bi(l), B<sub>2</sub>O<sub>3</sub>(l), and B(s). Alone, Bi(l) is expected to vaporize at 1846 K.

G1. 4.7% fuel, 87.92% gas produced, 1974.96 K—peak gas solids: none liquids: 12.01% B<sub>2</sub>O<sub>3</sub> gases: 45.17% Bi, 40.31% Bi<sub>2</sub>, 1.56% (BO)<sub>2</sub>, 0.85% B<sub>2</sub>O<sub>3</sub> simplified equation at 4.4% fuel: 2B + Bi<sub>2</sub>O<sub>3</sub> → B<sub>2</sub>O<sub>3</sub> + 2Bi

# 24 Aluminum–Oxidizer Systems

## 24.1 OVERVIEW

This chapter concerns the adiabatic properties of the aluminum–oxygen system and another thirtytwo aluminum–oxidizer combinations. Equation 24.1 is a general description of the chemical reactions in question, and Table 24.1 provides a broad overview of the most basic results. The thermochemical descriptions within this chapter were derived from the *FactPS* and *FToxid* databases of

TABLE 24.1 Aluminum-Oxidizer Systems			
24.2	804	$O_2$	4006
24.3	806	TiO <sub>2</sub>	2022
24.4	807	$V_2O_5$	3117
24.5	809	$Nb_2O_5$	2705
24.6	811	$Ta_2O_5$	2348
24.7	812	$Cr_2O_3$	2327
24.8	813	MoO <sub>3</sub>	3791
24.9	815	WO <sub>3</sub>	3874
24.10	817	MnO	2213
24.11	818	$Mn_3O_4$	2336
24.12	820	$Mn_2O_3$	2336
24.13	822	$MnO_2$	3380
24.14	824	FeO	2981
24.15	826	Fe <sub>3</sub> O <sub>4</sub>	3124
24.16	828	Fe <sub>2</sub> O <sub>3</sub>	3126
24.17	830	CoO	3189
24.18	832	$Co_3O_4$	3198
24.19	834	NiO	3182
24.20	836	Cu <sub>2</sub> O	2837
24.21	837	CuO	2839
24.22	839	$Ag_2O$	2427
24.23	840	ZnO	1580
24.24	841	CdO	2576
24.25	843	HgO	3650
24.26	845	$B_2O_3$	2327
24.27	847	SiO <sub>2</sub>	1759
24.28	848	SnO	2839
24.29	850	$SnO_2$	2835
24.30	851	PbO	2327
24.31	853	$Pb_3O_4$	3103
24.32	855	PbO <sub>2</sub>	3647
24.33	857	$Sb_2O_3$	2703
24.34	859	Bi <sub>2</sub> O <sub>3</sub>	3202

*FactSage 7.0.*\* Only pure substances were considered in the condensed phases. Gases were treated ideally, and ideal gas mixing was assumed. Charged species were not considered in any phase.

aluminum + oxidizer 
$$\rightarrow$$
 adiabatic equilibrium products  
( $P = 1 \text{ atm}, T_i = 298.15 \text{ K}, T_{ad} = adiabatic equilibrium temperature$ ) (24.1)

Within each of the following sections, you will find one or two general figures as well as written descriptions of certain fuel-to-oxidizer ratios. Temperature points (T1, T2, and so on) describe features and points of interest along adiabatic temperature profiles. Similarly, gas points (G1, G2, and so on) refer to adiabatic gas production profiles. Some adiabatic temperature charts contain flat regions where the adiabatic temperature remains constant despite variations in the stoichiometry of the system. Some of these plateaus are described and explained (see Chapter 2 and Tables 2.10–2.15 for more information). The first part of Chapter 5 is also about aluminum.

#### 24.2 ALUMINUM + $O_2$



**FIGURE 24.1** Adiabatic equilibrium temperature profile, Al (fuel) + O<sub>2</sub> (oxidizer).

**T1.** 36% fuel, 3889.65 K

solids: none liquids: 52.30% Al<sub>2</sub>O<sub>3</sub> major gases: 18.98% O, 16.19% O<sub>2</sub>, 8.12% AlO other gases: 1.44% Al<sub>2</sub>O<sub>2</sub>, 1.19% Al, 0.99% Al<sub>2</sub>O, 0.77% AlO<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (52.9% fuel)  $4Al + 3O_2 \rightarrow 2Al_2O_3$ (62.8% fuel)  $2Al + O_2 \rightarrow 2AlO$ 

<sup>\*</sup> Bale, C. W.; Pelton, A. D.; Thompson, W. T.; Eriksson, G.; Hack, K.; Chartrand, P.; Decterov, S.; Jung, I.-H.; Melançon, J.; Petersen, S. *FactSage*, version 7.0; CRCT ThermFact, Inc. and GTT-Technologies, 2015; www.factsage.com (accessed September, 2019).

- **T2.** 53% fuel, 4006.19 K—peak temperature solids: none liquids: 34.93% Al<sub>2</sub>O<sub>3</sub> major gases: 22.11% AlO, 12.47% O, 10.69% Al<sub>2</sub>O, 7.78% Al, 6.55% Al<sub>2</sub>O<sub>2</sub> other gases: 4.40% O<sub>2</sub>, 0.99% AlO<sub>2</sub> a combination of reactions with unreacted fuel and oxidizer remaining: (52.9% fuel) 4Al + 3O<sub>2</sub>  $\rightarrow$  2Al<sub>2</sub>O<sub>3</sub> (62.8% fuel) 2Al + O<sub>2</sub>  $\rightarrow$  2AlO (62.8% fuel) 2Al + O<sub>2</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>2</sub> (77.1% fuel) 4Al + O<sub>2</sub>  $\rightarrow$  2Al<sub>2</sub>O
- **T3.** 63% fuel, 3951.74 K

solids: none liquids: 38.06% Al<sub>2</sub>O<sub>3</sub> major gases: 20.56% Al<sub>2</sub>O, 17.66% AlO, 11.40% Al, 6.84% Al<sub>2</sub>O<sub>2</sub> other gases: 4.21% O, 0.81% O<sub>2</sub>, 0.41% AlO<sub>2</sub> a combination of reactions with unreacted fuel and oxidizer remaining: (52.9% fuel)  $4Al + 3O_2 \rightarrow 2Al_2O_3$ (62.8% fuel)  $2Al + O_2 \rightarrow 2AlO$ (62.8% fuel)  $2Al + O_2 \rightarrow Al_2O_2$ (77.1% fuel)  $4Al + O_2 \rightarrow 2Al_2O$ 

- **T4.** 77% fuel, 2534.93 K solids: none liquids: 8.35% Al<sub>2</sub>O<sub>3</sub> gases: 83.34% Al<sub>2</sub>O, 8.15% Al, 0.13% Al<sub>2</sub> a combination of two reactions with excess fuel remaining: (52.9% fuel) 4Al + 3O<sub>2</sub>  $\rightarrow$  2Al<sub>2</sub>O<sub>3</sub> (77.1% fuel) 4Al + O<sub>2</sub>  $\rightarrow$  2Al<sub>2</sub>O
- The first, third, and fourth points correspond to the maximum amounts of Al<sub>2</sub>O<sub>3</sub>, Al<sub>2</sub>O<sub>2</sub>, and Al<sub>2</sub>O, respectively. The second point corresponds to the maximum amounts of AlO and AlO<sub>2</sub>.
- From 78% to 91% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K. Pure Al(l) vaporizes at 2790 K.
- Al<sub>2</sub>O<sub>3</sub>(l) decomposes into a gaseous mixture of AlO, O, Al<sub>2</sub>O, Al, Al<sub>2</sub>O<sub>2</sub>, O<sub>2</sub>, and AlO<sub>2</sub> at 4006 K. This appears to limit any further increase in temperature.
- Al(g) is present from 26% to 91% fuel. The maximum amount, 15.69%, occurs at 72% fuel.

#### 24.3 ALUMINUM + $TiO_2$



**FIGURE 24.2** Adiabatic equilibrium temperature profile, Al (fuel) + TiO<sub>2</sub> (oxidizer).

**T1.** 10.1% fuel, 1358.95 K

solids: 80.32% Ti<sub>2</sub>O<sub>3</sub>, 19.08% Al<sub>2</sub>O<sub>3</sub> (corundum), 0.59% Ti<sub>3</sub>O<sub>5</sub> liquids: none gases: none simplified equation at 10.1% fuel:  $2AI + 6TiO_2 \rightarrow Al_2O_3 + 3Ti_2O_3$ 

- **T2.** 18.4% fuel, 1819.31 K solids: 65.22% TiO, 34.74%  $Al_2O_3$  (corundum) liquids: none gases: none simplified equation at 18.4% fuel:  $2Al + 3TiO_2 \rightarrow Al_2O_3 + 3TiO_3$
- T3. 44.1% fuel, 2022.42 K—peak temperature solids: 52.34% TiAl, 47.58% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: none simplified equation at 44.1% fuel: 7Al + 3TiO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3TiAl
- **T4.** 59.4% fuel, 1878.51 K solids: 65.39% TiAl<sub>3</sub>, 34.56% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: none simplified equation at 59.4% fuel:  $13Al + 3TiO_2 \rightarrow 2Al_2O_3 + 3TiAl_3$
- Elemental titanium is not predicted to occur at any point.

### 24.4 ALUMINUM + $V_2O_5$



**FIGURE 24.3** Adiabatic equilibrium temperature profile, Al (fuel) +  $V_2O_5$  (oxidizer).

- T1. 9.0% fuel, 1859.52 K solids: 17.01% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 82.99% VO<sub>2</sub> gases: none simplified equation at 9.0% fuel:  $2A1 + 3V_2O_5 \rightarrow Al_2O_3 + 6VO_2$
- **T2.** 16.5% fuel, 2744.20 K solids: none liquids: 68.68% V<sub>2</sub>O<sub>3</sub>, 31.18% Al<sub>2</sub>O<sub>3</sub>, 0.15% VO<sub>2</sub> gases: none simplified equation at 16.5% fuel: 4Al + 3V<sub>2</sub>O<sub>5</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3V<sub>2</sub>O<sub>3</sub>
- T3. 22.9% fuel, 3117.01 K—peak temperature solids: none liquids: 56.75% VO, 43.21% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 22.9% fuel: 2Al + V<sub>2</sub>O<sub>5</sub> → Al<sub>2</sub>O<sub>3</sub> + 2VO
- T4. 35.8% fuel, 7.45% gas produced, 3016.82 K solids: none liquids: 56.98% Al<sub>2</sub>O<sub>3</sub>, 35.58% V gases: 5.89% Al<sub>2</sub>O, 1.06% Al, 0.25% V, 0.16% VO a combination of two reactions with excess fuel remaining: (33.1% fuel) 10Al + 3V<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O<sub>3</sub> + 6V (59.7% fuel) 10Al + V<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O + 2V



**FIGURE 24.4** Adiabatic equilibrium gas production profile, Al (fuel) +  $V_2O_5$  (oxidizer).

- T4 corresponds to the maximum amount of V.
- From 6.0% to 7.6% fuel, the temperature is limited to 1633 K by the VO<sub>2</sub>(s-l) transition.
- From 66.3% to 67.3% fuel, the temperature is limited to 2190 K by the V(s-l) transition.
- From 11.3% to 12.1% and 58.1% to 64.1% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- From 12.3% to 13.5% fuel, the temperature is limited to 2340 K by the  $V_2O_3(s-1)$  transition.
- From 40.2% to 54.9% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
- From 23.7% to 35.7% fuel, the temperature appears to be limited to 3022 K by the reaction of V(l) and Al<sub>2</sub>O<sub>3</sub>(l) which forms VO(l-g), Al<sub>2</sub>O(g), and Al(g). Some of the V is vaporized as well.

G1. 40.2% fuel, 18.98% gas produced, 2469.55 K—peak gas solids: none liquids: 47.42% Al<sub>2</sub>O<sub>3</sub>, 33.49% V, 0.10% Al gases: 17.39% Al<sub>2</sub>O, 1.56% Al a combination of two reactions with excess fuel remaining: (33.1% fuel) 10Al + 3V<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O<sub>3</sub> + 6V (59.7% fuel) 10Al + V<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O + 2V

#### 24.5 ALUMINUM + $Nb_2O_5$



**FIGURE 24.5** Adiabatic equilibrium temperature profile, Al (fuel) +  $Nb_2O_5$  (oxidizer).

**FIGURE 24.6** Adiabatic equilibrium gas production profile, Al (fuel) +  $Nb_2O_5$  (oxidizer).

T1. 6.3% fuel, 1518.23 K

solids: 87.49% NbO<sub>2</sub>, 11.90% Al<sub>2</sub>O<sub>3</sub> (corundum), 0.60% Nb<sub>2</sub>O<sub>5</sub> liquids: none gases: none simplified equation at 6.3% fuel:  $2Al + 3Nb_2O_5 \rightarrow Al_2O_3 + 6NbO_2$ 

- **T2.** 16.9% fuel, 2221.56 K solids: 31.93%  $Al_2O_3$  (corundum), 0.15% Nb liquids: 67.92% NbO gases: none simplified equation at 16.9% fuel:  $2Al + Nb_2O_5 \rightarrow Al_2O_3 + 2NbO$
- T3. 25.3% fuel, 2704.64 K—peak temperature solids: 52.22% Nb liquids: 47.74% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 25.3% fuel: 10Al + 3Nb<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O<sub>3</sub> + 6Nb
  - T3 corresponds to the maximum amount of Nb.
  - From 11.2% to 13.3% fuel, the temperature is limited to 2175 K by the NbO<sub>2</sub>(s-l) transition.
  - From 13.6% to 16.8% fuel, the temperature is limited to 2210 K by the NbO(s-l) transition.
  - From 17.6% to 21.2% and 35.5% to 45.1% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
  - From 27.0% to 31.6% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.



G1. 27.0% fuel, 3.95% gas produced, 2469.66 K—peak gas solids: 51.03% Nb liquids: 44.91% Al<sub>2</sub>O<sub>3</sub>, 0.11% Al gases: 3.62% Al<sub>2</sub>O, 0.32% Al a combination of two reactions:
(25.3% fuel) 10Al + 3Nb<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O<sub>3</sub> + 6Nb (50.4% fuel) 10Al + Nb<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O + 2Nb

### 24.6 ALUMINUM + $Ta_2O_5$



FIGURE 24.7 Adiabatic equilibrium temperature profile, Al (fuel) + Ta<sub>2</sub>O<sub>5</sub> (oxidizer).

T1. 16.9% fuel, 2347.88 K—peak temperature solids: 68.00% Ta liquids: 31.93% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 16.9% fuel: 10A1 + 3Ta<sub>2</sub>O<sub>5</sub> → 5Al<sub>2</sub>O<sub>3</sub> + 6Ta

- T1 corresponds to the maximum amount of Ta.
- From 10.3% to 11.4% fuel, the temperature is limited to 2143 K by the  $Ta_2O_5(s-1)$  transition.
- From 12.7% to 16.6% and 17.4% to 27.3% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.

#### 24.7 ALUMINUM + $Cr_2O_3$



**FIGURE 24.8** Adiabatic equilibrium temperature profile, Al (fuel) +  $Cr_2O_3$  (oxidizer).

**T1.** 19.5% fuel, 1944.22 K

solids: 36.85% Al<sub>2</sub>O<sub>3</sub> (corundum), 28.95% Cr, 0.34% Cr<sub>2</sub>O<sub>3</sub> liquids: 33.86% CrO gases: none a combination of two reactions: (10.6% fuel) 2Al + 3Cr<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 6CrO (26.2% fuel) 2Al + Cr<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 2Cr

- **T2.** 26.2% fuel, 2327.02 K—*peak temperature* solids: 9.96% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 50.49% Cr, 39.54% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 26.2% fuel: 2Al + Cr<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 2Cr
  - T2 corresponds to the maximum amount of Cr.
  - From 14.5% to 19.5% fuel, the temperature appears to be limited by the formation of CrO(1) from Cr(s)/Cr<sub>2</sub>O<sub>3</sub>(s) mixtures, which occurs at 1944 K.
  - From 21.2% to 22.0% and 40.9% to 44.4% fuel, the temperature is limited to 2180 K by the Cr(s-l) transition.
  - From 23.2% to 36.9% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.

#### 24.8 ALUMINUM + MoO<sub>3</sub>



FIGURE 24.9 Adiabatic equilibrium temperature profile, Al (fuel) + MoO<sub>3</sub> (oxidizer).

FIGURE 24.10 Adiabatic equilibrium gas production profile, Al (fuel) +  $MoO_3$  (oxidizer).

40

50 60 70

fuel (wt-%)

80 90 100

AI + MoO<sub>3</sub>

- T1. 7.9% fuel, 28.90% gas produced, 2288.93 K solids: 56.17% MoO<sub>2</sub>, 14.93% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 23.68% (MoO<sub>3</sub>)<sub>3</sub>, 3.37% (MoO<sub>3</sub>)<sub>4</sub>, 1.54% (MoO<sub>3</sub>)<sub>2</sub>, 0.18% MoO<sub>3</sub>, 0.11% (MoO<sub>3</sub>)<sub>5</sub> one reaction with excess oxidizer remaining: (11.1% fuel)  $2A1 + 3MoO_3 \rightarrow Al_2O_3 + 3MoO_2$
- T2. 27.3% fuel, 8.28% gas produced, 3790.99 K—peak temperature solids: none liquids: 47.79% Al<sub>2</sub>O<sub>3</sub>, 43.93% Mo major gases: 3.38% MoO, 1.85% MoO<sub>2</sub>, 1.08% Al<sub>2</sub>O, 0.67% AlO other gases: 0.58% A1, 0.27% Al<sub>2</sub>O<sub>2</sub>, 0.17% MoO<sub>3</sub>, 0.14% Mo, 0.12% O simplified equation at 27.3% fuel:  $2A1 + MoO_3 \rightarrow Al_2O_3 + Mo$
- **T3.** 30.1% fuel, 8.70% gas produced, 3651.05 K solids: none liquids: 45.89% Al<sub>2</sub>O<sub>3</sub>, 45.41% Mo gases: 4.48% Al<sub>2</sub>O, 1.64% Al, 1.06% MoO, 0.72% AlO, 0.41% Al<sub>2</sub>O<sub>2</sub>, 0.24% MoO<sub>2</sub> a combination of two reactions with excess fuel remaining: (27.3% fuel) 2Al + MoO<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + Mo  $(52.9\% \text{ fuel}) 6\text{Al} + \text{MoO}_3 \rightarrow 3\text{Al}_2\text{O} + \text{Mo}$ 
  - T3 corresponds to the maximum amount of Mo.
  - From 8.0% to 11.1% fuel, the temperature appears to be limited by the vaporization of  $MoO_3$  from  $Mo(s)/MoO_2(s)$  mixtures, which occurs at 2308 K.

- From 11.2% to 12.6% and 62.3% to 66.1% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- From 39.3% to 59.8% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
- From 17.1% to 17.6% and 35.9% to 36.7% fuel, the temperature is limited to 2896 K by the Mo(s-l) transition.
- **G1.** 5.0% fuel, 54.98% gas produced, 1356.41 K solids: 35.57% MoO<sub>2</sub>, 9.45% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 31.05% (MoO<sub>3</sub>)<sub>4</sub>, 17.71% (MoO<sub>3</sub>)<sub>3</sub>, 6.20% (MoO<sub>3</sub>)<sub>5</sub> one reaction with excess oxidizer remaining: (11.1% fuel) 2Al + 3MoO<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3MoO<sub>2</sub>
- G2. 11.1% fuel, 59.29% gas produced, 2308.16 K—*peak gas* solids: 20.97% Al<sub>2</sub>O<sub>3</sub> (corundum), 19.71% Mo liquids: none gases: 48.59% (MoO<sub>3</sub>)<sub>3</sub>, 6.69% (MoO<sub>3</sub>)<sub>4</sub>, 3.31% (MoO<sub>3</sub>)<sub>2</sub>, 0.42% MoO<sub>3</sub>, 0.20% (MoO<sub>3</sub>)<sub>5</sub> one reaction with excess oxidizer remaining: (27.3% fuel) 2A1 + MoO<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + Mo
- G3. 39.3% fuel, 29.67% gas produced, 2469.66 K solids: 40.46% Mo liquids: 29.78% Al<sub>2</sub>O<sub>3</sub> gases: 27.19% Al<sub>2</sub>O, 2.43% Al a combination of two reactions with excess fuel remaining: (27.3% fuel) 2A1 + MoO<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + Mo (52.9% fuel) 6A1 + MoO<sub>3</sub> → 3Al<sub>2</sub>O + Mo

#### 24.9 ALUMINUM + $WO_3$



**FIGURE 24.11** Adiabatic equilibrium temperature profile, Al (fuel) + WO<sub>3</sub> (oxidizer).

100 90 80 70 gas products (wt-%) 60 50 40 30 20 10 0 70 0 10 20 30 40 50 60 80 90 100 fuel (wt-%)

AI + WO<sub>3</sub>

Adiabatic Equilibrium Gas Products

**FIGURE 24.12** Adiabatic equilibrium gas production profile, Al (fuel) + WO<sub>3</sub> (oxidizer).

T1. 4.3% fuel, 1920.99 K

solids: 54.70%  $W_{18}O_{49}$ , 37.17%  $WO_2$ , 8.12%  $Al_2O_3$  (corundum) liquids: none gases: none a combination of two reactions: (2.1% fuel)  $10Al + 54WO_3 \rightarrow 5Al_2O_3 + 3W_{18}O_{49}$ (7.2% fuel)  $2Al + 3WO_3 \rightarrow Al_2O_3 + 3WO_2$ 

- T2. 18.9% fuel, 3873.71 K—peak temperature solids: none liquids: 64.30% W, 35.63% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 18.9% fuel: 2Al + WO<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + W
  - T2 corresponds to the maximum amount of W.
  - From 4.8% to 6.6% fuel, the temperature appears to be limited by the  $3W_{18}O_{49}(s) \rightarrow 5W(s) + 49WO_3(l)$  decomposition, which occurs at 2011 K.
  - From 7.0% to 8.1% fuel, the temperature appears to be limited by the vaporization of WO<sub>3</sub> and W<sub>3</sub>O<sub>8</sub> from W(s)/WO<sub>3</sub>(l) mixtures, which occurs at 2087 K.
  - From 9.1% to 10.2% and 46.7% to 51.5% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
  - From 26.9% to 44.0% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
  - From 17.4% to 17.9% and 19.7% to 20.2% fuel, the temperature is limited to 3680 K by the W(s-l) transition.

G1. 8.1% fuel, 57.78% gas produced, 2087.07 K—peak gas solids: 26.76% W, 15.31% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 0.15% WO<sub>3</sub> gases: 29.26% (WO<sub>3</sub>)<sub>3</sub>, 11.90% (WO<sub>3</sub>)<sub>4</sub>, 9.25% W<sub>3</sub>O<sub>8</sub>, 7.37% (WO<sub>3</sub>)<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (2.5% fuel) 2A1 + 9WO<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 3W<sub>3</sub>O<sub>8</sub> (18.9% fuel) 2A1 + WO<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + W

**G2.** 26.9% fuel, 17.76% gas produced, 2469.66 K solids: 57.97% W liquids: 24.24% Al<sub>2</sub>O<sub>3</sub> gases: 16.27% Al<sub>2</sub>O, 1.46% Al a combination of two reactions with excess fuel remaining: (18.9% fuel) 2A1 + WO<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + W (41.1% fuel) 6A1 + WO<sub>3</sub>  $\rightarrow$  3Al<sub>2</sub>O + W

#### 24.10 ALUMINUM + MnO





**T1.** 16.0% fuel, 1966.89 K

solids: 50.94% MnAl<sub>2</sub>O<sub>4</sub> (galaxite), 0.19% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 48.87% Mn gases: none simplified equation at 16.0% fuel: 2Al + 4MnO  $\rightarrow$  MnAl<sub>2</sub>O<sub>4</sub> + 3Mn

- T2. 20.2% fuel, 2212.56 K—peak temperature solids: 37.97% Al<sub>2</sub>O<sub>3</sub> (corundum), 0.34% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: 61.70% Mn gases: none simplified equation at 20.2% fuel: 2Al + 3MnO → Al<sub>2</sub>O<sub>3</sub> + 3Mn
  - The maximum amount of manganese, 61.72% Mn(l), occurs at 20.3% fuel and 2211.89 K.
  - From 10.0% to 10.7% and 43.3% to 46.2% fuel, the temperature is limited to 1519 K by the Mn(s-l) transition.

#### 24.11 ALUMINUM + $Mn_3O_4$



**FIGURE 24.14** Adiabatic equilibrium temperature profile, Al (fuel) +  $Mn_3O_4$  (oxidizer).



**FIGURE 24.15** Adiabatic equilibrium gas production profile, Al (fuel) +  $Mn_3O_4$  (oxidizer).

**T1.** 7.3% fuel, 1927.71 K

solids: 76.57% MnO, 23.39% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: none gases: none simplified equation at 7.3% fuel:  $2Al + 3Mn_3O_4 \rightarrow MnAl_2O_4 + 8MnO_3O_4$ 

- T2. 19.1% fuel, 10.94% gas produced, 2335.90 K—peak temperature solids: 60.95% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: 27.97% Mn, 0.14% Al<sub>2</sub>O<sub>3</sub> gases: 10.94% Mn simplified equation at 19.1% fuel: 2Al + Mn<sub>3</sub>O<sub>4</sub> → MnAl<sub>2</sub>O<sub>4</sub> + 2Mn
- T3. 23.9% fuel, 4.04% gas produced, 2335.90 K—peak temperature solids: 0.29% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: 50.68% Mn, 44.98% Al<sub>2</sub>O<sub>3</sub> gases: 4.04% Mn simplified equation at 23.9% fuel: 8Al + 3Mn<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Mn
  - The maximum amount of manganese, 50.78% Mn(l) and 3.97% Mn(g), occurs at 24.0% fuel and 2327.68 K.
  - From 59.8% to 61.1% fuel, the temperature is limited to 1519 K by the Mn(s-l) transition.
  - From 9.8% to 13.5% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
  - The plateau from 25.8% to 40.8% fuel (2276 K) could not be attributed to a simple transition or reaction; species in this region include Mn(g), Al<sub>2</sub>O(g), Al(g), Mn(l), Al(l), and Al<sub>2</sub>O<sub>3</sub>(s).
  - From 15.4% to 23.9% fuel, the temperature is limited to 2336 K by the Mn(l-g) transition.

- **G1.** 19.1% fuel, 10.94% gas produced, 2335.90 K see T2 for details
- G2. 24.3% fuel, 16.29% gas produced, 2325.66 K—peak gas solids: 44.62% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 39.09% Mn gases: 15.44% Mn, 0.73% Al<sub>2</sub>O, 0.12% Al simplified equation at 23.9% fuel: 8Al + 3Mn<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Mn

#### 24.12 ALUMINUM + $Mn_2O_3$



**FIGURE 24.16** Adiabatic equilibrium temperature profile, Al (fuel) + Mn<sub>2</sub>O<sub>3</sub> (oxidizer).



**FIGURE 24.17** Adiabatic equilibrium gas production profile, Al (fuel) +  $Mn_2O_3$  (oxidizer).

**T1.** 4.1% fuel, 1488.91 K

solids: 86.84%  $Mn_3O_4$ , 13.14%  $MnAl_2O_4$  (galaxite) liquids: none gases: none simplified equation at 4.1% fuel:  $2Al + 8Mn_2O_3 \rightarrow MnAl_2O_4 + 5Mn_3O_4$ 

- **T2.** 10.2% fuel, 2200.29 K solids: 32.68% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: 67.29% MnO gases: none simplified equation at 10.2% fuel: 2A1 +  $3Mn_2O_3 \rightarrow MnAl_2O_4 + 5MnO$
- T3. 20.4% fuel, 25.51% gas produced, 2335.96 K—peak temperature solids: 65.36% MnAl<sub>2</sub>O<sub>4</sub> (galaxite) liquids: 9.09% Mn gases: 25.51% Mn simplified equation at 20.4% fuel: 6Al + 4Mn<sub>2</sub>O<sub>3</sub> → 3MnAl<sub>2</sub>O<sub>4</sub> + 5Mn
- **T4.** 25.5% fuel, 17.04% gas produced, 2335.25 K—*peak temperature* solids: none liquids: 48.10% Al<sub>2</sub>O<sub>3</sub>, 34.86% Mn gases: 16.99% Mn simplified equation at 25.5% fuel: 2A1 + Mn<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 2Mn
- T4 corresponds to the maximum amount of Mn.
- From 66.5% to 67.4% fuel, the temperature is limited to 1519 K by the Mn(s-l) transition.

- From 6.2% to 7.7% fuel, the temperature appears to be limited by the  $2Mn_3O_4(s) \rightarrow 6MnO(s) + O_2(g)$  decomposition, which occurs at 1925 K.
- From 8.4% to 9.9% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
- The plateau from 28.6% to 50.4% fuel (2276 K) could not be attributed to a simple transition or reaction; species in this region include Mn(g),  $Al_2O(g)$ , Al(g), Mn(l), Al(l), and  $Al_2O_3(s)$ .
- From 11.3% to 25.4% fuel, the temperature is limited to 2336 K by the Mn(l-g) transition.
- **G1.** 20.4% fuel, 25.51% gas produced, 2335.96 K see T3 for details
- G2. 26.1% fuel, 29.62% gas produced, 2326.37 K—peak gas solids: 47.13% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 23.26% Mn gases: 28.18% Mn, 1.24% Al<sub>2</sub>O, 0.20% Al simplified equation at 25.5% fuel: 2Al + Mn<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Mn

AI + MnO<sub>2</sub>

Adiabatic Equilibrium Gas Products

100

90

80

70

60 50

#### 24.13 ALUMINUM + $MnO_2$



**FIGURE 24.18** Adiabatic equilibrium temperature profile, Al (fuel) + MnO<sub>2</sub> (oxidizer).



**FIGURE 24.19** Adiabatic equilibrium gas production profile, Al (fuel) +  $MnO_2$  (oxidizer).

- **T1.** 5.4% fuel, 4.70% gas produced, 1620.31 K solids: 78.00%  $Mn_2O_3$  (bixbyite), 17.30%  $MnAl_2O_4$  (galaxite) liquids: none gases: 4.70%  $O_2$ a combination of two reactions: (11.0% fuel)  $2Al + 5MnO_2 \rightarrow MnAl_2O_4 + 2Mn_2O_3$ (decomposition)  $4MnO_2 \rightarrow 2Mn_2O_3 + O_2$
- **T2.** 7.0% fuel, 5.88% gas produced, 1915.37 K solids: 71.70%  $Mn_3O_4$ , 22.43%  $MnAl_2O_4$  (galaxite) liquids: none gases: 5.87%  $O_2$ a combination of two reactions: (13.4% fuel)  $2Al + 4MnO_2 \rightarrow MnAl_2O_4 + Mn_3O_4$ (decomposition)  $3MnO_2 \rightarrow Mn_3O_4 + O_2$
- **T3.** 12.5% fuel, 4.99% gas produced, 2637.95 K solids: 40.05%  $MnAl_2O_4$  (galaxite) liquids: 54.96% MnO gases: 4.92%  $O_2$  a combination of two reactions: (17.1% fuel)  $2Al + 3MnO_2 \rightarrow MnAl_2O_4 + 2MnO$  (decomposition)  $2MnO_2 \rightarrow 2MnO + O_2$

T4. 17.2% fuel, 0.28% gas produced, 3379.96 K—peak temperature solids: none liquids: 67.23% MnO, 32.50% Al<sub>2</sub>O<sub>3</sub> gases: 0.26% Mn simplified equation at 17.1% fuel: 2Al + 3MnO<sub>2</sub> → Al<sub>2</sub>O<sub>3</sub> + 3MnO

T5. 29.3% fuel, 44.74% gas produced, 2490.38 K solids: none liquids: 55.26% Al<sub>2</sub>O<sub>3</sub> gases: 44.68% Mn simplified equation at 29.3% fuel: 4Al + 3MnO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Mn

- T5 corresponds to the maximum amount of Mn.
- From 7.1% to 8.9% fuel, the temperature appears to be limited by the  $2Mn_3O_4(s) \rightarrow 6MnO(s) + O_2(g)$  decomposition, which occurs at 1925 K.
- From 9.6% to 10.9% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
- The plateau from 35.1% to 65.2% fuel (2276 K) could not be attributed to a simple transition or reaction; species in this region include Mn(g), Al<sub>2</sub>O(g), Al(g), Mn(l), Al(l), and Al<sub>2</sub>O<sub>3</sub>(s). Alone, Mn(l) is expected to boil at 2336 K.
- From 30.5% to 33.6% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
- From 12.6% to 14.1% and 27.2% to 28.5% fuel, the temperature appears to be limited by the  $MnAl_2O_4(s) \rightarrow MnO(l) + Al_2O_3(l)$  decomposition, which occurs at 2647 K.
- G1. 33.8% fuel, 53.23% gas produced, 2298.64 K—peak gas solids: 46.78% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 41.83% Mn, 10.26% Al<sub>2</sub>O, 1.12% Al a combination of two reactions with excess fuel remaining: (29.3% fuel) 4Al + 3MnO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Mn (55.4% fuel) 4Al + MnO<sub>2</sub> → 2Al<sub>2</sub>O + Mn

#### 24.14 ALUMINUM + FeO



**FIGURE 24.20** Adiabatic equilibrium temperature profile, Al (fuel) + FeO (oxidizer).

- **T1.** 12.2% fuel, 2355.59 K solids: 39.29% FeAl<sub>2</sub>O<sub>4</sub> (hercynite) liquids: 37.88% Fe, 22.83% FeO gases: none one reaction with excess oxidizer remaining: (15.8% fuel) 2Al + 4FeO  $\rightarrow$  FeAl<sub>2</sub>O<sub>4</sub> + 3Fe
- T2. 20.0% fuel, 2981.01 K—peak temperature solids: none liquids: 62.09% Fe, 37.79% Al<sub>2</sub>O<sub>3</sub>, 0.12% FeO gases: none simplified equation at 20.0% fuel: 2Al + 3FeO → Al<sub>2</sub>O<sub>3</sub> + 3Fe
- **T3.** 57.9% fuel, 2310.07 K

solids: 80.03% FeAl<sub>3</sub>, 19.92% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: none simplified equation at 57.9% fuel: 11Al + 3FeO  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3FeAl<sub>3</sub>

- The maximum amount of iron, 61.97% Fe(l) and 0.14% Fe(g), occurs at 20.1% fuel and 2966.79 K.
- From 6.8% to 8.0% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
- From 48.9% to 57.2% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- From 12.3% to 14.8% fuel, the temperature appears to be limited by the  $\text{FeAl}_2\text{O}_4(s) \rightarrow \text{FeO}(l) + \text{Al}_2\text{O}_3(l)$  decomposition, which occurs at 2360 K.
- From 23.4% to 38.0% fuel, the temperature appears to be limited to 2551 K by the reaction of FeAl<sub>3</sub>(s) and Al<sub>2</sub>O<sub>3</sub>(l) which forms Al<sub>2</sub>O(g), Al(g), and Fe(l-g).



**FIGURE 24.21** Adiabatic equilibrium gas production profile, Al (fuel) + FeO (oxidizer).

G1. 23.4% fuel, 7.65% gas produced, 2550.80 K—peak gas solids: 0.20% FeAl<sub>3</sub>
liquids: 59.15% Fe, 33.00% Al<sub>2</sub>O<sub>3</sub>
gases: 6.65% Al<sub>2</sub>O, 0.67% Al, 0.31% Fe a combination of two reactions:
(20.0% fuel) 2Al + 3FeO → Al<sub>2</sub>O<sub>3</sub> + 3Fe
(42.9% fuel) 2Al + FeO → Al<sub>2</sub>O + Fe

AI + Fe<sub>3</sub>O<sub>4</sub>

Adiabatic Equilibrium Gas Products

#### 24.15 ALUMINUM + $Fe_3O_4$



**FIGURE 24.22** Adiabatic equilibrium temperature profile, Al (fuel) +  $Fe_3O_4$  (oxidizer).

**FIGURE 24.23** Adiabatic equilibrium gas production profile, Al (fuel) +  $Fe_3O_4$  (oxidizer).

fuel (wt-%)

70

80 90 100

T1. 7.2% fuel, 1453.88 K

solids: 76.69% FeO (wüstite), 23.19%  $\text{FeAl}_2\text{O}_4$  (hercynite), 0.12%  $\text{Fe}_3\text{O}_4$  (magnetite) liquids: none gases: none simplified equation at 7.2% fuel:  $2\text{Al} + 3\text{Fe}_3\text{O}_4 \rightarrow \text{FeAl}_2\text{O}_4 + 8\text{FeO}$ 

100

90

80

70

60

50

40

30

20

10

0

0 10 20 30 40 50 60

- T2. 13.8% fuel, 2348.11 K
  - solids: 44.45% FeAl<sub>2</sub>O<sub>4</sub> (hercynite) liquids: 33.50% FeO, 22.05% Fe gases: none a combination of two reactions:  $(7.2\% \text{ fuel}) 2Al + 3Fe_3O_4 \rightarrow FeAl_2O_4 + 8FeO$  $(18.9\% \text{ fuel}) 2Al + Fe_3O_4 \rightarrow FeAl_2O_4 + 2Fe$

**T3.** 16.8% fuel, 2359.74 K solids: none liquids: 36.17% FeO, 32.09% Fe, 31.74%  $Al_2O_3$ gases: none a combination of two reactions: (7.2% fuel) 2A1 + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 9FeO (23.7% fuel) 8A1 + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4Al<sub>2</sub>O<sub>3</sub> + 9Fe

T4. 23.7% fuel, 0.86% gas produced, 3124.47 K—peak temperature solids: none liquids: 54.36% Fe, 44.78% Al<sub>2</sub>O<sub>3</sub> gases: 0.82% Fe simplified equation at 23.7% fuel: 8Al + 3Fe<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Fe

**T5.** 57.6% fuel, 2327.02 K solids: 75.07% FeAl<sub>3</sub>, 2.52% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 22.37% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 57.6% fuel:  $35Al + 3Fe_3O_4 \rightarrow 4Al_2O_3 + 9FeAl_3$ 

- T4 corresponds to the maximum amount of Fe.
- From 8.4% to 9.8% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
- From 56.8% to 61.3% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- From 13.9% to 16.7% fuel, the temperature appears to be limited by the FeAl<sub>2</sub>O<sub>4</sub>(s)  $\rightarrow$  FeO(l) + Al<sub>2</sub>O<sub>3</sub>(l) decomposition, which occurs at 2360 K.
- From 28.4% to 46.9% fuel, the temperature appears to be limited to 2551 K by the reaction of FeAl<sub>3</sub>(s) and Al<sub>2</sub>O<sub>3</sub>(l) which forms Al<sub>2</sub>O(g), Al(g), and Fe(l-g).
- **G1.** 28.4% fuel, 11.34% gas produced, 2550.80 K—*peak gas* solids: 0.11% FeAl<sub>3</sub> liquids: 51.31% Fe, 37.24% Al<sub>2</sub>O<sub>3</sub> gases: 9.87% Al<sub>2</sub>O, 1.00% Al, 0.46% Fe a combination of two reactions with excess fuel remaining: (23.7% fuel) 8Al + 3Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4Al<sub>2</sub>O<sub>3</sub> + 9Fe (48.2% fuel) 8Al + Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4Al<sub>2</sub>O + 3Fe

#### 24.16 ALUMINUM + $Fe_2O_3$



**FIGURE 24.24** Adiabatic equilibrium temperature profile, Al (fuel) +  $Fe_2O_3$  (oxidizer).

**FIGURE 24.25** Adiabatic equilibrium gas production profile, Al (fuel) +  $Fe_2O_3$  (oxidizer).

**T1.** 10.1% fuel, 1679.89 K

solids: 32.53%  $\text{FeAl}_2O_4$  (hercynite), 0.34%  $\text{Fe}_3O_4$  (magnetite) liquids: 67.13% FeOgases: none simplified equation at 10.1% fuel:  $2\text{Al} + 3\text{Fe}_2O_3 \rightarrow \text{FeAl}_2O_4 + 5\text{FeO}$ 

- **T2.** 13.8% fuel, 2353.85 K
  - solids: 44.45% FeAl<sub>2</sub>O<sub>4</sub> (hercynite) liquids: 42.85% FeO, 12.70% Fe gases: none a combination of two reactions: (10.1% fuel) 2Al + 3Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  FeAl<sub>2</sub>O<sub>4</sub> + 5FeO (20.2% fuel) 6Al + 4Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3FeAl<sub>2</sub>O<sub>4</sub> + 5Fe

**T3.** 16.8% fuel, 2364.24 K solids: none liquids: 45.20% FeO, 31.74%  $Al_2O_3$ , 23.06% Fe gases: none a combination of two reactions: (10.1% fuel)  $2Al + 3Fe_2O_3 \rightarrow Al_2O_3 + 6FeO$ (25.3% fuel)  $2Al + Fe_2O_3 \rightarrow Al_2O_3 + 2Fe$ 

**T4.** 25.3% fuel, 4.23% gas produced, 3126.19 K—*peak temperature* solids: none liquids: 48.13% Fe, 47.64%  $Al_2O_3$ gases: 4.10% Fe simplified equation at 25.3% fuel:  $2Al + Fe_2O_3 \rightarrow Al_2O_3 + 2Fe$ 



- **T5.** 57.5% fuel, 2419.30 K solids: 72.81% FeAl<sub>3</sub> liquids: 27.14% Al<sub>2</sub>O<sub>3</sub> gases: none simplified equation at 57.5% fuel:  $8Al + Fe_2O_3 \rightarrow Al_2O_3 + 2FeAl_3$ 
  - T4 corresponds to the maximum amount of Fe.
  - From 7.8% to 9.7% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
  - From 59.6% to 63.6% fuel, the temperature is limited to 2327 K by the  $Al_2O_3$ (s-l) transition.
  - From 13.9% to 16.7% fuel, the temperature appears to be limited by the FeAl<sub>2</sub>O<sub>4</sub>(s)  $\rightarrow$  FeO(l) + Al<sub>2</sub>O<sub>3</sub>(l) decomposition, which occurs at 2360 K.
  - From 31.1% to 52.3% fuel, the temperature appears to be limited to 2551 K by the reaction of FeAl<sub>3</sub>(s) and Al<sub>2</sub>O<sub>3</sub>(l) which forms Al<sub>2</sub>O(g), Al(g), and Fe(l-g).
  - From 23.3% to 25.1% fuel, the temperature appears to be limited by the vaporization of Fe and FeO from Fe(1)/FeO(1) mixtures, which occurs at 3120 K.

G1. 31.1% fuel, 14.40% gas produced, 2550.80 K—peak gas solids: 0.15% FeAl<sub>3</sub>
liquids: 47.55% Fe, 37.90% Al<sub>2</sub>O<sub>3</sub>
gases: 12.53% Al<sub>2</sub>O, 1.27% Al, 0.58% Fe a combination of two reactions with excess fuel remaining: (25.3% fuel) 2A1 + Fe<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Fe (50.3% fuel) 6A1 + Fe<sub>2</sub>O<sub>3</sub> → 3Al<sub>2</sub>O + 2Fe

AI + CoO

#### 24.17 ALUMINUM + CoO



**FIGURE 24.26** Adiabatic equilibrium temperature profile, Al (fuel) + CoO (oxidizer).



**FIGURE 24.27** Adiabatic equilibrium gas production profile, Al (fuel) + CoO (oxidizer).

- **T1.** 19.4% fuel, 2.15% gas produced, 3189.12 K—*peak temperature* solids: none liquids: 61.33% Co, 36.52%  $Al_2O_3$ gases: 2.06% Co simplified equation at 19.4% fuel: 2Al + 3CoO  $\rightarrow Al_2O_3$  + 3Co
- T2. 37.5% fuel, 3.83% gas produced, 3004.73 K solids: none liquids: 67.38% CoAl, 27.43% Al<sub>2</sub>O<sub>3</sub>, 1.36% Co gases: 1.86% Al<sub>2</sub>O, 1.57% Co, 0.37% Al simplified equation at 37.5% fuel: 5Al + 3CoO → Al<sub>2</sub>O<sub>3</sub> + 3CoAl
- **T3.** 66.6% fuel, 2300.19 K solids: 56.34% Co<sub>2</sub>Al<sub>5</sub>, 15.15% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 28.52% Al gases: none one reaction with excess fuel remaining: (53.3% fuel) 19Al + 6CoO  $\rightarrow$  2Al<sub>2</sub>O<sub>3</sub> + 3Co<sub>2</sub>Al<sub>5</sub>
- **T4.** 73.1% fuel, 1862.98 K solids: 50.22% CoAl<sub>3</sub>, 12.20% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 37.58% Al gases: none one reaction with excess fuel remaining: (56.9% fuel) 11Al + 3CoO  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3CoAl<sub>3</sub>

- **T5.** 76.0% fuel, 1721.95 K solids: 57.76%  $Co_2Al_9$ , 10.89%  $Al_2O_3$  (corundum) liquids: 31.35% Al gases: none one reaction with excess fuel remaining: (65.0% fuel) 31Al + 6CoO  $\rightarrow$  2Al<sub>2</sub>O<sub>3</sub> + 3Co<sub>2</sub>Al<sub>9</sub>
- The maximum amount of cobalt, 61.66% Co(l) and 1.89% Co(g), occurs at 19.2% fuel and 3158.75 K.
- From 74.9% to 75.9% fuel, the temperature appears to be limited by the  $Co_2Al_9(s) \rightarrow 2CoAl_3(s) + 3Al(l)$  decomposition, which occurs at 1728 K.
- From 72.5% to 73.0% fuel, the temperature appears to be limited by the  $2\text{CoAl}_3(s) \rightarrow \text{Co}_2\text{Al}_5(s) + \text{Al}(l)$  decomposition, which occurs at 1865 K.
- From 8.8% to 10.2% fuel, the temperature is limited to 2103 K by the CoO(s-l) transition.
- From 58.9% to 66.5% fuel, the temperature appears to be limited by the  $Co_2Al_5(s) \rightarrow 2CoAl(l) + 3Al(l)$  decomposition, which occurs at 2302 K.
- From 11.4% to 12.8% and 54.8% to 58.4% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- From 41.8% to 52.0% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
- From 20.8% to 37.8% fuel, the temperature appears to be limited to 3005 K by the reaction of CoAl(l) and Al<sub>2</sub>O<sub>3</sub>(l) which forms Co(l-g), Al<sub>2</sub>O(g), and Al(g).
- From 18.3% to 19.1% fuel, the temperature appears to be limited by the formation of Co(g) and O<sub>2</sub>(g) from Co(1)/CoO(1) mixtures, which occurs at 3150 K.
- G1. 41.8% fuel, 12.37% gas produced, 2469.57 K—*peak gas* solids: none liquids: 66.72% CoAl, 20.89% Al<sub>2</sub>O<sub>3</sub> gases: 11.33% Al<sub>2</sub>O, 1.01% Al a combination of two reactions with excess fuel remaining: (37.5% fuel) 5Al + 3CoO → Al<sub>2</sub>O<sub>3</sub> + 3CoAl (51.9% fuel) 3Al + CoO → Al<sub>2</sub>O + CoAl

#### 24.18 ALUMINUM + $Co_3O_4$



**FIGURE 24.28** Adiabatic equilibrium temperature profile, Al (fuel) +  $Co_3O_4$  (oxidizer).

- **T1.** 7.0% fuel, 1969.26 K solids: 86.60% CoO, 13.23% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 0.17% Co gases: none
- simplified equation at 7.0% fuel:  $2AI + 3Co_3O_4 \rightarrow Al_2O_3 + 9CoO$ **T2.** 23.0% fuel, 11.42% gas produced, 3198.33 K—*peak temperature*

solids: none liquids: 45.18% Co, 43.40%  $Al_2O_3$ gases: 11.36% Co simplified equation at 23.0% fuel:  $8Al + 3Co_3O_4 \rightarrow 4Al_2O_3 + 9Co$ 

**T3.** 38.8% fuel, 10.61% gas produced, 3004.73 K solids: none liquids: 53.54% CoAl, 32.00% Al<sub>2</sub>O<sub>3</sub>, 3.85% Co gases: 5.15% Al<sub>2</sub>O, 4.36% Co, 1.03% Al a combination of reactions with excess fuel remaining: (23.0% fuel) 8A1 +  $3Co_3O_4 \rightarrow 4Al_2O_3 + 9Co$  (38.8% fuel) 17A1 +  $3Co_3O_4 \rightarrow 4Al_2O_3 + 9CoAl$  (55.2% fuel) 11A1 +  $Co_3O_4 \rightarrow 4Al_2O + 3CoAl$ 

**T4.** 70.3% fuel, 2301.45 K solids: 46.77%  $Co_2Al_5$ , 16.77%  $Al_2O_3$  (corundum) liquids: 36.47% Al gases: none one reaction with excess fuel remaining: (53.3% fuel) 61Al + 6 $Co_3O_4 \rightarrow 8Al_2O_3 + 9Co_2Al_5$ 



**FIGURE 24.29** Adiabatic equilibrium gas production profile, Al (fuel) +  $Co_3O_4$  (oxidizer).
- **T5.** 76.1% fuel, 1863.60 K solids: 41.65% CoAl<sub>3</sub>, 13.49% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 44.86% Al gases: none one reaction with excess fuel remaining: (56.7% fuel)  $35Al + 3Co_3O_4 \rightarrow 4Al_2O_3 + 9CoAl_3$
- **T6.** 78.5% fuel, 1727.57 K solids: 48.30% Co<sub>2</sub>Al<sub>9</sub>, 12.14% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 39.56% Al gases: none one reaction with excess fuel remaining: (64.4% fuel) 97Al + 6Co<sub>3</sub>O<sub>4</sub>  $\rightarrow$  8Al<sub>2</sub>O<sub>3</sub> + 9Co<sub>2</sub>Al<sub>9</sub>
  - The maximum amount of cobalt, 49.13% Co(l) and 7.92% Co(g), occurs at 22.3% fuel and 3154.78 K.
  - From 3.6% to 4.7% fuel, the temperature appears to be limited by the  $2Co_3O_4(s) \rightarrow 6CoO(s) + O_2(g)$  decomposition, which occurs at 1213 K.
  - From 77.8% to 78.5% fuel, the temperature appears to be limited by the  $Co_2Al_9(s) \rightarrow 2CoAl_3(s) + 3Al(l)$  decomposition, which occurs at 1728 K.
  - From 7.9% to 10.1% fuel, the temperature is limited to 2103 K by the CoO(s-l) transition.
  - From 64.8% to 70.2% fuel, the temperature appears to be limited by the  $Co_2Al_5(s) \rightarrow 2CoAl(l) + 3Al(l)$  decomposition, which occurs at 2302 K.
  - From 11.3% to 12.7% and 61.1% to 64.4% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
  - From 45.3% to 58.6% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
  - From 26.5% to 39.8% fuel, the temperature appears to be limited to 3005 K by the reaction of CoAl(l) and Al<sub>2</sub>O<sub>3</sub>(l) which forms Co(l-g), Al<sub>2</sub>O(g), and Al(g).
  - From 18.5% to 22.2% fuel, the temperature appears to be limited by the formation of Co(g) and  $O_2(g)$  from Co(l)/CoO(l) mixtures, which occurs at 3150 K.
- G1. 45.2% fuel, 18.77% gas produced, 2472.21 K—peak gas solids: none liquids: 58.64% CoAl, 22.59% Al<sub>2</sub>O<sub>3</sub> gases: 17.19% Al<sub>2</sub>O, 1.54% Al a combination of two reactions with excess fuel remaining: (38.8% fuel) 17Al + 3Co<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9CoAl (55.2% fuel) 11Al + Co<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O + 3CoAl

#### 24.19 ALUMINUM + NiO



**FIGURE 24.30** Adiabatic equilibrium temperature profile, Al (fuel) + NiO (oxidizer).



**FIGURE 24.31** Adiabatic equilibrium gas production profile, Al (fuel) + NiO (oxidizer).

- T1. 19.4% fuel, 1.97% gas produced, 3181.54 K—peak temperature solids: none liquids: 61.39% Ni, 36.65% Al<sub>2</sub>O<sub>3</sub> gases: 1.93% Ni simplified equation at 19.4% fuel: 2Al + 3NiO → Al<sub>2</sub>O<sub>3</sub> + 3Ni
- T2. 37.6% fuel, 3.93% gas produced, 3055.87 K solids: none liquids: 68.37% NiAl, 27.70% Al<sub>2</sub>O<sub>3</sub> gases: 2.19% Ni, 1.39% Al<sub>2</sub>O, 0.32% Al simplified equation at 37.6% fuel: 5Al + 3NiO → Al<sub>2</sub>O<sub>3</sub> + 3NiAl
- **T3.** 66.3% fuel, 2281.12 K solids: 44.74% Ni<sub>2</sub>Al<sub>3</sub>, 15.33% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 39.92% Al gases: none one reaction with excess fuel remaining: (43.9% fuel) 13Al + 6NiO  $\rightarrow$  2Al<sub>2</sub>O<sub>3</sub> + 3Ni<sub>2</sub>Al<sub>3</sub>
- **T4.** 82.9% fuel, 1213.79 K solids: 31.97% NiAl<sub>3</sub>, 7.78% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 60.25% Al gases: none one reaction with excess fuel remaining: (57.0% fuel) 11Al + 3NiO  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3NiAl<sub>3</sub>

- The maximum amount of nickel, 63.69% Ni(l) and 0.58% Ni(g), occurs at 17.7% fuel and 2789.24 K.
- From 81.0% to 82.8% fuel, the temperature appears to be limited by the  $2NiAl_3(s) \rightarrow Ni_2Al_3(s) + 3Al(l)$  decomposition, which occurs at 1219 K.
- From 9.4% to 10.6% fuel, the temperature is limited to 2230 K by the NiO(s-l) transition.
- From 59.6% to 66.2% fuel, the temperature appears to be limited by the Ni<sub>2</sub>Al<sub>3</sub>(s)  $\rightarrow$  2NiAl(l) + Al(l) decomposition, which occurs at 2287 K.
- From 55.3% to 58.8% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
- From 42.1% to 52.5% fuel, the temperature appears to be limited by the vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 2470 K.
- From 12.4% to 14.8% fuel, the temperature appears to be limited by the (NiO)(Al<sub>2</sub>O<sub>3</sub>)(s)  $\rightarrow$  NiO(l) + Al<sub>2</sub>O<sub>3</sub>(l) decomposition, which occurs at 2621 K.
- From 15.9% to 17.6% fuel, the temperature appears to be limited by the 2NiO(1)  $\rightarrow$  2Ni(1-g) + O<sub>2</sub>(g) decomposition, which occurs at 2783 K. Some of the NiO is vaporized as well.
- From 20.3% to 37.5% fuel, the temperature appears to be limited to 3056 K by the reaction of NiAl(l) and  $Al_2O_3(l)$  which forms Ni(l-g),  $Al_2O(g)$ , and Al(g).

G1. 42.1% fuel, 12.83% gas produced, 2469.60 K—peak gas solids: none liquids: 66.41% NiAl, 20.64% Al<sub>2</sub>O<sub>3</sub>, 0.13% Al gases: 11.75% Al<sub>2</sub>O, 1.05% Al a combination of two reactions with excess fuel remaining: (37.6% fuel) 5Al + 3NiO → Al<sub>2</sub>O<sub>3</sub> + 3NiAl (52.0% fuel) 3Al + NiO → Al<sub>2</sub>O + NiAl

#### 24.20 ALUMINUM + $Cu_2O$



**FIGURE 24.32** Adiabatic equilibrium temperature profile, Al (fuel) + Cu<sub>2</sub>O (oxidizer).

**FIGURE 24.33** Adiabatic equilibrium gas production profile, Al (fuel) +  $Cu_2O$  (oxidizer).

- **T1.** 11.2% fuel, 6.38% gas produced, 2837.23 K—*peak temperature* solids: none liquids: 72.55% Cu, 21.07% Al<sub>2</sub>O<sub>3</sub> gases: 5.99% Cu, 0.33% Cu<sub>2</sub> simplified equation at 11.2% fuel: 2Al + 3Cu<sub>2</sub>O  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 6Cu
  - The maximum amount of copper, 77.47% Cu(l), 2.19% Cu(g), and 0.10% Cu<sub>2</sub>(g), occurs at 10.1% fuel and 2695.50 K.
  - From 56.4% to 58.5% fuel, the temperature is limited to 1358 K by the Cu(s-l) transition.
  - From 3.4% to 4.4% fuel, the temperature is limited to 1517 K by the Cu<sub>2</sub>O(s-l) transition.
  - From 7.2% to 7.8% and 29.7% to 34.3% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
  - The plateau from 15.2% to 26.9% fuel (2448 K) could not be attributed to a simple transition or reaction; species in this region include Al<sub>2</sub>O(g), Cu(g), Al(g), Cu(l), Al<sub>2</sub>O<sub>3</sub>(l), and Al(l). The vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2470 K.
  - From 9.2% to 10.0% fuel, the temperature appears to be limited by the  $2Cu_2O(l) \rightarrow 4Cu(l-g) + O_2(g)$  decomposition, which occurs at 2688 K.
- G1. 15.2% fuel, 9.23% gas produced, 2447.53 K—peak gas solids: none liquids: 74.11% Cu, 16.57% Al<sub>2</sub>O<sub>3</sub> gases: 7.35% Al<sub>2</sub>O, 1.18% Cu, 0.66% Al a combination of two reactions:
  (11.2% fuel) 2Al + 3Cu<sub>2</sub>O → Al<sub>2</sub>O<sub>3</sub> + 6Cu (27.4% fuel) 2Al + Cu<sub>2</sub>O → Al<sub>2</sub>O + 2Cu



#### 24.21 ALUMINUM + CuO



**FIGURE 24.34** Adiabatic equilibrium temperature profile, Al (fuel) + CuO (oxidizer).

- T1. 6.4% fuel, 3.72% gas produced, 1626.70 K solids: 29.06% Cu<sub>2</sub>Al<sub>2</sub>O<sub>4</sub> liquids: 67.22% Cu<sub>2</sub>O gases: 3.72% O<sub>2</sub> a combination of two reactions: (10.2% fuel) 2A1 + 6CuO → Cu<sub>2</sub>Al<sub>2</sub>O<sub>4</sub> + 2Cu<sub>2</sub>O (decomposition) 4CuO → 2Cu<sub>2</sub>O + O<sub>2</sub>
- T2. 10.2% fuel, 2640.41 K solids: none liquids: 80.40% Cu<sub>2</sub>O, 19.27% Al<sub>2</sub>O<sub>3</sub>, 0.33% Cu gases: none simplified equation at 10.2% fuel: 2Al + 6CuO → Al<sub>2</sub>O<sub>3</sub> + 3Cu<sub>2</sub>O
- T3. 14.1% fuel, 14.57% gas produced, 2688.56 K solids: none liquids: 58.79% Cu, 26.64% Al<sub>2</sub>O<sub>3</sub> gases: 9.04% Cu, 4.52% O<sub>2</sub>, 0.50% CuO, 0.39% Cu<sub>2</sub>, 0.11% O a combination of two reactions:
  (18.4% fuel) 2Al + 3CuO → Al<sub>2</sub>O<sub>3</sub> + 3Cu (decomposition) 2CuO → 2Cu + O<sub>2</sub>
- T4. 18.4% fuel, 33.57% gas produced, 2838.99 K—*peak temperature* solids: none liquids: 34.76% Al<sub>2</sub>O<sub>3</sub>, 31.66% Cu gases: 31.71% Cu, 1.76% Cu<sub>2</sub> simplified equation at 18.4% fuel: 2Al + 3CuO → Al<sub>2</sub>O<sub>3</sub> + 3Cu



**FIGURE 24.35** Adiabatic equilibrium gas production profile, Al (fuel) + CuO (oxidizer).

- T3 corresponds to the maximum amount of Cu.
- From 73.6% to 74.3% fuel, the temperature is limited to 1358 K by the Cu(s-l) transition.
- From 3.1% to 4.8% fuel, the temperature appears to be limited by the  $4\text{CuO}(s) \rightarrow 2\text{Cu}_2\text{O}(s) + O_2(g)$  decomposition, which occurs at 1397 K.
- From 5.2% to 6.1% fuel, the temperature is limited to 1517 K by the  $Cu_2O(s-1)$  transition.
- From 8.6% to 9.1% and 54.0% to 57.5% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-1)$  transition.
- The plateau from 29.2% to 51.8% fuel (2448 K) could not be attributed to a simple transition or reaction; species in this region include  $Al_2O(g)$ , Cu(g), Al(g), Cu(l),  $Al_2O_3(l)$ , and Al(l). The vaporization of  $Al_2O$  and Al from  $Al(l)/Al_2O_3(l)$  mixtures is expected to occur at 2470 K.
- From 10.5% to 14.0% fuel, the temperature appears to be limited by the  $2Cu_2O(l) \rightarrow 4Cu(l-g) + O_2(g)$  decomposition, which occurs at 2688 K.
- G1. 18.5% fuel, 33.71% gas produced, 2838.96 K—peak gas solids: none liquids: 34.78% Al<sub>2</sub>O<sub>3</sub>, 31.51% Cu gases: 31.84% Cu, 1.76% Cu<sub>2</sub> simplified equation at 18.4% fuel: 2A1 + 3CuO → Al<sub>2</sub>O<sub>3</sub> + 3Cu

**G2.** 29.1% fuel, 27.11% gas produced, 2447.93 K solids: none liquids: 53.08% Cu, 19.81% Al<sub>2</sub>O<sub>3</sub> gases: 21.57% Al<sub>2</sub>O, 3.46% Cu, 1.94% Al a combination of two reactions with excess fuel remaining: (18.4% fuel) 2Al + 3CuO  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3Cu (40.4% fuel) 2Al + CuO  $\rightarrow$  Al<sub>2</sub>O + Cu

#### 24.22 ALUMINUM + $Ag_2O$



Adiabatic Equilibrium Gas Products fuel (wt-%)

AI + Ag<sub>2</sub>O

**FIGURE 24.36** Adiabatic equilibrium temperature profile, Al (fuel) + Ag<sub>2</sub>O (oxidizer).

**FIGURE 24.37** Adiabatic equilibrium gas production profile, Al (fuel) +  $Ag_2O$  (oxidizer).

- T1. 7% fuel, 40.13% gas produced, 2427.04 K—*peak temperature* solids: none liquids: 46.64% Ag, 13.23% Al<sub>2</sub>O<sub>3</sub> gases: 37.77% Ag, 2.17% Ag<sub>2</sub>, 0.19% O<sub>2</sub> simplified equation at 7.2% fuel: 2Al + 3Ag<sub>2</sub>O → Al<sub>2</sub>O<sub>3</sub> + 6Ag
  - Ag<sub>2</sub>O(s) is unstable above 468 K. The maximum amount of silver, 92.17% Ag(s), occurs at just 1% fuel and 873.20 K.
  - From 33% to 35% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
  - The plateau from 12% to 32% fuel (2332 K) could not be attributed to a simple transition or reaction; species in this region include Ag(g), Al<sub>2</sub>O(g), Ag<sub>2</sub>(g), Al(g), Ag(l), Al<sub>2</sub>O<sub>3</sub>(l), and Al(l). Alone, Ag(l) is expected to vaporize at 2430 K. The vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2470 K.
- **G1.** 7% fuel, 40.13% gas produced, 2427.04 K—*peak gas* see T1 for details

#### 24.23 ALUMINUM + ZnO



**FIGURE 24.38** Adiabatic equilibrium temperature profile, Al (fuel) + ZnO (oxidizer).

- **T1.** 14.2% fuel, 51.61% gas produced, 1497.11 K solids: 48.25% ZnAl<sub>2</sub>O<sub>4</sub>, 0.14% ZnO (zincite) liquids: none gases: 51.61% Zn simplified equation at 14.2% fuel: 2Al + 4ZnO  $\rightarrow$  ZnAl<sub>2</sub>O<sub>4</sub> + 3Zn
- T2. 18.1% fuel, 65.79% gas produced, 1579.70 K—peak temperature solids: 34.18% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 65.79% Zn simplified equation at 18.1% fuel: 2Al + 3ZnO → Al<sub>2</sub>O<sub>3</sub> + 3Zn
  - T2 corresponds to the maximum amount of Zn.
  - From 67.4% to 75.9% fuel, the temperature is limited to 933 K by the Al(s-l) transition.
  - From 4.6% to 10.2% and 31.2% to 59.9% fuel, the temperature is limited to 1181 K by the Zn(1-g) transition.
- **G1.** 18.1% fuel, 65.79% gas produced, 1579.70 K—*peak gas* see T2 for details



**FIGURE 24.39** Adiabatic equilibrium gas production profile, Al (fuel) + ZnO (oxidizer).

#### 24.24 ALUMINUM + CdO



**FIGURE 24.40** Adiabatic equilibrium temperature profile, Al (fuel) + CdO (oxidizer).

- **T1.** 8.6% fuel, 63.29% gas produced, 1775.33 K solids: 36.71% (CdO)(Al<sub>2</sub>O<sub>3</sub>) liquids: none gases: 60.80% Cd, 1.48% CdO, 1.00% O<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (9.5% fuel) 2Al + 4CdO  $\rightarrow$  (CdO)(Al<sub>2</sub>O<sub>3</sub>) + 3Cd (decomposition) 2CdO  $\rightarrow$  2Cd + O<sub>2</sub>
- T2. 12.3% fuel, 76.79% gas produced, 2575.55 K—peak temperature solids: none liquids: 23.21% Al<sub>2</sub>O<sub>3</sub> gases: 76.77% Cd simplified equation at 12.3% fuel: 2Al + 3CdO → Al<sub>2</sub>O<sub>3</sub> + 3Cd
  - The maximum amount of cadmium, 76.96% Cd(g), occurs at 10.9% fuel and 2271.09 K.
  - From 1.9% to 2.8% and 52.2% to 63.5% fuel, the temperature is limited to 1040 K by the Cd(l-g) transition.
  - From 11.0% to 11.7% and 13.4% to 15.0% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- G1. 10.4% fuel, 80.35% gas produced, 1907.66 K—peak gas solids: 19.65% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 76.82% Cd, 1.85% CdO, 1.68% O<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (12.3% fuel) 2Al + 3CdO → Al<sub>2</sub>O<sub>3</sub> + 3Cd (decomposition) 2CdO → 2Cd + O<sub>2</sub>



**FIGURE 24.41** Adiabatic equilibrium gas production profile, Al (fuel) + CdO (oxidizer).

- G2. 15.4% fuel, 80.35% gas produced, 2213.28 K—peak gas solids: 19.64% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 74.06% Cd, 5.66% Al<sub>2</sub>O, 0.63% Al a combination of two reactions:
  (12.3% fuel) 2Al + 3CdO → Al<sub>2</sub>O<sub>3</sub> + 3Cd (29.6% fuel) 2Al + CdO → Al<sub>2</sub>O + Cd
- **G3.** 29.6% fuel, 62.03% gas produced, 1950.41 K solids: 18.47%  $Al_2O_3$  (corundum) liquids: 19.50% Al gases: 61.63% Cd, 0.35%  $Al_2O$  one reaction with excess fuel remaining: (12.3% fuel) 2Al + 3CdO  $\rightarrow Al_2O_3 + 3Cd$

#### 24.25 ALUMINUM + HgO



**FIGURE 24.42** Adiabatic equilibrium temperature profile, Al (fuel) + HgO (oxidizer).

- **T1.** 3.4% fuel, 93.58% gas produced, 2052.23 K solids: 6.42% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 88.25% Hg, 4.02% O<sub>2</sub>, 1.20% HgO, 0.11% Hg<sub>2</sub> a combination of two reactions with excess oxidizer remaining:  $(7.7\% \text{ fuel}) 2\text{Al} + 3\text{HgO} \rightarrow \text{Al}_2\text{O}_3 + 3\text{Hg}$  (decomposition)  $2\text{HgO} \rightarrow 2\text{Hg} + \text{O}_2$
- T2. 8.0% fuel, 88.45% gas produced, 3649.85 K—peak temperature solids: none liquids: 11.55% Al<sub>2</sub>O<sub>3</sub> major gases: 85.03% Hg, 1.07% AlO, 0.66% Al<sub>2</sub>O other gases: 0.54% O, 0.52% Al, 0.28% Al<sub>2</sub>O<sub>2</sub>, 0.14% O<sub>2</sub>, 0.13% HgO simplified equation at 7.7% fuel: 2Al + 3HgO → Al<sub>2</sub>O<sub>3</sub> + 3Hg
  - HgO(s) is unstable above 716 K.
  - T1 corresponds to the maximum amount of Hg.
- G1. 2.4% fuel, 95.46% gas produced, 715.47 K—*peak gas* solids: 4.53% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 80.10% Hg, 10.47% HgO, 4.30% O<sub>2</sub>, 0.59% Hg<sub>2</sub>



**FIGURE 24.43** Adiabatic equilibrium gas production profile, Al (fuel) + HgO (oxidizer).

**G2.** 15.6% fuel, 93.55% gas produced, 2324.76 K solids: 6.42%  $Al_2O_3$  (corundum) liquids: none gases: 78.10% Hg, 14.05%  $Al_2O$ , 1.31% A1 a combination of two reactions with excess fuel remaining: (7.7% fuel)  $2Al + 3HgO \rightarrow Al_2O_3 + 3Hg$  (19.9% fuel)  $2Al + HgO \rightarrow Al_2O + Hg$ 

**G3.** 19.9% fuel, 86.39% gas produced, 2310.26 K solids: 7.16% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 6.45% Al gases: 74.12% Hg, 11.14% Al<sub>2</sub>O, 1.06% Al a combination of two reactions with excess fuel remaining: (7.7% fuel) 2A1 + 3HgO  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3Hg (19.9% fuel) 2A1 + HgO  $\rightarrow$  Al<sub>2</sub>O + Hg

#### 24.26 ALUMINUM + $B_2O_3$





**FIGURE 24.44** Adiabatic equilibrium temperature profile, Al (fuel) +  $B_2O_3$  (oxidizer).

**FIGURE 24.45** Adiabatic equilibrium gas production profile, Al (fuel) +  $B_2O_3$  (oxidizer).

- **T1.** 40.0% fuel, 2.12% gas produced, 2302.21 K solids: 80.21% (Al<sub>2</sub>O<sub>3</sub>)<sub>9</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>2</sub>, 17.67% AlB<sub>12</sub> liquids: none gases: 1.09% (BO)<sub>2</sub>, 0.72% B<sub>2</sub>O<sub>3</sub>, 0.25% AlBO<sub>2</sub> simplified equation at 40.7% fuel: 39Al + 22B<sub>2</sub>O<sub>3</sub> → 2(Al<sub>2</sub>O<sub>3</sub>)<sub>9</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>2</sub> + 3AlB<sub>12</sub>
- **T2.** 45.7% fuel, 2327.02 K—peak temperature solids: 36.31% Al<sub>2</sub>O<sub>3</sub> (corundum), 20.37% AlB<sub>12</sub> liquids: 43.22% Al<sub>2</sub>O<sub>3</sub>, 0.10% Al gases: none simplified equation at 45.6% fuel: 13Al + 6B<sub>2</sub>O<sub>3</sub>  $\rightarrow$  6Al<sub>2</sub>O<sub>3</sub> + AlB<sub>12</sub>
- **T3.** 64.2% fuel, 2101.22 K solids: 52.43% Al<sub>2</sub>O<sub>3</sub> (corundum), 24.99% AlB<sub>2</sub> liquids: 22.58% Al gases: none one reaction with excess fuel remaining: (53.8% fuel)  $3Al + B_2O_3 \rightarrow Al_2O_3 + AlB_2$ 
  - Elemental boron is not predicted to occur at any point.
  - From 60.1% to 64.1% fuel, the temperature appears to be limited by the  $6AlB_2(s) \rightarrow AlB_{12}(s) + 5Al(l)$  decomposition, which occurs at 2104 K.
  - From 37.0% to 39.3% fuel, the temperature appears to be limited to 2208 K by the reaction of B<sub>2</sub>O<sub>3</sub>(l) and AlB<sub>12</sub>(s) which forms (BO)<sub>2</sub>(g) and AlBO<sub>2</sub>(g). Some of the B<sub>2</sub>O<sub>3</sub> is also vaporized.

- From 40.1% to 43.5% fuel, the temperature appears to be limited to 2310 K by the reaction of AlB<sub>12</sub>(s) and (Al<sub>2</sub>O<sub>3</sub>)<sub>9</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>2</sub>(s) which forms Al<sub>2</sub>O<sub>3</sub>(s), (BO)<sub>2</sub>(g), B<sub>2</sub>O<sub>3</sub>(g), AlBO<sub>2</sub>(g), and BO(g).
- From 43.8% to 54.2% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
- **G1.** 39.3% fuel, 3.75% gas produced, 2207.85 K solids: 78.92%  $(Al_2O_3)_9(B_2O_3)_2$ , 17.25%  $AlB_{12}$  liquids: none gases: 1.90% (BO)<sub>2</sub>, 1.62% B<sub>2</sub>O<sub>3</sub>, 0.17%  $AlBO_2$  one reaction with excess oxidizer remaining:  $(40.7\% \text{ fuel}) 39Al + 22B_2O_3 \rightarrow 2(Al_2O_3)_9(B_2O_3)_2 + 3AlB_{12}$
- **G2.** 43.5% fuel, 5.37% gas produced, 2309.51 K—*peak gas* solids: 74.34% Al<sub>2</sub>O<sub>3</sub> (corundum), 18.92% AlB<sub>12</sub>, 1.37% (Al<sub>2</sub>O<sub>3</sub>)<sub>9</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>2</sub> liquids: none gases: 2.75% (BO)<sub>2</sub>, 1.77% B<sub>2</sub>O<sub>3</sub>, 0.69% AlBO<sub>2</sub>, 0.15% BO one reaction with excess oxidizer remaining: (45.6% fuel) 13Al + 6B<sub>2</sub>O<sub>3</sub>  $\rightarrow$  6Al<sub>2</sub>O<sub>3</sub> + AlB<sub>12</sub>

### 24.27 ALUMINUM + $SiO_2$



FIGURE 24.46 Adiabatic equilibrium temperature profile, Al (fuel) + SiO<sub>2</sub> (oxidizer).

**T1.** 26.4% fuel, 1671.55 K

solids: 79.28% Al<sub>2</sub>SiO<sub>5</sub> (sillimanite), 20.61% Si, 0.11% SiO<sub>2</sub> (tridymite) liquids: none gases: none simplified equation at 26.4% fuel:  $4A1 + 5SiO_2 \rightarrow 2Al_2SiO_5 + 3Si$ 

- T2. 37.5% fuel, 1759.40 K—peak temperature solids: 70.71% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 29.22% Si gases: none simplified equation at 37.5% fuel: 4Al + 3SiO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Si
  - T2 corresponds to the maximum amount of Si.
  - From 26.7% to 35.3% and 40.3% to 52.4% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.

AI + SnO

Adiabatic Equilibrium Gas Products

#### 24.28 ALUMINUM + SnO



gas products (wt-%) fuel (wt-%)

**FIGURE 24.47** Adiabatic equilibrium temperature profile, Al (fuel) + SnO (oxidizer).

**FIGURE 24.48** Adiabatic equilibrium gas production profile, Al (fuel) + SnO (oxidizer).

- T1. 11.8% fuel, 8.98% gas produced, 2839.43 K—peak temperature solids: none liquids: 68.95% Sn, 22.07% Al<sub>2</sub>O<sub>3</sub> gases: 7.38% Sn, 0.93% Sn<sub>2</sub>, 0.52% SnO, 0.11% Al<sub>2</sub>O simplified equation at 11.8% fuel: 2Al + 3SnO → Al<sub>2</sub>O<sub>3</sub> + 3Sn
  - The maximum amount of tin, 68.77% Sn(l), 7.59% Sn(g), and 0.96% Sn<sub>2</sub>(g), occurs at 11.9% fuel and 2834.99 K.
  - From 4.4% to 7.1% fuel, the temperature appears to be limited by the vaporization of SnO from Sn(1)/SnO<sub>2</sub>(s) mixtures, which occurs at about 1820 K.
  - From 9.2% to 9.8% and 26.7% to 32.0% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
  - The plateau from 14.9% to 24.3% fuel (2449 K) could not be attributed to a simple transition or reaction; species in this region include Al<sub>2</sub>O(g), Al(g), Sn(g), Sn<sub>2</sub>(g), Sn(l), Al<sub>2</sub>O<sub>3</sub>(l), and Al(l). The vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2470 K.
- G1. 7.2% fuel, 38.89% gas produced, 1828.56 K—peak gas solids: 13.60% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 47.50% Sn gases: 17.49% (SnO)<sub>2</sub>, 7.62% SnO, 7.31% (SnO)<sub>4</sub>, 6.45% (SnO)<sub>3</sub> one reaction with excess oxidizer remaining: (11.8% fuel) 2Al + 3SnO → Al<sub>2</sub>O<sub>3</sub> + 3Sn

**G2.** 14.9% fuel, 8.05% gas produced, 2448.81 K solids: none liquids: 73.29% Sn, 18.65%  $Al_2O_3$  gases: 5.81%  $Al_2O$ , 1.59% Sn, 0.52% Al, 0.11% Sn<sub>2</sub> a combination of two reactions: (11.8% fuel)  $2Al + 3SnO \rightarrow Al_2O_3 + 3Sn$  (28.6% fuel)  $2Al + SnO \rightarrow Al_2O + Sn$ 

AI + SnO<sub>2</sub>

#### 24.29 ALUMINUM + $SnO_2$



**FIGURE 24.49** Adiabatic equilibrium temperature profile, Al (fuel) +  $SnO_2$  (oxidizer).



**FIGURE 24.50** Adiabatic equilibrium gas production profile, Al (fuel) +  $SnO_2$  (oxidizer).

- T1. 19% fuel, 31.36% gas produced, 2835.21 K—peak temperature solids: none liquids: 35.66% Al<sub>2</sub>O<sub>3</sub>, 32.98% Sn gases: 24.82% Sn, 3.26% SnO, 3.13% Sn<sub>2</sub> a combination of two reactions:
  (10.7% fuel) 2Al + 3SnO<sub>2</sub> → Al<sub>2</sub>O<sub>3</sub> + 3SnO (19.3% fuel) 4Al + 3SnO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Sn
  - The maximum amount of tin, 35.80% Sn(1), 23.57% Sn(g), and 2.93% Sn<sub>2</sub>(g), occurs at 20% fuel and 2825.04 K.
  - From 6% to 11% fuel, the temperature appears to be limited by the vaporization of SnO from Sn(l)/SnO<sub>2</sub>(s) mixtures, which occurs at about 1820 K.
  - From 45% to 49% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
  - The plateau from 26% to 41% fuel (2449 K) could not be attributed to a simple transition or reaction; species in this region include Al<sub>2</sub>O(g), Al(g), Sn(g), Sn<sub>2</sub>(g), Sn(l), Al<sub>2</sub>O<sub>3</sub>(l), and Al(l). The vaporization of Al<sub>2</sub>O and Al from Al(l)/Al<sub>2</sub>O<sub>3</sub>(l) mixtures is expected to occur at 2470 K.
- G1. 11% fuel, 76.49% gas produced, 1821.42 K—peak gas solids: 20.78% Al<sub>2</sub>O<sub>3</sub> (corundum), 0.15% SnO<sub>2</sub> (cassiterite) liquids: 2.58% Sn gases: 33.88% (SnO)<sub>2</sub>, 15.38% (SnO)<sub>4</sub>, 14.20% SnO, 13.01% (SnO)<sub>3</sub> a combination of two reactions:
  (10.7% fuel) 2A1 + 3SnO<sub>2</sub> → Al<sub>2</sub>O<sub>3</sub> + 3SnO (19.3% fuel) 4A1 + 3SnO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Sn
- **G2.** 19% fuel, 31.36% gas produced, 2835.21 K see T1 for details

#### 24.30 ALUMINUM + PbO





**FIGURE 24.51** Adiabatic equilibrium temperature profile, Al (fuel) + PbO (oxidizer).

**FIGURE 24.52** Adiabatic equilibrium gas production profile, Al (fuel) + PbO (oxidizer).

- T1. 7.5% fuel, 85.94% gas produced, 2327.01 K—peak temperature solids: 9.49% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 4.57% Al<sub>2</sub>O<sub>3</sub> gases: 85.39% Pb, 0.48% Pb<sub>2</sub> simplified equation at 7.5% fuel: 2A1 + 3PbO → Al<sub>2</sub>O<sub>3</sub> + 3Pb
  - T1 corresponds to the maximum amount of Pb.
  - From 1.2% to 1.5% fuel, the temperature is limited to 1159 K by the PbO(s-l) transition.
  - From 2.6% to 4.5% fuel, the temperature appears to be limited by the vaporization of Pb and PbO from Pb(1)/PbO(1) mixtures, which occurs at 1780 K.
  - The plateau from 11.8% to 32.9% fuel (2016 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), Al<sub>2</sub>O(g), Al(l), Pb(l), and Al<sub>2</sub>O<sub>3</sub>(s). Alone, Pb(l) is expected to vaporize at 2020 K.
  - From 7.2% to 7.8% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- **G1.** 6.8% fuel, 87.15% gas produced, 2043.14 K—*peak gas* solids: 12.85%  $Al_2O_3$  (corundum) liquids: none gases: 77.70% Pb, 8.82% PbO, 0.63% Pb<sub>2</sub> one reaction with excess oxidizer remaining: (7.5% fuel) 2A1 + 3PbO  $\rightarrow Al_2O_3 + 3Pb$

G2. 8.3% fuel, 86.72% gas produced, 2135.65 K solids: 13.28% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 84.52% Pb, 1.41% Al<sub>2</sub>O, 0.61% Pb<sub>2</sub>, 0.18% Al a combination of two reactions: (7.5% fuel) 2Al + 3PbO → Al<sub>2</sub>O<sub>3</sub> + 3Pb (19.5% fuel) 2Al + PbO → Al<sub>2</sub>O + Pb

#### 24.31 ALUMINUM + $Pb_3O_4$



**FIGURE 24.53** Adiabatic equilibrium temperature profile, Al (fuel) +  $Pb_3O_4$  (oxidizer).

- **FIGURE 24.54** Adiabatic equilibrium gas production profile, Al (fuel) +  $Pb_3O_4$  (oxidizer).
- **T1.** 2.6% fuel, 16.09% gas produced, 1806.15 K solids: 6.70% (PbO)(Al<sub>2</sub>O<sub>3</sub>)<sub>6</sub> liquids: 77.21% PbO gases: 15.22% PbO, 0.84% Pb simplified equation at 2.6% fuel: 12Al + 18Pb<sub>3</sub>O<sub>4</sub> → (PbO)(Al<sub>2</sub>O<sub>3</sub>)<sub>6</sub> + 53PbO
- **T2.** 9.5% fuel, 82.32% gas produced, 3102.99 K—*peak temperature* solids: none liquids: 17.68% Al<sub>2</sub>O<sub>3</sub> gases: 80.78% Pb, 1.19% PbO, 0.17% Pb<sub>2</sub> simplified equation at 9.5% fuel: 8Al + 3Pb<sub>3</sub>O<sub>4</sub>  $\rightarrow$  4Al<sub>2</sub>O<sub>3</sub> + 9Pb
- T3. 9.9% fuel, 82.46% gas produced, 3031.17 K solids: none liquids: 17.54% Al<sub>2</sub>O<sub>3</sub> gases: 81.22% Pb, 0.47% Al<sub>2</sub>O, 0.31% PbO, 0.22% Al, 0.18% Pb<sub>2</sub> simplified equation at 9.5% fuel: 8Al + 3Pb<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Pb
  - T3 corresponds to the maximum amount of Pb.
  - From 3.1% to 5.1% fuel, the temperature appears to be limited by the vaporization of Pb and PbO from Pb(1)/PbO(1) mixtures, which occurs at 1780 K.
  - The plateau from 29.8% to 43.5% fuel (2016 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), Al<sub>2</sub>O(g), Al(l), Pb(l), and Al<sub>2</sub>O<sub>3</sub>(s). Alone, Pb(l) is expected to vaporize at 2020 K.
  - From 6.7% to 7.4% and 12.5% to 13.5% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.



G1. 6.1% fuel, 88.47% gas produced, 1906.21 K—peak gas solids: 11.53% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 46.57% PbO, 41.67% Pb, 0.24% Pb<sub>2</sub> a combination of two reactions:
(2.6% fuel) 2A1 + 3Pb<sub>3</sub>O<sub>4</sub> → Al<sub>2</sub>O<sub>3</sub> + 9PbO (9.5% fuel) 8A1 + 3Pb<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Pb

**G2.** 13.7% fuel, 86.56% gas produced, 2277.61 K solids: 13.44% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 77.90% Pb, 7.55% Al<sub>2</sub>O, 0.75% Al, 0.35% Pb<sub>2</sub> a combination of two reactions: (9.5% fuel) 8Al + 3Pb<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O<sub>3</sub> + 9Pb (23.9% fuel) 8Al + Pb<sub>3</sub>O<sub>4</sub> → 4Al<sub>2</sub>O + 3Pb

#### 24.32 ALUMINUM + $PbO_2$



**FIGURE 24.55** Adiabatic equilibrium temperature profile, Al (fuel) + PbO<sub>2</sub> (oxidizer).

- **T1.** 7.0% fuel, 86.77% gas produced, 2388.59 K solids: none liquids: 13.23% Al<sub>2</sub>O<sub>3</sub> gases: 69.68% PbO, 15.86% Pb, 1.20% O<sub>2</sub> a combination of reactions: (7.0% fuel) 2A1 + 3PbO<sub>2</sub> → Al<sub>2</sub>O<sub>3</sub> + 3PbO (13.1% fuel) 4A1 + 3PbO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Pb (decomposition) PbO<sub>2</sub> → Pb + O<sub>2</sub>
- T2. 13.1% fuel, 78.53% gas produced, 3646.89 K—*peak temperature* solids: none liquids: 21.47% Al<sub>2</sub>O<sub>3</sub> major gases: 70.15% Pb, 5.45% PbO, 0.94% AlO, 0.64% Al<sub>2</sub>O other gases: 0.49% Al, 0.42% O, 0.26% Al<sub>2</sub>O<sub>2</sub>, 0.10% O<sub>2</sub> simplified equation at 13.1% fuel: 4Al + 3PbO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Pb
- T3. 15.8% fuel, 78.92% gas produced, 3508.84 K solids: none liquids: 21.08% Al<sub>2</sub>O<sub>3</sub> major gases: 71.52% Pb, 3.16% Al<sub>2</sub>O, 1.46% Al, 1.45% PbO other gases: 0.81% AlO, 0.36% Al<sub>2</sub>O<sub>2</sub> a combination of two reactions with excess fuel remaining: (13.1% fuel) 4Al + 3PbO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Pb (31.1% fuel) 4Al + PbO<sub>2</sub> → 2Al<sub>2</sub>O + Pb



**FIGURE 24.56** Adiabatic equilibrium gas production profile, Al (fuel) + PbO<sub>2</sub> (oxidizer).

- T3 corresponds to the maximum amount of Pb.
- The plateau from 49.4% to 56.6% fuel (2016 K) could not be attributed to a simple transition or reaction; species in this region include Pb(g), Pb<sub>2</sub>(g), Al<sub>2</sub>O(g), Al(l), Pb(l), and Al<sub>2</sub>O<sub>3</sub>(s). Alone, Pb(l) is expected to vaporize at 2020 K.
- From 6.4% to 6.8% and 27.6% to 31.9% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.
- **G1.** 5.6% fuel, 89.42% gas produced, 1873.26 K—*peak gas* solids: 10.58% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 85.74% PbO, 2.17% Pb, 1.50% O<sub>2</sub> a combination of reactions: (7.0% fuel) 2A1 + 3PbO<sub>2</sub>  $\rightarrow$  Al<sub>2</sub>O<sub>3</sub> + 3PbO (decomposition) 2PbO<sub>2</sub>  $\rightarrow$  2PbO + O<sub>2</sub> (decomposition) PbO<sub>2</sub>  $\rightarrow$  Pb + O<sub>2</sub>
- **G2.** 21.5% fuel, 85.42% gas produced, 2360.54 K solids: none liquids: 14.58% Al<sub>2</sub>O<sub>3</sub> gases: 67.80% Pb, 15.91% Al<sub>2</sub>O, 1.49% Al, 0.19% Pb<sub>2</sub> a combination of two reactions with excess fuel remaining: (13.1% fuel) 4Al + 3PbO<sub>2</sub> → 2Al<sub>2</sub>O<sub>3</sub> + 3Pb (31.1% fuel) 4Al + PbO<sub>2</sub> → 2Al<sub>2</sub>O + Pb

#### 24.33 ALUMINUM + $Sb_2O_3$



FIGURE 24.57 Adiabatic equilibrium temperature profile, Al (fuel) +  $Sb_2O_3$  (oxidizer).

FIGURE 24.58 Adiabatic equilibrium gas production profile, Al (fuel) +  $Sb_2O_3$  (oxidizer).

**T1.** 15.5% fuel, 71.13% gas produced, 2703.45 K—peak temperature solids: none liquids: 28.87% Al<sub>2</sub>O<sub>3</sub> gases: 36.21% Sb, 32.21% Sb<sub>2</sub>, 2.39% SbO, 0.18% Al<sub>2</sub>O simplified equation at 15.6% fuel:  $2Al + Sb_2O_3 \rightarrow Al_2O_3 + 2Sb$ 

T2. 27.0% fuel, 37.83% gas produced, 2348.74 K solids: none liquids: 38.32% AlSb, 21.88% Al<sub>2</sub>O<sub>3</sub>, 1.97% Al gases: 21.01% Sb<sub>2</sub>, 8.39% Sb, 7.51% Al<sub>2</sub>O, 0.69% Al, 0.20% Sb<sub>4</sub> a combination of reactions with excess fuel remaining:  $(15.6\% \text{ fuel}) 2\text{Al} + \text{Sb}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2\text{Sb}$  $(27.0\% \text{ fuel}) 4\text{Al} + \text{Sb}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2\text{AlSb}$  $(35.7\% \text{ fuel}) 6\text{Al} + \text{Sb}_2\text{O}_3 \rightarrow 3\text{Al}_2\text{O} + 2\text{Sb}$ 

T3. 42.4% fuel, 2344.37 K solids: none liquids: 58.78% AlSb, 21.08% Al, 20.15% Al<sub>2</sub>O<sub>3</sub> gases: none one reaction with excess fuel remaining:  $(27.0\% \text{ fuel}) 4\text{Al} + \text{Sb}_2\text{O}_3 \rightarrow \text{Al}_2\text{O}_3 + 2\text{AlSb}$ 

- The maximum amount of antimony, 34.26% Sb(g) and 34.98% Sb<sub>2</sub>(g), occurs at 16.3% fuel • and 2663.40 K.
- From 65.1% to 68.9% fuel, the temperature is limited to 1333 K by the AlSb(s-l) transition.

80

90 100

- From 11.7% to 12.8%, 19.6% to 20.0%, and 42.8% to 47.2% fuel, the temperature is limited to 2327 K by the Al<sub>2</sub>O<sub>3</sub>(s-l) transition.
- From 25.5% to 42.3% fuel, the temperature appears to be limited by the vaporization of Sb,  $Al_2O$ , and Al from  $AlSb(l)/Al_2O_3(l)$  mixtures, which occurs at 2349 K.
- **G1.** 3.4% fuel, 78.44% gas produced, 1092.86 K solids: 6.42% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 15.14% Sb gases: 78.19% Sb<sub>4</sub>O<sub>6</sub>, 0.18% Sb<sub>4</sub> one reaction with excess oxidizer remaining: (15.6% fuel)  $2Al + Sb_2O_3 \rightarrow Al_2O_3 + 2Sb$
- G2. 9.4% fuel, 82.24% gas produced, 1581.32 K—peak gas solids: 17.76% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 55.64% SbO, 15.30% Sb<sub>4</sub>, 10.55% Sb<sub>2</sub>, 0.57% Sb<sub>4</sub>O<sub>6</sub>, 0.18% Sb a combination of two reactions:
  (5.8% fuel) 2Al + 3Sb<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 6SbO (15.6% fuel) 2Al + Sb<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Sb
- **G3.** 19.7% fuel, 75.73% gas produced, 2327.02 K solids: 1.32% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: 22.95% Al<sub>2</sub>O<sub>3</sub> gases: 50.65% Sb<sub>2</sub>, 15.62% Sb, 7.85% Al<sub>2</sub>O, 0.80% Sb<sub>4</sub>, 0.79% Al a combination of two reactions: (15.6% fuel) 2Al + Sb<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Sb (35.7% fuel) 6Al + Sb<sub>2</sub>O<sub>3</sub> → 3Al<sub>2</sub>O + 2Sb

#### 24.34 ALUMINUM + $Bi_2O_3$



Adiabatic Equilibrium Gas Products fuel (wt-%)

AI + Bi<sub>2</sub>O<sub>3</sub>

FIGURE 24.59 Adiabatic equilibrium temperature profile, Al (fuel) +  $Bi_2O_3$  (oxidizer).

**FIGURE 24.60** Adiabatic equilibrium gas production profile, Al (fuel) +  $Bi_2O_3$  (oxidizer).

- T1. 10.4% fuel, 80.56% gas produced, 3201.96 K—peak temperature solids: none liquids: 19.44% Al<sub>2</sub>O<sub>3</sub> gases: 79.32% Bi, 0.82% Bi<sub>2</sub>, 0.25% BiO simplified equation at 10.4% fuel: 2Al + Bi<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Bi
  - The maximum amount of bismuth, 79.31% Bi(g) and 0.85% Bi<sub>2</sub>(g), occurs at 10.5% fuel and 3189.63 K.
  - From 3.1% to 4.0% fuel, the temperature appears to be limited by the vaporization of BiO and Bi from Bi(l)/Bi<sub>2</sub>O<sub>3</sub>(l) mixtures, which occurs at 1827 K.
  - From 40.3% to 47.9% fuel, the temperature appears to be limited to 1845 K by the vaporization of Bi(l). Alone, Bi(l) is expected to vaporize at 1846 K.
  - From 8.0% to 8.5% and 13.9% to 15.0% fuel, the temperature is limited to 2327 K by the  $Al_2O_3(s-l)$  transition.

G1. 7.2% fuel, 86.40% gas produced, 1992.12 K—peak gas solids: 13.60% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 37.74% Bi, 23.28% Bi<sub>2</sub>, 22.93% BiO, 1.42% O<sub>2</sub>, 1.03% Bi<sub>2</sub>O<sub>3</sub> a combination of reactions with excess oxidizer remaining: (3.7% fuel) 2Al + 3Bi<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 6BiO (10.4% fuel) 2Al + Bi<sub>2</sub>O<sub>3</sub> → Al<sub>2</sub>O<sub>3</sub> + 2Bi (decomposition) 2Bi<sub>2</sub>O<sub>3</sub> → 4Bi + 3O<sub>2</sub>

**G2.** 15.1% fuel, 85.60% gas produced, 2307.77 K solids: 14.40% Al<sub>2</sub>O<sub>3</sub> (corundum) liquids: none gases: 66.27% Bi, 9.88% Bi<sub>2</sub>, 8.59% Al<sub>2</sub>O, 0.84% Al a combination of two reactions: (10.4% fuel)  $2Al + Bi_2O_3 \rightarrow Al_2O_3 + 2Bi$ (25.8% fuel)  $6Al + Bi_2O_3 \rightarrow 3Al_2O + 2Bi$ 

# 25 Silicon–Oxidizer Systems

## 25.1 OVERVIEW

This chapter concerns the adiabatic properties of the silicon–oxygen system and another thirty-one silicon–oxidizer combinations. Equation 25.1 is a general description of the chemical reactions in question, and Table 25.1 provides a broad overview of the most basic results. The thermochemical descriptions within this chapter were derived from the *FactPS* and *FToxid* databases of

TABLE 25.1 Silicon–Oxidizer Systems			
Section	Pages	Oxidizer	Maximum T <sub>ad</sub> (K)
25.2	862	$O_2$	3147
25.3	864	TiO <sub>2</sub>	1272
25.4	865	V <sub>2</sub> O <sub>5</sub>	2633
25.5	867	Nb <sub>2</sub> O <sub>5</sub>	2334
25.6	869	Ta <sub>2</sub> O <sub>5</sub>	1705
25.7	870	$Cr_2O_3$	1941
25.8	871	MoO <sub>3</sub>	2905
25.9	873	WO <sub>3</sub>	2875
25.10	875	MnO	1770
25.11	877	$Mn_3O_4$	2168
25.12	879	$Mn_2O_3$	2304
25.13	881	$MnO_2$	3045
25.14	884	FeO	2481
25.15	886	Fe <sub>3</sub> O <sub>4</sub>	2644
25.16	888	$Fe_2O_3$	2812
25.17	890	CoO	2862
25.18	892	$Co_3O_4$	3039
25.19	894	NiO	2843
25.20	896	Cu <sub>2</sub> O	2791
25.21	897	CuO	2814
25.22	899	Ag <sub>2</sub> O	2430
25.23	900	ZnO	1181
25.24	901	CdO	1781
25.25	902	HgO	2923
25.26	904	$B_2O_3$	1090
-	-	$SiO_2$	-
25.27	905	SnO	2573
25.28	906	$SnO_2$	2574
25.29	908	PbO	2019
25.30	909	$Pb_3O_4$	2411
25.31	911	PbO <sub>2</sub>	2876
25.32	913	$Sb_2O_3$	2262
25.33	915	$Bi_2O_3$	2559

*FactSage 7.0.*\* Only pure substances were considered in the condensed phases. Gases were treated ideally, and ideal gas mixing was assumed. Charged species were not considered in any phase.

silicon + oxidizer 
$$\rightarrow$$
 adiabatic equilibrium products  
(P = 1 atm,  $T_i = 298.15$  K,  $T_{ad}$  = adiabatic equilibrium temperature) (25.1)

Within each of the following sections, you will find one or two general figures as well as written descriptions of certain fuel-to-oxidizer ratios. Temperature points (T1, T2, and so on) describe features and points of interest along adiabatic temperature profiles. Similarly, gas points (G1, G2, and so on) refer to adiabatic gas production profiles. Some adiabatic temperature charts contain flat regions where the adiabatic temperature remains constant despite variations in the stoichiometry of the system. Some of these plateaus are described and explained (see Chapter 2 and Tables 2.10–2.15 for additional information).

#### 25.2 SILICON + $O_2$



FIGURE 25.1 Adiabatic equilibrium temperature profile, Si (fuel) + O<sub>2</sub> (oxidizer).

**T1.** 21% fuel, 3043.55 K solids: none liquids: 21.51% SiO<sub>2</sub> gases: 55.99% O<sub>2</sub>, 14.31% SiO, 4.28% O, 3.92% SiO<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (46.7% fuel) Si + O<sub>2</sub>  $\rightarrow$  SiO<sub>2</sub> (63.7% fuel) 2Si + O<sub>2</sub>  $\rightarrow$  2SiO

<sup>&</sup>lt;sup>\*</sup> Bale, C. W.; Pelton, A. D.; Thompson, W. T.; Eriksson, G.; Hack, K.; Chartrand, P.; Decterov, S.; Jung, I.-H.; Melançon, J.; Petersen, S. *FactSage*, version 7.0; CRCT ThermFact, Inc. and GTT-Technologies, 2015; www.factsage.com (accessed September, 2019).

**T2.** 47% fuel, 3147.42 K—*peak temperature* solids: none liquids: 0.85% SiO<sub>2</sub> gases: 67.02% SiO, 20.11% O<sub>2</sub>, 8.36% SiO<sub>2</sub>, 3.67% O a combination of two reactions with excess oxidizer remaining: (46.7% fuel) Si + O<sub>2</sub>  $\rightarrow$  SiO<sub>2</sub> (63.7% fuel) 2Si + O<sub>2</sub>  $\rightarrow$  2SiO

**T3.** 64% fuel, 2859.63 K solids: none liquids: none gases: 99.19% SiO, 0.76% Si simplified equation at 63.7% fuel:  $2Si + O_2 \rightarrow 2SiO$ 

- The first and third points correspond to the maximum amounts of SiO<sub>2</sub> and SiO, respectively.
- From 91% to 95% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 71% to 88% fuel, the temperature appears to be limited by the vaporization of SiO from Si(l)/SiO<sub>2</sub>(l) mixtures, which occurs at 2145 K.
- SiO<sub>2</sub>(l) vaporizes and partially decomposes into gaseous SiO, O<sub>2</sub>, and O at 3147 K. This appears to limit any further increase in temperature. SiO(g) is stable at much higher temperatures, with only minor decomposition expected at 4500 K.
- Si(l) is present from 65% to 95% fuel with the maximum amount (81.22%) occurring at 90% fuel. Si(g) is present from 64% to 68% fuel with the maximum amount (0.98%) occurring at 65% fuel. Pure Si(l) vaporizes at 3462 K.

### 25.3 SILICON + $TiO_2$



FIGURE 25.2 Adiabatic equilibrium temperature profile, Si (fuel) + TiO<sub>2</sub> (oxidizer).

T1. 41.3% fuel, 1271.61 K—peak temperature solids: 55.78% TiSi, 44.16% SiO<sub>2</sub> (tridymite) liquids: none gases: none simplified equation at 41.3% fuel: 2Si + TiO<sub>2</sub> → SiO<sub>2</sub> + TiSi

**T2.** 51.3% fuel, 1245.38 K solids: 63.15% TiSi<sub>2</sub>, 36.64% SiO<sub>2</sub> (tridymite), 0.21% TiSi liquids: none gases: none simplified equation at 51.3% fuel:  $3Si + TiO_2 \rightarrow SiO_2 + TiSi_2$ 

- Elemental titanium is not predicted to occur at any point.
- From 31.1% to 31.9% and 57.4% to 57.9% fuel, the temperature is limited to 1140 K by the quartz  $\rightarrow$  tridymite transition of SiO<sub>2</sub>(s).

#### 25.4 SILICON + $V_2O_5$



**FIGURE 25.3** Adiabatic equilibrium temperature profile, Si (fuel) +  $V_2O_5$  (oxidizer).

**FIGURE 25.4** Adiabatic equilibrium gas production profile, Si (fuel)  $+ V_2O_5$  (oxidizer).

**T1.** 7.2% fuel, 1633.00 K

solids: 26.98% VO<sub>2</sub>, 15.40% SiO<sub>2</sub> (tridymite), 0.37% V<sub>2</sub>O<sub>3</sub> liquids: 57.25% VO<sub>2</sub> gases: none simplified equation at 7.2% fuel: Si +  $2V_2O_5 \rightarrow SiO_2 + 4VO_2$ 

- **T2.** 13.4% fuel, 2342.25 K solids: none liquids: 71.07% V<sub>2</sub>O<sub>3</sub>, 28.67% SiO<sub>2</sub>, 0.26% VO gases: none simplified equation at 13.4% fuel: Si + V<sub>2</sub>O<sub>5</sub> → SiO<sub>2</sub> + V<sub>2</sub>O<sub>3</sub>
- T3. 18.8% fuel, 2632.68 K—peak temperature solids: none liquids: 59.69% VO, 40.22% SiO<sub>2</sub> gases: none simplified equation at 18.8% fuel: 3Si + 2V<sub>2</sub>O<sub>5</sub> → 3SiO<sub>2</sub> + 4VO
- **T4.** 36.4% fuel, 12.17% gas produced, 2375.23 K solids: 39.05% V<sub>5</sub>Si<sub>3</sub> liquids: 40.53% SiO<sub>2</sub>, 8.25% VO gases: 12.16% SiO a combination of reactions: (18.8% fuel)  $3Si + 2V_2O_5 \rightarrow 3SiO_2 + 4VO$ (36.4% fuel)  $37Si + 10V_2O_5 \rightarrow 25SiO_2 + 4V_5Si_3$ (48.9% fuel)  $31Si + 5V_2O_5 \rightarrow 25SiO + 2V_5Si_3$



**T5.** 62.4% fuel, 1954.01 K

solids: 44.29% VSi<sub>2</sub>, 31.05% SiO<sub>2</sub> (cristobalite) liquids: 24.66% Si gases: none one reaction with excess fuel remaining:  $(50.1\% \text{ fuel}) \ 13\text{Si} + 2\text{V}_2\text{O}_5 \rightarrow 5\text{SiO}_2 + 4\text{VSi}_2$ 

- Elemental vanadium is not predicted to occur at any point.
- From 5.9% to 7.9% fuel, the temperature is limited to 1633 K by the VO<sub>2</sub>(s-l) transition.
- From 65.5% to 75.8% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 57.5% to 62.3% fuel, the temperature appears to be limited by the  $5VSi_2(s) \rightarrow V_5Si_3(s) + 7Si(l)$  decomposition, which occurs at 1958 K.
- From 56.3% to 57.0% fuel, the temperature is limited to 1996 K by the SiO<sub>2</sub>(s-1) transition.
- From 39.7% to 54.2% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 11.4% to 13.3% fuel, the temperature is limited to 2340 K by the  $V_2O_3(s-1)$  transition.
- From 19.8% to 39.1% fuel, the temperature appears to be limited by the  $V_5Si_3(s) + 8SiO_2(l) \rightarrow 5VO(l) + 11SiO(g)$  reaction, which occurs at 2375 K.

**G1.** 39.7% fuel, 16.32% gas produced, 2144.86 K—*peak gas* solids: 44.95% V<sub>5</sub>Si<sub>3</sub> liquids: 38.68% SiO<sub>2</sub> gases: 16.32% SiO a combination of two reactions: (36.4% fuel) 37Si + 10V<sub>2</sub>O<sub>5</sub> → 25SiO<sub>2</sub> + 4V<sub>5</sub>Si<sub>3</sub> (48.9% fuel) 31Si + 5V<sub>2</sub>O<sub>5</sub> → 25SiO + 2V<sub>5</sub>Si<sub>3</sub>

#### 25.5 SILICON + Nb<sub>2</sub>O<sub>5</sub>



**FIGURE 25.5** Adiabatic equilibrium temperature profile, Si (fuel) +  $Nb_2O_5$  (oxidizer).

**FIGURE 25.6** Adiabatic equilibrium gas production profile, Si (fuel) +  $Nb_2O_5$  (oxidizer).

fuel (wt-%)

100

90

80

70

20

10

0

0 10 20 30 40 50 60 70 80 90 100

- **T1.** 5.0% fuel, 1087.81 K solids: 88.95% NbO<sub>2</sub>, 10.70% SiO<sub>2</sub> (quartz), 0.36% Nb<sub>2</sub>O<sub>5</sub> liquids: none gases: none simplified equation at 5.0% fuel: Si + 2Nb<sub>2</sub>O<sub>5</sub> → SiO<sub>2</sub> + 4NbO<sub>2</sub>
- T2. 13.7% fuel, 1768.76 K solids: 70.64% NbO, 29.28% SiO<sub>2</sub> (cristobalite) liquids: none gases: none simplified equation at 13.7% fuel: 3Si + 2Nb<sub>2</sub>O<sub>5</sub> → 3SiO<sub>2</sub> + 4NbO
- T3. 28.1% fuel, 2333.82 K—peak temperature solids: 59.35% Nb<sub>5</sub>Si<sub>3</sub> liquids: 40.62% SiO<sub>2</sub> gases: none simplified equation at 28.1% fuel: 37Si + 10Nb<sub>2</sub>O<sub>5</sub> → 25SiO<sub>2</sub> + 4Nb<sub>5</sub>Si<sub>3</sub>

**T4.** 40.7% fuel, 1860.13 K

solids: 33.51% SiO<sub>2</sub> (cristobalite), 29.62% NbSi<sub>2</sub>, 27.17% Nb<sub>5</sub>Si<sub>3</sub> liquids: 9.71% Si gases: none a combination of two reactions with excess fuel remaining: (28.1% fuel)  $37Si + 10Nb_2O_5 \rightarrow 25SiO_2 + 4Nb_5Si_3$ (40.7% fuel)  $13Si + 2Nb_2O_5 \rightarrow 5SiO_2 + 4NbSi_2$ 



**T5.** 44.8% fuel, 1855.78 K solids: 61.92% NbSi<sub>2</sub>, 31.19% SiO<sub>2</sub> (cristobalite) liquids: 6.89% Si gases: none one reaction with excess fuel remaining: (40.7% fuel) 13Si + 2Nb<sub>2</sub>O<sub>5</sub>  $\rightarrow$  5SiO<sub>2</sub> + 4NbSi<sub>2</sub>

- Elemental niobium is not predicted to occur at any point.
- From 47.3% to 54.2% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 37.1% to 44.7% fuel, the temperature appears to be limited by the  $5NbSi_2(s) \rightarrow Nb_5Si_3(s) + 7Si(l)$  decomposition, which occurs at 1860 K.
- From 18.4% to 19.8% and 33.8% to 34.9% fuel, the temperature is limited to 1996 K by the  $SiO_2(s-1)$  transition.
- From 28.6% to 31.2% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 25.1% to 26.6% fuel, the temperature is limited to 2210 K by the NbO(s-1) transition.

G1. 28.6% fuel, 1.99% gas produced, 2144.86 K—peak gas solids: 58.97% Nb<sub>5</sub>Si<sub>3</sub> liquids: 38.99% SiO<sub>2</sub> gases: 1.99% SiO a combination of two reactions:
(28.1% fuel) 37Si + 10Nb<sub>2</sub>O<sub>5</sub> → 25SiO<sub>2</sub> + 4Nb<sub>5</sub>Si<sub>3</sub> (39.6% fuel) 31Si + 5Nb<sub>2</sub>O<sub>5</sub> → 25SiO + 2Nb<sub>5</sub>Si<sub>3</sub>
## 25.6 SILICON + $Ta_2O_5$



**FIGURE 25.7** Adiabatic equilibrium temperature profile, Si (fuel) +  $Ta_2O_5$  (oxidizer).

**T1.** 18.2% fuel, 1687.43 K

solids: 71.94% Ta<sub>2</sub>Si, 27.81% SiO<sub>2</sub> (tridymite), 0.26% Ta<sub>5</sub>Si<sub>3</sub> liquids: none gases: none simplified equation at 18.2% fuel:  $7Si + 2Ta_2O_5 \rightarrow 5SiO_2 + 2Ta_2Si$ 

- **T2.** 19.1% fuel, 1691.64 K solids: 72.05% Ta<sub>5</sub>Si<sub>3</sub>, 27.50% SiO<sub>2</sub> (tridymite), 0.45% TaSi<sub>2</sub> liquids: none gases: none simplified equation at 19.0% fuel:  $37Si + 10Ta_2O_5 \rightarrow 25SiO_2 + 4Ta_5Si_3$
- T3. 29.2% fuel, 1705.10 K—peak temperature solids: 75.69% TaSi<sub>2</sub>, 24.07% SiO<sub>2</sub> (tridymite), 0.25% Ta<sub>5</sub>Si<sub>3</sub> liquids: none gases: none simplified equation at 29.2% fuel: 13Si + 2Ta<sub>2</sub>O<sub>5</sub> → 5SiO<sub>2</sub> + 4TaSi<sub>2</sub>
  - Elemental tantalum is not predicted to occur at any point.
  - From 29.5% to 29.8% fuel, the temperature is limited to 1685 K by the Si(s-1) transition.

# 25.7 SILICON + $Cr_2O_3$



**FIGURE 25.8** Adiabatic equilibrium temperature profile, Si (fuel) +  $Cr_2O_3$  (oxidizer).

**T1.** 21.7% fuel, 1698.18 K solids: 53.57% Cr, 46.42% SiO<sub>2</sub> (tridymite) liquids: none gases: none simplified equation at 21.7% fuel:  $3Si + 2Cr_2O_3 \rightarrow 3SiO_2 + 4Cr$ 

- **T2.** 28.6% fuel, 1913.83 K solids: 57.54% Cr<sub>3</sub>Si, 42.34% SiO<sub>2</sub> (cristobalite), 0.13% Cr<sub>5</sub>Si<sub>3</sub> liquids: none gases: none simplified equation at 28.6% fuel:  $13Si + 6Cr_2O_3 \rightarrow 9SiO_2 + 4Cr_3Si$
- T3. 33.3% fuel, 1941.33 K—peak temperature solids: 60.39% Cr<sub>5</sub>Si<sub>3</sub>, 39.55% SiO<sub>2</sub> (cristobalite) liquids: none gases: none simplified equation at 33.3% fuel: 27Si + 10Cr<sub>2</sub>O<sub>3</sub> → 15SiO<sub>2</sub> + 4Cr<sub>5</sub>Si<sub>3</sub>
- **T4.** 50.4% fuel, 1729.34 K solids: 70.57% CrSi<sub>2</sub>, 29.41% SiO<sub>2</sub> (tridymite) liquids: none gases: none simplified equation at 50.4% fuel:  $11Si + 2Cr_2O_3 \rightarrow 3SiO_2 + 4CrSi_2$ 
  - T1 corresponds to the maximum amount of Cr.
  - From 51.2% to 52.1% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.

## 25.8 SILICON + $MoO_3$



**FIGURE 25.9** Adiabatic equilibrium temperature profile, Si (fuel) + MoO<sub>3</sub> (oxidizer).

**T1.** 9% fuel, 18.18% gas produced, 2308.05 K



**FIGURE 25.10** Adiabatic equilibrium gas production profile, Si (fuel) + MoO<sub>3</sub> (oxidizer).

- solids: 56.10% MoO<sub>2</sub>, 6.47% Mo liquids: 19.25% SiO<sub>2</sub> gases: 14.90% (MoO<sub>3</sub>)<sub>3</sub>, 2.05% (MoO<sub>3</sub>)<sub>4</sub>, 1.02% (MoO<sub>3</sub>)<sub>2</sub>, 0.13% MoO<sub>3</sub> a combination of two reactions with excess oxidizer remaining: (8.9% fuel) Si + 2MoO<sub>3</sub>  $\rightarrow$  SiO<sub>2</sub> + 2MoO<sub>2</sub> (22.6% fuel) 3Si + 2MoO<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 2Mo
- T2. 23% fuel, 14.92% gas produced, 2904.58 K—peak temperature solids: none liquids: 46.21% Mo, 38.87% SiO<sub>2</sub> major gases: 7.49% SiO, 2.38% MoO<sub>3</sub>, 2.25% MoO<sub>2</sub>, 1.23% (MoO<sub>3</sub>)<sub>3</sub>, 1.03% (MoO<sub>3</sub>)<sub>2</sub> other gases: 0.37% MoO, 0.13% SiO<sub>2</sub> a combination of two reactions with excess oxidizer remaining: (22.6% fuel) 3Si + 2MoO<sub>3</sub> → 3SiO<sub>2</sub> + 2Mo (36.9% fuel) 3Si + MoO<sub>3</sub> → 3SiO + Mo
- **T3.** 27% fuel, 17.72% gas produced, 2584.49 K solids: 48.66% Mo liquids: 33.63% SiO<sub>2</sub> gases: 17.70% SiO a combination of two reactions: (22.6% fuel) 3Si + 2MoO<sub>3</sub> → 3SiO<sub>2</sub> + 2Mo (36.9% fuel) 3Si + MoO<sub>3</sub> → 3SiO + Mo
- **T4.** 31% fuel, 19.52% gas produced, 2458.84 K solids: 49.01% Mo<sub>3</sub>Si, 1.57% Mo<sub>5</sub>Si<sub>3</sub>

```
liquids: 29.90% SiO<sub>2</sub>
gases: 19.51% SiO
a combination of two reactions:
(26.3% fuel) 11Si + 6MoO<sub>3</sub> \rightarrow 9SiO<sub>2</sub> + 2Mo<sub>3</sub>Si
(39.4% fuel) 10Si + 3MoO<sub>3</sub> \rightarrow 9SiO + Mo<sub>3</sub>Si
```

- **T5.** 34% fuel, 21.21% gas produced, 2233.73 K solids: 51.14% Mo<sub>5</sub>Si<sub>3</sub>, 0.79% MoSi<sub>2</sub> liquids: 26.87% SiO<sub>2</sub> gases: 21.20% SiO a combination of two reactions: (29.1% fuel) 21Si + 10MoO<sub>3</sub> → 15SiO<sub>2</sub> + 2Mo<sub>5</sub>Si<sub>3</sub> (41.3% fuel) 18Si + 5MoO<sub>3</sub> → 15SiO + Mo<sub>5</sub>Si<sub>3</sub>
- **T6.** 44% fuel, 18.08% gas produced, 2230.10 K solids: 59.18% MoSi<sub>2</sub> liquids: 22.74% SiO<sub>2</sub> gases: 18.08% SiO a combination of two reactions: (40.6% fuel) 7Si + 2MoO<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 2MoSi<sub>2</sub> (49.4% fuel) 5Si + MoO<sub>3</sub>  $\rightarrow$  3SiO + MoSi<sub>2</sub>
  - T3 corresponds to the maximum amount of Mo.
  - From 65% to 77% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
  - From 45% to 59% fuel, the temperature appears to be limited by the vaporization of SiO from Si(l)/SiO<sub>2</sub>(l) mixtures, which occurs at 2145 K.
  - From 34% to 43% fuel, the temperature appears to be limited by the  $5MoSi_2(s) + 7SiO_2(l) \rightarrow Mo_5Si_3(s) + 14SiO(g)$  reaction, which occurs at 2234 K.
  - From 8% to 12% fuel, the temperature appears to be limited by the vaporization of MoO<sub>3</sub> from Mo(s)/MoO<sub>2</sub>(s) mixtures, which occurs at 2308 K.
  - From 31% to 33% fuel, the temperature appears to be limited by the  $3Mo_5Si_3(s) + 4SiO_2(l) \rightarrow 5Mo_3Si(s) + 8SiO(g)$  reaction, which occurs at 2459 K.
  - From 28% to 30% fuel, the temperature appears to be limited by the  $Mo_3Si(s) + SiO_2(l) \rightarrow 3Mo(s) + 2SiO(g)$  reaction, which occurs at 2477 K.
- G1. 5% fuel, 43.74% gas produced, 1388.70 K—peak gas solids: 45.56% MoO<sub>2</sub>, 10.70% SiO<sub>2</sub> (tridymite) liquids: none gases: 23.85% (MoO<sub>3</sub>)<sub>4</sub>, 15.54% (MoO<sub>3</sub>)<sub>3</sub>, 4.33% (MoO<sub>3</sub>)<sub>5</sub> one reaction with excess oxidizer remaining: (8.9% fuel) Si + 2MoO<sub>3</sub> → SiO<sub>2</sub> + 2MoO<sub>2</sub>
- G2. 13% fuel, 42.65% gas produced, 2403.78 K solids: 29.57% Mo liquids: 27.78% SiO<sub>2</sub> major gases: 34.81% (MoO<sub>3</sub>)<sub>3</sub>, 4.07% (MoO<sub>3</sub>)<sub>4</sub>, 3.00% (MoO<sub>3</sub>)<sub>2</sub> other gases: 0.52% MoO<sub>3</sub>, 0.11% (MoO<sub>3</sub>)<sub>5</sub>, 0.11% MoO<sub>2</sub> one reaction with excess oxidizer remaining: (22.6% fuel) 3Si + 2MoO<sub>3</sub> → 3SiO<sub>2</sub> + 2Mo
- **G3.** 34% fuel, 21.21% gas produced, 2233.73 K See T5 for details

#### 25.9 SILICON + $WO_3$



**FIGURE 25.11** Adiabatic equilibrium temperature profile, Si (fuel) + WO<sub>3</sub> (oxidizer).

**FIGURE 25.12** Adiabatic equilibrium gas production profile, Si (fuel) + WO<sub>3</sub> (oxidizer).

- T1. 15% fuel, 11.97% gas produced, 2875.17 K—peak temperature solids: 60.65% W
  liquids: 27.39% SiO<sub>2</sub>
  gases: 7.22% (WO<sub>3</sub>)<sub>2</sub>, 3.42% SiO, 0.74% W<sub>3</sub>O<sub>8</sub>, 0.40% (WO<sub>3</sub>)<sub>3</sub>
  a combination of two reactions with excess oxidizer remaining: (15.4% fuel) 3Si + 2WO<sub>3</sub> → 3SiO<sub>2</sub> + 2W
  (26.7% fuel) 3Si + WO<sub>3</sub> → 3SiO + W
- **T2.** 17% fuel, 6.83% gas produced, 2834.00 K solids: 65.43% W liquids: 27.74% SiO<sub>2</sub> gases: 6.30% SiO, 0.42% (WO<sub>3</sub>)<sub>2</sub> a combination of two reactions: (15.4% fuel)  $3Si + 2WO_3 \rightarrow 3SiO_2 + 2W$  (26.7% fuel)  $3Si + WO_3 \rightarrow 3SiO + W$
- **T3.** 23% fuel, 10.25% gas produced, 2185.53 K solids: 65.91% W<sub>5</sub>Si<sub>3</sub>, 0.89% WSi<sub>2</sub> liquids: 22.95% SiO<sub>2</sub> gases: 10.25% SiO a combination of two reactions: (20.3% fuel) 21Si + 10WO<sub>3</sub> → 15SiO<sub>2</sub> + 2W<sub>5</sub>Si<sub>3</sub> (30.4% fuel) 18Si + 5WO<sub>3</sub> → 15SiO + W<sub>5</sub>Si<sub>3</sub>



- **T4.** 32% fuel, 9.25% gas produced, 2144.86 K solids: 70.40% WSi<sub>2</sub> liquids: 20.13% SiO<sub>2</sub>, 0.22% Si gases: 9.25% SiO a combination of two reactions: (29.8% fuel) 7Si + 2WO<sub>3</sub> → 3SiO<sub>2</sub> + 2WSi<sub>2</sub> (37.7% fuel) 5Si + WO<sub>3</sub> → 3SiO + WSi<sub>2</sub>
- T2 corresponds to the maximum amount of W.
- From 49% to 62% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 32% to 42% fuel, the temperature appears to be limited by the vaporization of SiO from Si(l)/SiO<sub>2</sub>(l) mixtures, which occurs at 2145 K.
- From 23% to 31% fuel, the temperature appears to be limited by the  $5WSi_2(s) + 7SiO_2(l) \rightarrow W_5Si_3(s) + 14SiO(g)$  reaction, which occurs at 2186 K.
- From 19% to 22% fuel, the temperature appears to be limited by the  $W_5Si_3(s) + 3SiO_2(l) \rightarrow 5W(s) + 6SiO(g)$  reaction, which occurs at 2316 K.
- G1. 10% fuel, 35.63% gas produced, 2261.46 K—peak gas solids: 42.99% W
  liquids: 21.39% SiO<sub>2</sub>
  gases: 15.33% (WO<sub>3</sub>)<sub>3</sub>, 9.30% (WO<sub>3</sub>)<sub>2</sub>, 7.20% W<sub>3</sub>O<sub>8</sub>, 3.78% (WO<sub>3</sub>)<sub>4</sub>
  a combination of two reactions with excess oxidizer remaining:
  (2.0% fuel) Si + 6WO<sub>3</sub> → SiO<sub>2</sub> + 2W<sub>3</sub>O<sub>8</sub>
  (15.4% fuel) 3Si + 2WO<sub>3</sub> → 3SiO<sub>2</sub> + 2W

## 25.10 SILICON + MnO



FIGURE 25.13 Adiabatic equilibrium temperature profile, Si (fuel) + MnO (oxidizer).

**T1.** 9.0% fuel. 1083.88 K solids: 64.72% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite), 35.21% Mn liquids: none gases: none simplified equation at 9.0% fuel:  $Si + 4MnO \rightarrow Mn_2SiO_4 + 2Mn$ T2. 14.2% fuel, 1321.23 K solids: 60.47% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite), 39.01% Mn<sub>3</sub>Si, 0.51% MnSiO<sub>3</sub> (rhodonite) liquids: none gases: none simplified equation at 14.2% fuel:  $5Si + 12MnO \rightarrow 3Mn_2SiO_4 + 2Mn_3Si$ **T3.** 18.0% fuel, 1457.50 K solids: 50.08% MnSiO<sub>3</sub> (rhodonite), 49.45% Mn<sub>3</sub>Si, 0.47% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite) liquids: none gases: none simplified equation at 18.0% fuel:  $5Si + 9MnO \rightarrow 3MnSiO_3 + 2Mn_3Si$ **T4.** 22.5% fuel, 1546.19 K solids: 52.27% Mn<sub>5</sub>Si<sub>3</sub>, 47.71% MnSiO<sub>3</sub> (rhodonite) liquids: none gases: none

simplified equation at 22.5% fuel:  $11Si + 15MnO \rightarrow 5MnSiO_3 + 2Mn_5Si_3$ 

- **T5.** 30.3% fuel, 1728.04 K solids: 70.41%  $Mn_5Si_3$ , 29.36% SiO<sub>2</sub> (tridymite), 0.23%  $MnSiO_3$  (rhodonite) liquids: none gases: none simplified equation at 30.3% fuel: 11Si + 10MnO →  $5SiO_2 + 2Mn_5Si_3$
- T6. 37.2% fuel, 1769.62 K—peak temperature solids: 72.79% MnSi, 26.60% SiO<sub>2</sub> (cristobalite), 0.61% Mn<sub>5</sub>Si<sub>3</sub> liquids: none gases: none simplified equation at 37.3% fuel: 3Si + 2MnO → SiO<sub>2</sub> + 2MnSi
  - T1 corresponds to the maximum amount of Mn.
  - From 39.0% to 41.1% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.

## 25.11 SILICON + $Mn_3O_4$



**FIGURE 25.14** Adiabatic equilibrium temperature profile, Si (fuel) +  $Mn_3O_4$  (oxidizer).

**FIGURE 25.15** Adiabatic equilibrium gas production profile, Si (fuel) +  $Mn_3O_4$  (oxidizer).

- **T1.** 5.8% fuel, 1578.16 K solids: 58.22% MnO, 41.71%  $Mn_2SiO_4$  (tephroite) liquids: none gases: none simplified equation at 5.8% fuel: Si +  $2Mn_3O_4 \rightarrow Mn_2SiO_4 + 4MnO$
- **T2.** 10.9% fuel, 1805.90 K solids: 78.38%  $Mn_2SiO_4$  (tephroite), 0.37% MnO liquids: 21.25% Mn gases: none simplified equation at 10.9% fuel: Si +  $Mn_3O_4 \rightarrow Mn_2SiO_4 + Mn_3O_4$
- **T3.** 14.1% fuel, 1967.61 K solids: 75.28%  $Mn_2SiO_4$  (tephroite), 24.25%  $Mn_3Si$ , 0.47%  $MnSiO_3$  (rhodonite) liquids: none gases: none simplified equation at 14.1% fuel:  $4Si + 3Mn_3O_4 \rightarrow 3Mn_2SiO_4 + Mn_3Si$
- **T4.** 18.8% fuel, 2058.87 K solids: 62.00% MnSiO<sub>3</sub> (rhodonite), 37.85% Mn<sub>3</sub>Si liquids: 0.15% Mn gases: none simplified equation at 18.8% fuel:  $17Si + 9Mn_3O_4 \rightarrow 12MnSiO_3 + 5Mn_3Si$



- **T5.** 22.3% fuel, 2098.06 K solids: 59.13% MnSiO<sub>3</sub> (rhodonite), 40.74% Mn<sub>5</sub>Si<sub>3</sub> liquids: 0.14% SiO<sub>2</sub> gases: none simplified equation at 22.3% fuel: 7Si +  $3Mn_3O_4 \rightarrow 4MnSiO_3 + Mn_5Si_3$
- **T6.** 31.8% fuel, 2168.18 K—*peak temperature* solids: 64.17%  $Mn_5Si_3$ liquids: 35.79%  $SiO_2$ gases: none simplified equation at 31.8% fuel: 19Si +  $5Mn_3O_4 \rightarrow 10SiO_2 + 3Mn_5Si_3$
- **T7.** 39.0% fuel, 2115.38 K solids: 66.40% MnSi liquids: 32.04% SiO<sub>2</sub>, 1.56% Si gases: none one reaction with excess fuel remaining: (38.0% fuel) 5Si + Mn<sub>3</sub>O<sub>4</sub>  $\rightarrow$  2SiO<sub>2</sub> + 3MnSi
- T2 corresponds to the maximum amount of Mn.
- From 47.5% to 56.7% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 15.4% to 17.4% fuel, the temperature appears to be limited by the  $Mn_3Si(s) + 3Mn_2SiO_4(s) \rightarrow 5Mn(l) + 4MnSiO_3(s)$  reaction, which occurs at 1992 K.
- From 41.3% to 42.0% fuel, the temperature is limited to 1996 K by the SiO<sub>2</sub>(s-l) transition.
- From 32.9% to 38.9% fuel, the temperature appears to be limited by the 5MnSi(s)  $\rightarrow$  Mn<sub>5</sub>Si<sub>3</sub>(s) + 2Si(l) decomposition, which occurs at 2119 K.

G1. 31.9% fuel, 0.40% gas produced, 2138.46 K—peak gas solids: 64.07% Mn<sub>5</sub>Si<sub>3</sub> liquids: 35.51% SiO<sub>2</sub> gases: 0.38% SiO simplified equation at 31.8% fuel: 19Si + 5Mn<sub>3</sub>O<sub>4</sub> → 10SiO<sub>2</sub> + 3Mn<sub>5</sub>Si<sub>3</sub>

#### 25.12 SILICON + $Mn_2O_3$



**FIGURE 25.16** Adiabatic equilibrium temperature profile, Si (fuel) +  $Mn_2O_3$  (oxidizer).



FIGURE 25.17 Adiabatic equilibrium gas production profile, Si (fuel) +  $Mn_2O_3$  (oxidizer).

- **T1.** 8% fuel, 0.21% gas produced, 2115.15 K solids: 57.53%  $Mn_2SiO_4$  (tephroite), 26.51% MnO liquids: 15.75% MnO gases: 0.21%  $O_2$ simplified equation at 8.2% fuel: Si +  $2Mn_2O_3 \rightarrow Mn_2SiO_4 + 2MnO$
- **T2.** 11% fuel, 2304.34 K—peak temperature solids: 79.10%  $Mn_2SiO_4$  (tephroite) liquids: 12.06% Mn, 8.84% MnO gases: none a combination of two reactions: (8.2% fuel) Si + 2Mn\_2O\_3  $\rightarrow$  Mn\_2SiO<sub>4</sub> + 2MnO (11.8% fuel) 3Si + 4Mn\_2O\_3  $\rightarrow$  3Mn\_2SiO<sub>4</sub> + 2Mn
- **T3.** 12% fuel, 2.38% gas produced, 2275.12 K solids: 83.81% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite) liquids: 13.81% Mn gases: 1.84% Mn, 0.54% SiO simplified equation at 11.8% fuel:  $3Si + 4Mn_2O_3 \rightarrow 3Mn_2SiO_4 + 2Mn_2O_3$
- **T4.** 15% fuel, 2.43% gas produced, 2255.15 K solids: 61.90% MnSiO<sub>3</sub> (rhodonite), 9.18% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite) liquids: 26.50% Mn gases: 1.71% Mn, 0.72% SiO a combination of two reactions: (11.8% fuel)  $3Si + 4Mn_2O_3 \rightarrow 3Mn_2SiO_4 + 2Mn$ (15.1% fuel)  $Si + Mn_2O_3 \rightarrow MnSiO_3 + Mn$

- **T5.** 22% fuel, 5.70% gas produced, 2230.54 K solids: 62.63% MnSiO<sub>3</sub> (rhodonite), 30.77% Mn<sub>5</sub>Si<sub>3</sub> liquids: 0.90% Mn gases: 3.58% Mn, 2.12% SiO simplified equation at 22.2% fuel: 8Si + 5Mn<sub>2</sub>O<sub>3</sub> → 5MnSiO<sub>3</sub> + Mn<sub>5</sub>Si<sub>3</sub>
- **T6.** 46% fuel, 2077.55 K solids: 56.80% MnSi liquids: 30.83% SiO<sub>2</sub>, 12.38% Si gases: none one reaction with excess fuel remaining: (38.4% fuel) 7Si + 2Mn<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 4MnSi
  - T4 corresponds to the maximum amount of Mn.
  - From 53% to 64% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
  - From 8% to 9% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
  - From 41% to 45% fuel, the temperature appears to be limited by the 5MnSi(s)  $\rightarrow$  Mn<sub>5</sub>Si<sub>3</sub>(s) + 2Si(1) decomposition, which occurs at 2119 K.
  - The plateau from 34% to 40% fuel (2138 K) could not be attributed to a simple transition or reaction; species in this region include SiO(g), Mn(g),  $SiO_2(l)$ , Si(l), and  $Mn_5Si_3(s)$ . The vaporization of SiO from  $Si(l)/SiO_2(l)$  mixtures is expected to occur at 2145 K.
  - From 23% to 32% fuel, the temperature appears to be limited by the  $Mn_5Si_3(s) + 3SiO_2(l) \rightarrow 5Mn(g) + 6SiO(g)$  reaction, which occurs at 2227 K.
  - From 16% to 22% fuel, the temperature appears to be limited by the  $2Mn_5Si_3(s) + 3MnSiO_3(s) \rightarrow 13Mn(l-g) + 9SiO(g)$  reaction, which occurs at 2231 K.
  - From 13% to 15% fuel, the temperature appears to be limited by the  $Mn(l) + 3MnSiO_3(s) \rightarrow 2Mn_2SiO_4(s) + SiO(g)$  reaction, which occurs at 2255 K.
- G1. 22% fuel, 5.70% gas produced, 2230.54 K—*peak gas* See T5 for details
- **G2.** 31% fuel, 5.70% gas produced, 2226.96 K—*peak gas* solids: 54.00% Mn<sub>5</sub>Si<sub>3</sub>, 8.77% MnSiO<sub>3</sub> (rhodonite) liquids: 31.54% SiO<sub>2</sub> gases: 3.02% Mn, 2.67% SiO a combination of two reactions: (22.2% fuel) 8Si + 5Mn<sub>2</sub>O<sub>3</sub> → 5MnSiO<sub>3</sub> + Mn<sub>5</sub>Si<sub>3</sub> (32.4% fuel) 27Si + 10Mn<sub>2</sub>O<sub>3</sub> → 15SiO<sub>2</sub> + 4Mn<sub>5</sub>Si<sub>3</sub>

### 25.13 SILICON + $MnO_2$



**FIGURE 25.18** Adiabatic equilibrium temperature profile, Si (fuel) +  $MnO_2$  (oxidizer).



FIGURE 25.19 Adiabatic equilibrium gas production profile, Si (fuel) +  $MnO_2$  (oxidizer).

- **T1.** 5.7% fuel, 5.43% gas produced, 1606.24 K solids: 53.58%  $Mn_2O_3$  (bixbyite), 40.99%  $Mn_2SiO_4$  (tephroite) liquids: none gases: 5.43%  $O_2$ a combination of two reactions: (13.9% fuel) Si + 2MnO<sub>2</sub>  $\rightarrow$  Mn<sub>2</sub>SiO<sub>4</sub> (decomposition) 4MnO<sub>2</sub>  $\rightarrow$  2Mn<sub>2</sub>O<sub>3</sub> + O<sub>2</sub>
- **T2.** 7.1% fuel, 6.01% gas produced, 1898.53 K solids: 51.06% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite), 42.94% Mn<sub>3</sub>O<sub>4</sub> liquids: none gases: 6.00% O<sub>2</sub> a combination of two reactions: (13.9% fuel) Si + 2MnO<sub>2</sub> → Mn<sub>2</sub>SiO<sub>4</sub> (decomposition) 3MnO<sub>2</sub> → Mn<sub>3</sub>O<sub>4</sub> + O<sub>2</sub>
- **T3.** 10.9% fuel, 4.00% gas produced, 2646.04 K solids: 78.33%  $Mn_2SiO_4$  (tephroite) liquids: 17.67% MnO gases: 3.93%  $O_2$  a combination of two reactions: (13.9% fuel) Si + 2MnO<sub>2</sub>  $\rightarrow$  Mn<sub>2</sub>SiO<sub>4</sub> (decomposition) 2MnO<sub>2</sub>  $\rightarrow$  2MnO + O<sub>2</sub>

- **T4.** 12.0% fuel, 2.60% gas produced, 2792.14 K solids: 55.85% MnSiO<sub>3</sub> (rhodonite) liquids: 41.55% MnO gases: 2.47% O<sub>2</sub> a combination of two reactions: (13.9% fuel) Si + 2MnO<sub>2</sub>  $\rightarrow$  MnSiO<sub>3</sub> + MnO (decomposition) 2MnO<sub>2</sub>  $\rightarrow$  2MnO + O<sub>2</sub>
- T5. 13.9% fuel, 3044.64 K—peak temperature solids: none liquids: 70.25% MnO, 29.73% SiO<sub>2</sub> gases: none simplified equation at 13.9% fuel: Si + 2MnO<sub>2</sub> → SiO<sub>2</sub> + 2MnO
- **T6.** 21.2% fuel, 26.85% gas produced, 2230.98 K solids: 69.31% MnSiO<sub>3</sub> (rhodonite) liquids: 3.84% Mn gases: 16.89% Mn, 9.96% SiO a combination of two reactions: (17.7% fuel) 2Si + 3MnO<sub>2</sub> → 2MnSiO<sub>3</sub> + Mn (39.3% fuel) 2Si + MnO<sub>2</sub> → 2SiO + Mn
- **T7.** 37.5% fuel, 18.81% gas produced, 2144.16 K solids: 49.94%  $Mn_5Si_3$  liquids: 31.25% SiO<sub>2</sub> gases: 17.53% SiO, 1.28% Mn a combination of two reactions: (34.1% fuel) 8Si + 5MnO<sub>2</sub>  $\rightarrow$  5SiO<sub>2</sub> + Mn<sub>5</sub>Si<sub>3</sub> (45.6% fuel) 13Si + 5MnO<sub>2</sub>  $\rightarrow$  10SiO + Mn<sub>5</sub>Si<sub>3</sub>
- **T8.** 57.1% fuel, 2116.31 K solids: 40.97% MnSi liquids: 29.65% SiO<sub>2</sub>, 29.38% Si gases: none one reaction with excess fuel remaining: (39.3% fuel) 2Si + MnO<sub>2</sub>  $\rightarrow$  SiO<sub>2</sub> + MnSi
  - T6 corresponds to the maximum amount of Mn.
  - From 63.1% to 76.1% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
  - From 7.2% to 8.2% fuel, the temperature appears to be limited by the  $2Mn_3O_4(s) \rightarrow 6MnO(s) + O_2(g)$  decomposition, which occurs at 1925 K.
  - From 58.7% to 59.2% fuel, the temperature is limited to 1996 K by the  $SiO_2(s-1)$  transition.
  - From 8.8% to 9.3% fuel, the temperature is limited to 2115 K by the MnO(s-l) transition.
  - From 54.6% to 57.0% fuel, the temperature appears to be limited by the 5MnSi(s)  $\rightarrow$  Mn<sub>5</sub>Si<sub>3</sub>(s) + 2Si(l) decomposition, which occurs at 2119 K.
  - The plateau from 37.6% to 54.2% fuel (2138 K) could not be attributed to a simple transition or reaction; species in this region include SiO(g), Mn(g), SiO<sub>2</sub>(l), Si(l), and Mn<sub>5</sub>Si<sub>3</sub>(s). The vaporization of SiO from Si(l)/SiO<sub>2</sub>(l) mixtures is expected to occur at 2145 K.

- From 23.8% to 33.9% fuel, the temperature appears to be limited by the  $Mn_5Si_3(s) + 3SiO_2(1) \rightarrow 5Mn(g) + 6SiO(g)$  reaction, which occurs at 2227 K.
- From 21.3% to 22.1% fuel, the temperature appears to be limited by the  $2Mn_5Si_3(s) + 3MnSiO_3(s) \rightarrow 13Mn(l-g) + 9SiO(g)$  reaction, which occurs at 2231 K.
- From 11.0% to 11.6% and 17.3% to 18.1% fuel, the temperature appears to be limited by the Mn<sub>2</sub>SiO<sub>4</sub>(s) → MnSiO<sub>3</sub>(s) + MnO(l) decomposition, which occurs at 2665 K.
- From 12.1% to 13.2% and 14.9% to 16.3% fuel, the temperature appears to be limited by the MnSiO<sub>3</sub>(s) → MnO(l) + SiO<sub>2</sub>(l) decomposition, which occurs at 2818 K.

**G1.** 20.6% fuel, 28.17% gas produced, 2255.15 K—*peak gas* solids: 71.10% MnSiO<sub>3</sub> (rhodonite), 0.53% Mn<sub>2</sub>SiO<sub>4</sub> (tephroite) liquids: 0.20% Mn gases: 19.87% Mn, 8.30% SiO a combination of two reactions: (17.7% fuel) 2Si + 3MnO<sub>2</sub>  $\rightarrow$  2MnSiO<sub>3</sub> + Mn (39.3% fuel) 2Si + MnO<sub>2</sub>  $\rightarrow$  2SiO + Mn

## 25.14 SILICON + FeO



**FIGURE 25.20** Adiabatic equilibrium temperature profile, Si (fuel) + FeO (oxidizer).



**FIGURE 25.21** Adiabatic equilibrium gas production profile, Si (fuel) + FeO (oxidizer).

- **T1.** 8.9% fuel, 1810.95 K solids: 64.57%  $Fe_2SiO_4$  (fayalite), 23.15% Fe liquids: 12.25% Fe gases: none simplified equation at 8.9% fuel: Si + 4FeO  $\rightarrow$  Fe<sub>2</sub>SiO<sub>4</sub> + 2Fe
- **T2.** 16.3% fuel, 2480.66 K—*peak temperature* solids: none liquids: 64.82% Fe, 34.87% SiO<sub>2</sub>, 0.31% FeO gases: none simplified equation at 16.4% fuel: Si + 2FeO → SiO<sub>2</sub> + 2Fe
- **T3.** 38.1% fuel, 5.75% gas produced, 2280.81 K solids: 72.26% FeSi liquids: 21.99% SiO<sub>2</sub> gases: 5.72% SiO a combination of two reactions: (37.0% fuel)  $3Si + 2FeO \rightarrow SiO_2 + 2FeSi$  (43.9% fuel)  $2Si + FeO \rightarrow SiO + FeSi$
- **T4.** 43.9% fuel, 2.19% gas produced, 2144.85 K solids: 65.54% FeSi liquids: 21.97% SiO<sub>2</sub>, 10.31% Si gases: 2.19% SiO a combination of two reactions with excess fuel remaining: (37.0% fuel) 3Si + 2FeO → SiO<sub>2</sub> + 2FeSi (43.9% fuel) 2Si + FeO → SiO + FeSi

**T5.** 52.6% fuel, 1852.10 K

- solids: 41.07% FeSi, 20.69% Fe<sub>3</sub>Si<sub>7</sub>, 19.82% SiO<sub>2</sub> (cristobalite) liquids: 18.42% Si gases: none
- a combination of two reactions with excess fuel remaining: (37.0% fuel)  $3Si + 2FeO \rightarrow SiO_2 + 2FeSi$
- (52.6% fuel) 17Si + 6FeO  $\rightarrow$  3SiO<sub>2</sub> + 2Fe<sub>3</sub>Si<sub>7</sub>
- **T6.** 56.6% fuel, 1845.17 K
  - solids: 73.32%  $Fe_3Si_7$ , 18.15%  $SiO_2$  (cristobalite) liquids: 8.53% Si gases: none one reaction with excess fuel remaining: (52.6% fuel) 17Si + 6FeO  $\rightarrow$  3SiO<sub>2</sub> + 2Fe<sub>3</sub>Si<sub>7</sub>
- **T7.** 78.3% fuel, 1232.64 K solids: 57.09% Si, 33.83% FeSi<sub>2</sub>, 9.07% SiO<sub>2</sub> (tridymite) liquids: none gases: none one reaction with excess fuel remaining: (49.4% fuel) 5Si + 2FeO  $\rightarrow$  SiO<sub>2</sub> + 2FeSi<sub>2</sub>
- The maximum amount of iron, 64.98% Fe(1), occurs at 16.4% fuel and 2472.88 K.
- From 76.9% to 78.2% fuel, the temperature appears to be limited by the  $3\text{FeSi}_2(s) + \text{Si}(s) \rightarrow \text{Fe}_3\text{Si}_7(s)$  reaction, which occurs at 1233 K.
- From 58.7% to 64.9% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 8.8% to 9.4% fuel, the temperature is limited to 1811 K by the Fe(s-l) transition.
- From 51.1% to 56.5% fuel, the temperature appears to be limited by the Fe<sub>3</sub>Si<sub>7</sub>(s)  $\rightarrow$  3FeSi(s) + 4Si(l) decomposition, which occurs at 1852 K.
- From 10.7% to 12.1% fuel, the temperature appears to be limited by the  $Fe_2SiO_4(s) \rightarrow 2FeO(l) + SiO_2(s)$  decomposition, which occurs at 1933 K.
- From 38.5% to 46.1% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 17.1% to 38.0% fuel, the temperature appears to be limited by the  $FeSi(s) + SiO_2(l) \rightarrow Fe(l) + 2SiO(g)$  reaction, which occurs at 2290 K.
- G1. 38.5% fuel, 7.34% gas produced, 2144.85 K—peak gas solids: 71.84% FeSi liquids: 20.71% SiO<sub>2</sub> gases: 7.34% SiO a combination of two reactions: (37.0% fuel) 3Si + 2FeO → SiO<sub>2</sub> + 2FeSi (43.9% fuel) 2Si + FeO → SiO + FeSi

## 25.15 SILICON + $Fe_3O_4$



**FIGURE 25.22** Adiabatic equilibrium temperature profile, Si (fuel) +  $Fe_3O_4$  (oxidizer).

**FIGURE 25.23** Adiabatic equilibrium gas production profile, Si (fuel) +  $Fe_3O_4$  (oxidizer).

**T1.** 5.7% fuel, 1087.52 K solids: 58.32% FeO (wüstite), 41.36%  $\text{Fe}_2\text{SiO}_4$  (fayalite), 0.32%  $\text{Fe}_3\text{O}_4$  (magnetite) liquids: none gases: none

simplified equation at 5.7% fuel:  $Si + 2Fe_3O_4 \rightarrow Fe_2SiO_4 + 4FeO_3O_4$ 

- **T2.** 10.8% fuel, 1810.95 K solids: 78.36%  $Fe_2SiO_4$  (fayalite), 0.57% Fe liquids: 20.87% Fe, 0.21% FeO gases: none simplified equation at 10.8% fuel: Si +  $Fe_3O_4 \rightarrow Fe_2SiO_4 + Fe$
- T3. 19.5% fuel, 2644.32 K—peak temperature solids: none liquids: 58.13% Fe, 41.72% SiO<sub>2</sub>, 0.15% FeO gases: none simplified equation at 19.5% fuel: 2Si + Fe<sub>3</sub>O<sub>4</sub> → 2SiO<sub>2</sub> + 3Fe
- **T4.** 39.2% fuel, 7.38% gas produced, 2266.17 K solids: 66.07% FeSi liquids: 26.55% SiO<sub>2</sub> gases: 7.34% SiO a combination of two reactions: (37.8% fuel)  $5Si + Fe_3O_4 \rightarrow 2SiO_2 + 3FeSi$  (45.9% fuel)  $7Si + Fe_3O_4 \rightarrow 4SiO + 3FeSi$



- **T5.** 45.9% fuel, 2.51% gas produced, 2144.85 K solids: 58.83% FeSi liquids: 26.37% SiO<sub>2</sub>, 12.29% Si gases: 2.51% SiO a combination of two reactions with excess fuel remaining: (37.8% fuel) 5Si + Fe<sub>3</sub>O<sub>4</sub> → 2SiO<sub>2</sub> + 3FeSi (45.9% fuel) 7Si + Fe<sub>3</sub>O<sub>4</sub> → 4SiO + 3FeSi
- **T6.** 58.0% fuel, 1848.31 K solids: 66.05% Fe<sub>3</sub>Si<sub>7</sub>, 21.80% SiO<sub>2</sub> (cristobalite) liquids: 12.15% Si gases: none one reaction with excess fuel remaining: (52.2% fuel) 9Si + Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  2SiO<sub>2</sub> + Fe<sub>3</sub>Si<sub>7</sub>
- **T7.** 79.9% fuel, 1230.12 K solids: 60.40% Si, 29.17%  $\text{FeSi}_2$ , 10.43% SiO<sub>2</sub> (tridymite) liquids: none gases: none one reaction with excess fuel remaining: (49.2% fuel) 8Si + Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  2SiO<sub>2</sub> + 3FeSi<sub>2</sub>
- The maximum amount of iron, 58.15% Fe(1), occurs at 19.6% fuel and 2623.95 K.
- From 78.8% to 79.8% fuel, the temperature appears to be limited by the  $3\text{FeSi}_2(s) + \text{Si}(s) \rightarrow \text{Fe}_3\text{Si}_7(s)$  reaction, which occurs at 1233 K.
- From 60.1% to 67.5% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 53.3% to 57.9% fuel, the temperature appears to be limited by the  $Fe_3Si_7(s) \rightarrow 3FeSi(s) + 4Si(l)$  decomposition, which occurs at 1852 K.
- From 12.1% to 14.0% fuel, the temperature appears to be limited by the  $Fe_2SiO_4(s) \rightarrow 2FeO(l) + SiO_2(s)$  decomposition, which occurs at 1933 K.
- From 14.5% to 14.8% and 50.7% to 51.2% fuel, the temperature is limited to 1996 K by the  $SiO_2(s-l)$  transition.
- From 39.6% to 48.4% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 20.8% to 39.1% fuel, the temperature appears to be limited by the  $FeSi(s) + SiO_2(l) \rightarrow Fe(l) + 2SiO(g)$  reaction, which occurs at 2290 K.
- G1. 39.5% fuel, 8.81% gas produced, 2149.83 K—peak gas solids: 65.79% FeSi liquids: 25.40% SiO<sub>2</sub> gases: 8.81% SiO a combination of two reactions:
  (37.8% fuel) 5Si + Fe<sub>3</sub>O<sub>4</sub> → 2SiO<sub>2</sub> + 3FeSi (45.9% fuel) 7Si + Fe<sub>3</sub>O<sub>4</sub> → 4SiO + 3FeSi

## 25.16 SILICON + $Fe_2O_3$



**FIGURE 25.24** Adiabatic equilibrium temperature profile, Si (fuel) +  $Fe_2O_3$  (oxidizer).

**FIGURE 25.25** Adiabatic equilibrium gas production profile, Si (fuel) +  $Fe_2O_3$  (oxidizer).

T1. 8.1% fuel, 1521.76 K

solids: 58.77%  $\text{Fe}_2\text{SiO}_4$  (fayalite), 41.16% FeO (wüstite) liquids: none gases: none simplified equation at 8.1% fuel:  $\text{Si} + 2\text{Fe}_2\text{O}_3 \rightarrow \text{Fe}_2\text{SiO}_4 + 2\text{FeO}$ 

- **T2.** 11.4% fuel, 1920.47 K solids: 82.71%  $Fe_2SiO_4$  (fayalite) liquids: 14.35% Fe, 2.94% FeO gases: none a combination of two reactions: (8.1% fuel) Si + 2Fe\_2O\_3  $\rightarrow$  Fe\_2SiO<sub>4</sub> + 2FeO (11.7% fuel) 3Si + 4Fe\_2O\_3  $\rightarrow$  3Fe\_2SiO<sub>4</sub> + 2Fe
- T3. 20.9% fuel, 0.22% gas produced, 2812.05 K—peak temperature solids: none liquids: 55.20% Fe, 44.50% SiO<sub>2</sub> gases: 0.16% SiO simplified equation at 20.9% fuel: 3Si + 2Fe<sub>2</sub>O<sub>3</sub> → 3SiO<sub>2</sub> + 4Fe
- **T4.** 39.9% fuel, 9.22% gas produced, 2265.12 K solids: 63.12% FeSi liquids: 27.67% SiO<sub>2</sub> gases: 9.18% SiO a combination of two reactions: (38.1% fuel) 7Si + 2Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 4FeSi (46.8% fuel) 5Si + Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO + 2FeSi



- **T5.** 46.8% fuel, 3.86% gas produced, 2144.85 K solids: 55.92% FeSi liquids: 27.40% SiO<sub>2</sub>, 12.82% Si gases: 3.86% SiO a combination of two reactions with excess fuel remaining: (38.1% fuel) 7Si + 2Fe<sub>2</sub>O<sub>3</sub> → 3SiO<sub>2</sub> + 4FeSi (46.8% fuel) 5Si + Fe<sub>2</sub>O<sub>3</sub> → 3SiO + 2FeSi
- **T6.** 59.5% fuel, 1844.79 K solids: 61.57% Fe<sub>3</sub>Si<sub>7</sub>, 22.86% SiO<sub>2</sub> (cristobalite) liquids: 15.58% Si gases: none one reaction with excess fuel remaining: (52.0% fuel) 37Si + 6Fe<sub>2</sub>O<sub>3</sub> → 9SiO<sub>2</sub> + 4Fe<sub>3</sub>Si<sub>7</sub>
- **T7.** 81.2% fuel, 1231.95 K solids: 63.01% Si, 26.38% FeSi<sub>2</sub>, 10.61% SiO<sub>2</sub> (tridymite) liquids: none gases: none one reaction with excess fuel remaining: (49.2% fuel) 11Si + 2Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 4FeSi<sub>2</sub>
- T3 corresponds to the maximum amount of Fe.
- From 80.3% to 81.1% fuel, the temperature appears to be limited by the  $3\text{FeSi}_2(s) + \text{Si}(s) \rightarrow \text{Fe}_3\text{Si}_7(s)$  reaction, which occurs at 1233 K.
- From 9.0% to 9.6% fuel, the temperature is limited to 1644 K by the FeO(s-l) transition.
- From 61.5% to 69.7% fuel, the temperature is limited to 1685 K by the Si(s-l) transition.
- From 55.3% to 59.4% fuel, the temperature appears to be limited by the  $Fe_3Si_7(s) \rightarrow 3FeSi(s) + 4Si(l)$  decomposition, which occurs at 1852 K.
- From 11.5% to 13.9% fuel, the temperature appears to be limited by the  $Fe_2SiO_4(s) \rightarrow 2FeO(l) + SiO_2(s)$  decomposition, which occurs at 1933 K.
- From 52.7% to 53.2% fuel, the temperature is limited to 1996 K by the  $SiO_2(s-1)$  transition.
- From 40.3% to 50.5% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 22.7% to 39.8% fuel, the temperature appears to be limited by the  $FeSi(s) + SiO_2(l) \rightarrow Fe(l) + 2SiO(g)$  reaction, which occurs at 2290 K.

**G1.** 40.2% fuel, 10.64% gas produced, 2149.33 K—*peak gas* solids: 62.86% FeSi liquids: 26.50% SiO<sub>2</sub> gases: 10.64% SiO a combination of two reactions: (38.1% fuel) 7Si + 2Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO<sub>2</sub> + 4FeSi (46.8% fuel) 5Si + Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  3SiO + 2FeSi

## 25.17 SILICON + CoO



**FIGURE 25.26** Adiabatic equilibrium temperature profile, Si (fuel) + CoO (oxidizer).



**FIGURE 25.27** Adiabatic equilibrium gas production profile, Si (fuel) + CoO (oxidizer).

- **T1.** 8.6% fuel, 1991.29 K solids: 63.76%  $Co_2SiO_4$ , 0.15%  $SiO_2$  (cristobalite) liquids: 36.09% Co gases: none simplified equation at 8.6% fuel: Si + 4CoO  $\rightarrow$  Co<sub>2</sub>SiO<sub>4</sub> + 2Co
- T2. 15.8% fuel, 2861.89 K—peak temperature solids: none liquids: 66.20% Co, 33.71% SiO<sub>2</sub> gases: none simplified equation at 15.8% fuel: Si + 2CoO → SiO<sub>2</sub> + 2Co
- T3. 37.7% fuel, 8.50% gas produced, 2336.94 K solids: 72.29% CoSi liquids: 19.22% SiO<sub>2</sub> gases: 8.46% SiO a combination of two reactions: (36.0% fuel) 3Si + 2CoO → SiO<sub>2</sub> + 2CoSi (42.8% fuel) 2Si + CoO → SiO + CoSi
- **T4.** 42.8% fuel, 6.00% gas produced, 2144.86 K solids: 66.43% CoSi liquids: 18.84% SiO<sub>2</sub>, 8.73% Si gases: 6.00% SiO a combination of two reactions with excess fuel remaining: (36.0% fuel) 3Si + 2CoO → SiO<sub>2</sub> + 2CoSi (42.8% fuel) 2Si + CoO → SiO + CoSi

- T2 corresponds to the maximum amount of cobalt.
- From 55.6% to 68.7% fuel, the temperature is limited to 1685 K by the Si(s-1) transition.
- From 6.9% to 7.3% fuel, the temperature is limited to 1768 K by the Co(s-l) transition.
- From 50.9% to 51.3% fuel, the temperature is limited to 1996 K by the  $\rm SiO_2(s\text{-}l)$  transition.
- From 9.4% to 10.4% fuel, the temperature appears to be limited by the  $Co_2SiO_4(s) \rightarrow 2CoO(s) + SiO_2(l)$  decomposition, which occurs at 2096 K.
- From 10.6% to 11.5% fuel, the temperature is limited to 2103 K by the CoO(s-l) transition.
- From 38.2% to 48.7% fuel, the temperature appears to be limited by the vaporization of SiO from Si(1)/SiO<sub>2</sub>(1) mixtures, which occurs at 2145 K.
- From 17.4% to 37.6% fuel, the temperature appears to be limited by the  $CoSi(s) + SiO_2(l) \rightarrow Co(l) + 2SiO(g)$  reaction, which occurs at 2354 K.
- **G1.** 38.2% fuel, 10.62% gas produced, 2144.86 K—*peak gas* solids: 71.77% CoSi liquids: 17.55% SiO<sub>2</sub> gases: 10.61% SiO a combination of two reactions: (36.0% fuel)  $3Si + 2CoO \rightarrow SiO_2 + 2CoSi$  (42.8% fuel)  $2Si + CoO \rightarrow SiO + CoSi$