

CONCLUSIONS AND RECOMMENDATIONS

Based on the experimental results and theoretical analysis, the following conclusions are derived:

- HTSR-1, a catalyst proprietary to Haldor-Topsøe A/S, Copenhagen, Denmark, exhibited excellent activity for the decomposition of NH_3 in hot coal gas streams. The tolerance of this catalyst to H_2S increased with increasing temperatures.
- MoS_2 -based catalysts showed only a moderate activity for NH_3 decomposition. These catalysts required surface area stabilization.
- Many catalysts containing Ni, Co, Mo, and W on a high surface TiO_2 support showed only a moderate activity for NH_3 decomposition.
- Mixing the catalysts with a zinc titanate sorbent allowed the catalysts to function for an extended period of time. As the sorbent gets loaded with H_2S , the residual H_2S level increases thereby decreasing the activity of the catalyst for NH_3 decomposition.
- The titania support sinters excessively at a temperature of 725°C in the presence of steam. Adding ZrO_2 to the titania decrease the rate of sintering.

The following recommendations are made for further investigation into the removal of fuel-bound nitrogen from hot coal gas streams.

- The HTSR-1 should be tested using hot coal gas streams from an operating coal gasifier. The effects of trace components of the hot coal gas stream that could not be simulated in the laboratory must be determined.
- Alternative catalysts that have a high NH_3 decomposition activity at a temperature of about 550°C in the presence of H_2S must be developed.
- The regeneration of sulfur-poisoned HTSR-1 must be investigated. Although this catalyst can tolerate significant levels of H_2S at 800°C , it is slowly poisoned at low temperatures. Regeneration of the catalyst will allow continued use of this catalyst in a hot coal gas cleanup process.

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APPENDIX A

THERMODYNAMIC CALCULATIONS OF THE VAPORIZATION OF METAL OXIDES

TABLE 1.

CALCULATED PARTIAL PRESSURES OF SPECIES OVER MoO₃(c) AND SOME
MMoO₄(c) IN PRESENCE OF PURE O₂ AT 0.02 ATM TOTAL PRESSURE

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	MoO₃(c)				
Mo	1.21 x 10 ⁻⁸¹	1.23 x 10 ⁻⁶⁸	1.53 x 10 ⁻⁵⁸	1.84 x 10 ⁻⁵⁰	6.11 x 10 ⁻⁴⁴
MoO	4.76 x 10 ⁻⁶²	7.35 x 10 ⁻⁵²	5.89 x 10 ⁻⁴⁴	1.21 x 10 ⁻³⁷	1.34 x 10 ⁻³²
MoO ₂	5.48 x 10 ⁻³⁹	2.76 x 10 ⁻³²	4.30 x 10 ⁻²⁷	5.97 x 10 ⁻²³	9.86 x 10 ⁻²⁰
MoO ₃	5.93 x 10 ⁻¹⁹	1.76 x 10 ⁻¹⁵	8.52 x 10 ⁻¹³	1.16 x 10 ⁻¹⁰	3.98 x 10 ⁻⁹
Mo ₂ O ₆	3.01 x 10 ⁻¹⁴	3.63 x 10 ⁻¹¹	8.59 x 10 ⁻⁹	6.52 x 10 ⁻⁷	8.76 x 10 ⁻⁶
Mo ₃ O ₉	2.20 x 10 ⁻¹¹	2.19 x 10 ⁻⁸	4.42 x 10 ⁻⁶	2.92 x 10 ⁻⁴	2.20 x 10 ⁻³
Mo ₄ O ₁₂	9.37 x 10 ⁻¹²	1.45 x 10 ⁻⁸	4.07 x 10 ⁻⁶	3.46 x 10 ⁻⁴	2.02 x 10 ⁻³
Mo ₅ O ₁₅	1.10 x 10 ⁻¹³	4.04 x 10 ⁻¹⁰	2.20 x 10 ⁻⁷	3.13 x 10 ⁻⁵	1.76 x 10 ⁻⁴
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.54 x 10 ⁻¹³	2.17 x 10 ⁻¹¹	3.09 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	1.93 x 10 ⁻²	1.56 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.44 x 10 ⁻¹⁵	2.34 x 10 ⁻¹⁴	7.81 x 10 ⁻¹⁴
Σ P(Mo) (atm)	3.15 x 10⁻¹¹	3.68 x 10⁻⁸	8.72 x 10⁻⁶	6.70 x 10⁻⁴	4.41 x 10⁻³
Mo(2896 ^a)	0	0	0	0	0
MoO ₂ (c)	0	0	0	0	0
MoO ₃ (1075)	1 ^b	1	1	1	0
Mo ₄ O ₁₁ (c)	0	0	0	0	0
Mo ₈ O ₂₃ (c)	0	0	0	0	0
Mo ₉ O ₂₆ (c)	0	0	0	0	0

TABLE 1. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	CuMoO₄(c)				
Cu	5.02×10^{-25}	1.77×10^{-20}	5.96×10^{-17}	3.86×10^{-14}	7.68×10^{-12}
CuO	2.38×10^{-25}	4.33×10^{-21}	8.70×10^{-18}	3.73×10^{-15}	5.21×10^{-13}
Mo	4.49×10^{-83}	5.71×10^{-70}	8.44×10^{-60}	1.10×10^{-51}	4.61×10^{-45}
MoO	1.76×10^{-63}	3.41×10^{-53}	3.24×10^{-45}	7.38×10^{-39}	1.15×10^{-33}
MoO ₂	2.03×10^{-40}	1.28×10^{-33}	2.37×10^{-28}	3.70×10^{-24}	9.55×10^{-21}
MoO ₃	2.19×10^{-20}	8.18×10^{-17}	4.69×10^{-14}	7.29×10^{-12}	4.36×10^{-10}
Mo ₂ O ₆	4.11×10^{-17}	7.82×10^{-14}	2.61×10^{-11}	2.59×10^{-9}	1.05×10^{-7}
Mo ₃ O ₉	1.11×10^{-15}	2.19×10^{-12}	7.40×10^{-10}	7.30×10^{-8}	2.90×10^{-6}
Mo ₄ O ₁₂	1.75×10^{-17}	6.72×10^{-14}	3.75×10^{-11}	5.44×10^{-9}	2.92×10^{-7}
Mo ₅ O ₁₅	7.63×10^{-21}	8.72×10^{-17}	1.12×10^{-13}	3.11×10^{-11}	2.78×10^{-9}
O	5.02×10^{-17}	1.12×10^{-14}	7.54×10^{-13}	2.20×10^{-11}	3.50×10^{-10}
O ₂	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}
O ₃	1.45×10^{-17}	3.14×10^{-16}	3.45×10^{-15}	2.46×10^{-14}	1.14×10^{-13}
$\Sigma P(\text{Mo})$ (atm)	1.17×10^{-15}	2.34×10^{-12}	8.04×10^{-10}	8.10×10^{-8}	3.30×10^{-6}
Cu(1358)	0	0	0	0	0
CuO(c)	0	0	0	0	0
Cu ₂ O(1517)	0	0	0	0	0
CuMoO ₄ (c)	1	1	1	1	1
Mo(2896)	0	0	0	0	0
MoO ₂ (c)	0	0	0	0	0
MoO ₃ (1075)	0	0	0	0	0
Mo ₄ O ₁₁ (c)	0	0	0	0	0
Mo ₈ O ₂₃ (c)	0	0	0	0	0
Mo ₉ O ₂₆ (c)	0	0	0	0	0

TABLE 1. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	FeMoO₄(c)				
Fe	2.95 x 10 ⁻⁴⁶	1.32 x 10 ⁻³⁸	1.12 x 10 ⁻³²	6.04 x 10 ⁻²⁸	5.28 x 10 ⁻²⁴
FeO	7.94 x 10 ⁻³⁸	1.15 x 10 ⁻³¹	6.74 x 10 ⁻²⁷	4.21 x 10 ⁻²³	5.51 x 10 ⁻²⁰
FeO ₂	3.61 x 10 ⁻²⁸	6.86 x 10 ⁻²⁴	1.39 x 10 ⁻²⁰	5.83 x 10 ⁻¹⁸	7.44 x 10 ⁻¹⁶
Mo	1.21 x 10 ⁻⁸¹	1.23 x 10 ⁻⁶⁸	1.53 x 10 ⁻⁵⁸	1.84 x 10 ⁻⁵⁰	7.20 x 10 ⁻⁴⁴
MoO	4.76 x 10 ⁻⁶²	7.35 x 10 ⁻⁵²	5.89 x 10 ⁻⁴⁴	1.21 x 10 ⁻³⁷	1.53 x 10 ⁻³²
MoO ₂	5.48 x 10 ⁻³⁹	2.76 x 10 ⁻³²	4.30 x 10 ⁻²⁷	5.97 x 10 ⁻²³	1.08 x 10 ⁻¹⁹
MoO ₃	5.93 x 10 ⁻¹⁹	1.76 x 10 ⁻¹⁵	8.51 x 10 ⁻¹³	1.16 x 10 ⁻¹⁰	4.23 x 10 ⁻⁹
Mo ₂ O ₆	3.01 x 10 ⁻¹⁴	3.63 x 10 ⁻¹¹	8.59 x 10 ⁻⁹	6.52 x 10 ⁻⁷	9.88 x 10 ⁻⁶
Mo ₃ O ₉	2.20 x 10 ⁻¹¹	2.19 x 10 ⁻⁸	4.42 x 10 ⁻⁶	2.92 x 10 ⁻⁴	2.64 x 10 ⁻³
Mo ₄ O ₁₂	9.37 x 10 ⁻¹²	1.45 x 10 ⁻⁸	4.07 x 10 ⁻⁶	3.46 x 10 ⁻⁴	2.57 x 10 ⁻³
Mo ₅ O ₁₅	1.10 x 10 ⁻¹³	4.04 x 10 ⁻¹⁰	2.20 x 10 ⁻⁷	3.13 x 10 ⁻⁵	2.37 x 10 ⁻⁴
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.54 x 10 ⁻¹³	2.17 x 10 ⁻¹¹	2.98 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	1.93 x 10 ⁻²	1.45 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.44 x 10 ⁻¹⁵	2.34 x 10 ⁻¹⁴	7.04 x 10 ⁻¹⁴
$\Sigma P(\text{Mo})$ (atm)	3.15 x 10 ⁻¹¹	3.68 x 10 ⁻⁸	8.72 x 10 ⁻⁶	6.70 x 10 ⁻⁴	5.45 x 10 ⁻³
Fe(1809)	0	0	0	0	0
FeO(1650)	0	0	0	0	0
Fe ₂ O ₃ (c)	1	1	1	1	1
Fe ₃ O ₄ (c)	0	0	0	0	0
FeMoO ₄ (c)	0	0	0	0	0
Mo(2896)	0	0	0	0	0
MoO ₂ (c)	0	0	0	0	0
MoO ₃ (1075)	1	1	1	1	0
Mo ₄ O ₁₁ (c)	0	0	0	0	0
Mo ₈ O ₂₃ (c)	0	0	0	0	0
Mo ₉ O ₂₆ (c)	0	0	0	0	0

TABLE 1. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	NiMoO₄(c)				
Mo	7.26×10^{-83}	8.62×10^{-69}	1.53×10^{-58}	1.84×10^{-50}	6.11×10^{-44}
MoO	2.85×10^{-63}	5.15×10^{-52}	5.89×10^{-44}	1.21×10^{-37}	1.34×10^{-32}
MoO ₂	3.28×10^{-40}	1.94×10^{-32}	4.30×10^{-27}	5.97×10^{-23}	9.86×10^{-20}
MoO ₃	3.55×10^{-20}	1.23×10^{-15}	8.51×10^{-13}	1.16×10^{-10}	3.98×10^{-9}
Mo ₂ O ₆	1.08×10^{-16}	1.78×10^{-11}	8.59×10^{-9}	6.52×10^{-7}	8.76×10^{-6}
Mo ₃ O ₉	4.72×10^{-15}	7.53×10^{-9}	4.42×10^{-6}	2.92×10^{-4}	2.20×10^{-3}
Mo ₄ O ₁₂	1.20×10^{-16}	3.49×10^{-9}	4.07×10^{-6}	3.46×10^{-4}	2.02×10^{-3}
Mo ₅ O ₁₅	8.47×10^{-20}	6.82×10^{-11}	2.20×10^{-7}	3.13×10^{-5}	1.76×10^{-4}
Ni	3.61×10^{-37}	5.60×10^{-31}	3.55×10^{-26}	2.49×10^{-22}	3.79×10^{-19}
NiO	2.45×10^{-31}	2.80×10^{-26}	2.33×10^{-22}	3.18×10^{-19}	1.14×10^{-16}
O	5.02×10^{-17}	1.12×10^{-14}	7.54×10^{-13}	2.17×10^{-11}	3.09×10^{-10}
O ₂	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	1.93×10^{-2}	1.56×10^{-2}
O ₃	1.45×10^{-17}	3.14×10^{-16}	3.44×10^{-15}	2.34×10^{-14}	7.82×10^{-14}
$\Sigma P(\text{Mo})$ (atm)	4.94×10^{-15}	1.11×10^{-8}	8.72×10^{-6}	6.70×10^{-4}	4.41×10^{-3}
Ni(1728)	0	0	0	0	0
NiO(c)	0	0	1	1	1
NiMoO ₄ (c)	1	1	0	0	0
Mo(2896)	0	0	0	0	0
MoO ₂ (c)	0	0	0	0	0
MoO ₃ (1075)	0	0	1	1	0
Mo ₄ O ₁₁ (c)	0	0	0	0	0
Mo ₈ O ₂₃ (c)	0	0	0	0	0
Mo ₉ O ₂₆ (c)	0	0	0	0	0

TABLE 1. (Concluded)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	CoMoO₄(c)				
Co	1.38 x 10 ⁻³⁹	8.43 x 10 ⁻³³	1.57 x 10 ⁻²⁷	2.57 x 10 ⁻²³	8.24 x 10 ⁻²⁰
CoO	4.47 x 10 ⁻³³	1.45 x 10 ⁻²⁷	2.71 x 10 ⁻²³	6.91 x 10 ⁻²⁰	4.27 x 10 ⁻¹⁷
Mo	1.21 x 10 ⁻⁸¹	1.23 x 10 ⁻⁶⁸	1.53 x 10 ⁻⁵⁸	1.84 x 10 ⁻⁵⁰	6.77 x 10 ⁻⁴⁴
MoO	4.76 x 10 ⁻⁶²	7.35 x 10 ⁻⁵²	5.89 x 10 ⁻⁴⁴	1.21 x 10 ⁻³⁷	1.45 x 10 ⁻³²
MoO ₂	5.48 x 10 ⁻³⁹	2.76 x 10 ⁻³²	4.30 x 10 ⁻²⁷	5.97 x 10 ⁻²³	1.05 x 10 ⁻¹⁹
MoO ₃	5.93 x 10 ⁻¹⁹	1.76 x 10 ⁻¹⁵	8.51 x 10 ⁻¹³	1.16 x 10 ⁻¹⁰	4.14 x 10 ⁻⁹
Mo ₂ O ₆	3.01 x 10 ⁻¹⁴	3.63 x 10 ⁻¹¹	8.59 x 10 ⁻⁹	6.52 x 10 ⁻⁷	9.46 x 10 ⁻⁶
Mo ₃ O ₉	2.20 x 10 ⁻¹¹	2.19 x 10 ⁻⁸	4.42 x 10 ⁻⁶	2.92 x 10 ⁻⁴	2.47 x 10 ⁻³
Mo ₄ O ₁₂	9.37 x 10 ⁻¹²	1.45 x 10 ⁻⁸	4.07 x 10 ⁻⁶	3.46 x 10 ⁻⁴	2.36 x 10 ⁻³
Mo ₅ O ₁₅	1.10 x 10 ⁻¹³	4.04 x 10 ⁻¹⁰	2.20 x 10 ⁻⁷	3.13 x 10 ⁻⁵	2.13 x 10 ⁻⁴
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.54 x 10 ⁻¹³	2.17 x 10 ⁻¹¹	3.03 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	1.93 x 10 ⁻²	1.49 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.44 x 10 ⁻¹⁵	2.34 x 10 ⁻¹⁴	7.34 x 10 ⁻¹⁴
$\Sigma P(\text{Mo})$ (atm)	3.15 x 10 ⁻¹¹	3.68 x 10 ⁻⁸	8.72 x 10 ⁻⁶	6.70 x 10 ⁻⁴	5.05 x 10 ⁻³
Co(1768)	0	0	0	0	0
CoO(c)	0	0	0	0	0
Co ₃ O ₄ (c)	1	1	1	1	1
CoMoO ₄ (c)	0	0	0	0	0
Mo(2896)	0	0	0	0	0
MoO ₂ (c)	0	0	0	0	0
MoO ₃ (1075)	1	1	1	1	0
Mo ₄ O ₁₁ (c)	0	0	0	0	0
Mo ₈ O ₂₃ (c)	0	0	0	0	0
Mo ₉ O ₂₆ (c)	0	0	0	0	0

a: Melting point.

b: Mole fraction of condensed phase.

TABLE 2.

TOTAL MO-CONTAINING SPECIES PRESSURE OVER $\text{MoO}_3(\text{c})$ AND SOME
 $\text{MMoO}_4(\text{c})$ IN PRESENCE OF PURE O_2 AT 0.02 ATM TOTAL PRESSURE

Oxide	Total Mo-containing Species Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
$\text{MoO}_3(\text{c})$	3.15×10^{-11}	3.68×10^{-8}	8.72×10^{-6}	6.70×10^{-4}	4.41×10^{-3}
$\text{CuMoO}_4(\text{c})$	1.17×10^{-15}	2.34×10^{-12}	8.04×10^{-10}	8.10×10^{-8}	3.30×10^{-6}
$\text{FeMoO}_4(\text{c})$	3.15×10^{-11}	3.68×10^{-8}	8.72×10^{-6}	6.70×10^{-4}	5.45×10^{-3}
$\text{NiMoO}_4(\text{c})$	4.94×10^{-15}	1.11×10^{-8}	8.72×10^{-6}	6.70×10^{-4}	4.41×10^{-3}
$\text{CoMoO}_4(\text{c})$	3.15×10^{-11}	3.68×10^{-8}	8.72×10^{-6}	6.70×10^{-4}	5.05×10^{-3}

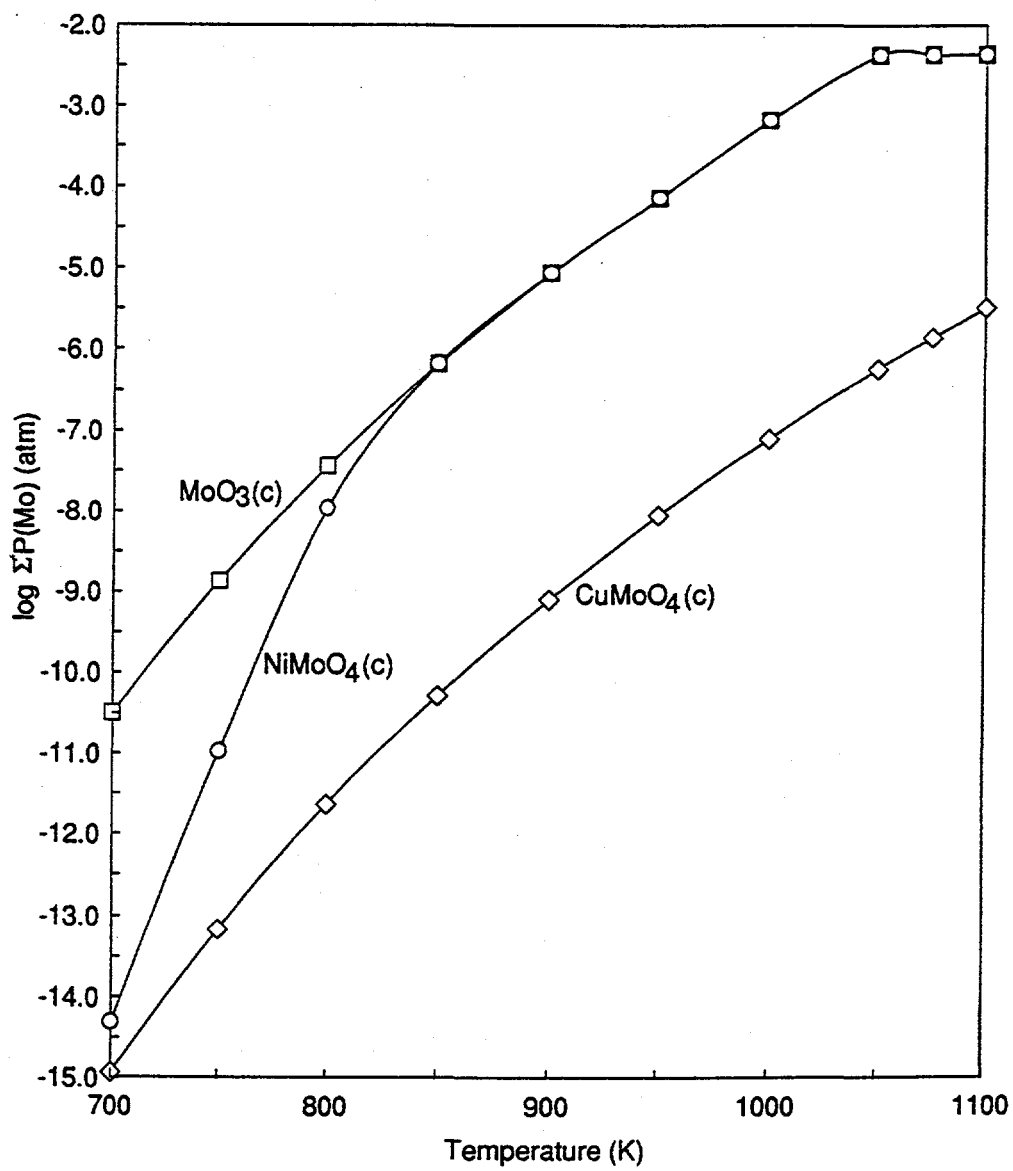


Figure 1. Plot of total Mo-containing species pressure vs temperature over MoO₃(c) and NiMoO₄(c) in presence of pure O₂ at 0.02 atm total pressure.

TABLE 3.

CALCULATED PARTIAL PRESSURES OF SPECIES OVER $\text{WO}_3(\text{c})$ AND SOME $\text{MWO}_4(\text{c})$ IN PRESENCE OF PURE O_2 AT 0.02 ATM TOTAL PRESSURE

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	$\text{WO}_3(\text{c})$				
W	8.79×10^{-104}	4.71×10^{-88}	7.95×10^{-76}	4.73×10^{-66}	4.61×10^{-58}
WO	6.85×10^{-73}	2.15×10^{-61}	1.79×10^{-52}	2.34×10^{-45}	1.49×10^{-39}
WO_2	7.07×10^{-50}	7.43×10^{-42}	1.23×10^{-35}	1.12×10^{-30}	1.22×10^{-26}
WO_3	1.98×10^{-29}	1.22×10^{-24}	6.28×10^{-21}	5.65×10^{-18}	1.42×10^{-15}
W_2O_6	3.55×10^{-24}	7.29×10^{-20}	1.57×10^{-16}	6.98×10^{-14}	9.72×10^{-12}
W_3O_8	2.01×10^{-42}	6.75×10^{-35}	4.56×10^{-29}	1.98×10^{-24}	1.15×10^{-20}
W_3O_9	6.80×10^{-25}	3.15×10^{-20}	1.26×10^{-16}	9.14×10^{-14}	1.86×10^{-11}
W_4O_{12}	9.90×10^{-27}	9.86×10^{-22}	7.12×10^{-18}	8.13×10^{-15}	2.37×10^{-12}
W_5O_{15}	7.26×10^{-34}	7.05×10^{-28}	2.97×10^{-23}	1.37×10^{-19}	1.23×10^{-16}
O	5.02×10^{-17}	1.12×10^{-14}	7.55×10^{-13}	2.20×10^{-11}	3.50×10^{-10}
O_2	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}	2.00×10^{-2}
O_3	1.45×10^{-17}	3.14×10^{-16}	3.45×10^{-15}	2.46×10^{-14}	1.14×10^{-13}
$\Sigma P(\text{W})$ (atm)	4.24×10^{-24}	1.05×10^{-19}	2.91×10^{-16}	1.69×10^{-13}	3.07×10^{-11}
W(3695a)	0	0	0	0	0
$\text{WO}_2(\text{c})$	0	0	0	0	0
$\text{WO}_3(1747)$	1b	1	1	1	1
$\text{W}_{18}\text{O}_{49}(\text{c})$	0	0	0	0	0
$\text{W}_{20}\text{O}_{58}(\text{c})$	0	0	0	0	0
$\text{W}_{25}\text{O}_{74}(\text{c})$	0	0	0	0	0

TABLE 3. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
			CoWO₄(c)		
Co	1.37 x 10 ⁻³⁹	8.26 x 10 ⁻³³	1.47 x 10 ⁻²⁷	2.14 x 10 ⁻²³	4.73 x 10 ⁻²⁰
CoO	4.44 x 10 ⁻³³	1.42 x 10 ⁻²⁷	2.55 x 10 ⁻²³	5.84 x 10 ⁻²⁰	2.83 x 10 ⁻¹⁷
W	3.75 x 10 ⁻¹⁰⁶	1.63 x 10 ⁻⁹⁰	2.40 x 10 ⁻⁷⁸	1.38 x 10 ⁻⁶⁸	1.46 x 10 ⁻⁶⁰
WO	2.92 x 10 ⁻⁷⁵	7.41 x 10 ⁻⁶⁴	5.41 x 10 ⁻⁵⁵	6.82 x 10 ⁻⁴⁸	4.71 x 10 ⁻⁴²
WO ₂	3.02 x 10 ⁻⁵²	2.56 x 10 ⁻⁴⁴	3.72 x 10 ⁻³⁸	3.25 x 10 ⁻³³	3.85 x 10 ⁻²⁹
WO ₃	8.46 x 10 ⁻³²	4.23 x 10 ⁻²⁷	1.90 x 10 ⁻²³	1.65 x 10 ⁻²⁰	4.50 x 10 ⁻¹⁸
W ₂ O ₆	6.46 x 10 ⁻²⁹	8.68 x 10 ⁻²⁵	1.44 x 10 ⁻²¹	5.94 x 10 ⁻¹⁹	9.73 x 10 ⁻¹⁷
W ₃ O ₈	1.56 x 10 ⁻⁴⁹	2.78 x 10 ⁻⁴²	1.26 x 10 ⁻³⁶	4.92 x 10 ⁻³²	3.65 x 10 ⁻²⁸
W ₃ O ₉	5.28 x 10 ⁻³²	1.29 x 10 ⁻²⁷	3.50 x 10 ⁻²⁴	2.27 x 10 ⁻²¹	5.90 x 10 ⁻¹⁹
W ₄ O ₁₂	3.28 x 10 ⁻³⁶	1.40 x 10 ⁻³¹	5.96 x 10 ⁻²⁸	5.88 x 10 ⁻²⁵	2.37 x 10 ⁻²²
W ₅ O ₁₅	1.02 x 10 ⁻⁴⁵	3.45 x 10 ⁻⁴⁰	7.51 x 10 ⁻³⁶	2.89 x 10 ⁻³²	3.90 x 10 ⁻²⁹
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.55 x 10 ⁻¹³	2.20 x 10 ⁻¹¹	3.50 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.45 x 10 ⁻¹⁵	2.46 x 10 ⁻¹⁴	1.14 x 10 ⁻¹³
Σ P(W) (atm)	6.47 x 10⁻²⁹	8.74 x 10⁻²⁵	1.46 x 10⁻²¹	6.13 x 10⁻¹⁹	1.02 x 10⁻¹⁶
Co(1768)	0	0	0	0	0
CoO(c)	0	0	0	0	0
Co ₃ O ₄ (c)	0	0	0	0	0
CoWO ₄ (c)	1	1	1	1	1
W(3695)	0	0	0	0	0
WO ₂ (c)	0	0	0	0	0
WO ₃ (1747)	0	0	0	0	0
W ₁₈ O ₄₉ (c)	0	0	0	0	0
W ₂₀ O ₅₈ (c)	0	0	0	0	0
W ₂₅ O ₇₄ (c)	0	0	0	0	0

TABLE 3. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	CuWO₄(c)				
Cu	5.01 x 10 ⁻²⁵	1.77 x 10 ⁻²⁰	5.96 x 10 ⁻¹⁷	3.86 x 10 ⁻¹⁴	7.68 x 10 ⁻¹²
CuO	2.38 x 10 ⁻²⁵	4.33 x 10 ⁻²¹	8.70 x 10 ⁻¹⁸	3.73 x 10 ⁻¹⁵	5.21 x 10 ⁻¹³
W	8.79 x 10 ⁻¹⁰⁴	4.71 x 10 ⁻⁸⁸	7.95 x 10 ⁻⁷⁶	4.73 x 10 ⁻⁶⁶	4.61 x 10 ⁻⁵⁸
WO	6.85 x 10 ⁻⁷³	2.15 x 10 ⁻⁶¹	1.79 x 10 ⁻⁵²	2.34 x 10 ⁻⁴⁵	1.49 x 10 ⁻³⁹
WO ₂	7.07 x 10 ⁻⁵⁰	7.43 x 10 ⁻⁴²	1.23 x 10 ⁻³⁵	1.12 x 10 ⁻³⁰	1.22 x 10 ⁻²⁶
WO ₃	1.98 x 10 ⁻²⁹	1.22 x 10 ⁻²⁴	6.28 x 10 ⁻²¹	5.65 x 10 ⁻¹⁸	1.42 x 10 ⁻¹⁵
W ₂ O ₆	3.55 x 10 ⁻²⁴	7.29 x 10 ⁻²⁰	1.57 x 10 ⁻¹⁶	6.98 x 10 ⁻¹⁴	9.72 x 10 ⁻¹²
W ₃ O ₈	2.01 x 10 ⁻⁴²	6.75 x 10 ⁻³⁵	4.56 x 10 ⁻²⁹	1.98 x 10 ⁻²⁴	1.15 x 10 ⁻²⁰
W ₃ O ₉	6.80 x 10 ⁻²⁵	3.15 x 10 ⁻²⁰	1.26 x 10 ⁻¹⁶	9.14 x 10 ⁻¹⁴	1.86 x 10 ⁻¹¹
W ₄ O ₁₂	9.90 x 10 ⁻²⁷	9.86 x 10 ⁻²²	7.12 x 10 ⁻¹⁸	8.13 x 10 ⁻¹⁵	2.37 x 10 ⁻¹²
W ₅ O ₁₅	7.26 x 10 ⁻³⁴	7.05 x 10 ⁻²⁸	2.97 x 10 ⁻²³	1.37 x 10 ⁻¹⁹	1.23 x 10 ⁻¹⁶
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.55 x 10 ⁻¹³	2.20 x 10 ⁻¹¹	3.50 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.45 x 10 ⁻¹⁵	2.46 x 10 ⁻¹⁴	1.14 x 10 ⁻¹³
Σ P(W) (atm)	4.24 x 10⁻²⁴	1.05 x 10⁻¹⁹	2.91 x 10⁻¹⁶	1.69 x 10⁻¹³	3.07 x 10⁻¹¹
Cu(1358)	0	0	0	0	0
CuO(c)	1	1	1	1	1
Cu ₂ O(1517)	0	0	0	0	0
CuWO ₄ (c)	0	0	0	0	0
W(3695)	0	0	0	0	0
WO ₂ (c)	0	0	0	0	0
WO ₃ (1747)	1	1	1	1	1
W ₁₈ O ₄₉ (c)	0	0	0	0	0
W ₂₀ O ₅₈ (c)	0	0	0	0	0
W ₂₅ O ₇₄ (c)	0	0	0	0	0

TABLE 3. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
			FeWO₄(c)		
Fe	2.95 x 10 ⁻⁴⁶	1.32 x 10 ⁻³⁸	1.12 x 10 ⁻³²	5.89 x 10 ⁻²⁸	4.16 x 10 ⁻²⁴
FeO	7.94 x 10 ⁻³⁸	1.15 x 10 ⁻³¹	6.74 x 10 ⁻²⁷	4.17 x 10 ⁻²³	5.09 x 10 ⁻²⁰
FeO ₂	3.61 x 10 ⁻²⁸	6.86 x 10 ⁻²⁴	1.39 x 10 ⁻²⁰	5.88 x 10 ⁻¹⁸	8.05 x 10 ⁻¹⁶
W	8.79 x 10 ⁻¹⁰⁴	4.71 x 10 ⁻⁸⁸	7.95 x 10 ⁻⁷⁶	4.73 x 10 ⁻⁶⁶	4.61 x 10 ⁻⁵⁸
WO	6.85 x 10 ⁻⁷³	2.15 x 10 ⁻⁶¹	1.79 x 10 ⁻⁵²	2.34 x 10 ⁻⁴⁵	1.49 x 10 ⁻³⁹
WO ₂	7.07 x 10 ⁻⁵⁰	7.43 x 10 ⁻⁴²	1.23 x 10 ⁻³⁵	1.12 x 10 ⁻³⁰	1.22 x 10 ⁻²⁶
WO ₃	1.98 x 10 ⁻²⁹	1.22 x 10 ⁻²⁴	6.28 x 10 ⁻²¹	5.65 x 10 ⁻¹⁸	1.42 x 10 ⁻¹⁵
W ₂ O ₆	3.55 x 10 ⁻²⁴	7.29 x 10 ⁻²⁰	1.57 x 10 ⁻¹⁶	6.98 x 10 ⁻¹⁴	9.72 x 10 ⁻¹²
W ₃ O ₈	2.01 x 10 ⁻⁴²	6.75 x 10 ⁻³⁵	4.56 x 10 ⁻²⁹	1.98 x 10 ⁻²⁴	1.15 x 10 ⁻²⁰
W ₃ O ₉	6.80 x 10 ⁻²⁵	3.15 x 10 ⁻²⁰	1.26 x 10 ⁻¹⁶	9.14 x 10 ⁻¹⁴	1.86 x 10 ⁻¹¹
W ₄ O ₁₂	9.90 x 10 ⁻²⁷	9.86 x 10 ⁻²²	7.12 x 10 ⁻¹⁸	8.13 x 10 ⁻¹⁵	2.37 x 10 ⁻¹²
W ₅ O ₁₅	7.26 x 10 ⁻³⁴	7.05 x 10 ⁻²⁸	2.97 x 10 ⁻²³	1.37 x 10 ⁻¹⁹	1.23 x 10 ⁻¹⁶
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.55 x 10 ⁻¹³	2.20 x 10 ⁻¹¹	3.50 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.45 x 10 ⁻¹⁵	2.46 x 10 ⁻¹⁴	1.14 x 10 ⁻¹³
Σ P(W) (atm)	4.24 x 10 ⁻²⁴	1.05 x 10 ⁻¹⁹	2.91 x 10 ⁻¹⁶	1.69 x 10 ⁻¹³	3.07 x 10 ⁻¹¹
Fe(1809)	0	0	0	0	0
FeO(1650)	0	0	0	0	0
Fe ₂ O ₃ (c)	1	1	1	1	1
Fe ₃ O ₄ (c)	0	0	0	0	0
FeWO ₄ (c)	0	0	0	0	0
W(3695)	0	0	0	0	0
WO ₂ (c)	0	0	0	0	0
WO ₃ (1747)	1	1	1	1	1
W ₁₈ O ₄₉ (c)	0	0	0	0	0
W ₂₀ O ₅₈ (c)	0	0	0	0	0
W ₂₅ O ₇₄ (c)	0	0	0	0	0

TABLE 3. (Continued)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	NiWO₄(c)				
Ni	3.61 x 10 ⁻³⁷	5.59 x 10 ⁻³¹	3.54 x 10 ⁻²⁶	2.44 x 10 ⁻²²	3.32 x 10 ⁻¹⁹
NiO	2.45 x 10 ⁻³¹	2.80 x 10 ⁻²⁶	2.32 x 10 ⁻²²	3.16 x 10 ⁻¹⁹	1.13 x 10 ⁻¹⁶
W	2.26 x 10 ⁻¹⁰⁸	3.73 x 10 ⁻⁹¹	1.57 x 10 ⁻⁷⁸	1.97 x 10 ⁻⁶⁸	3.65 x 10 ⁻⁶⁰
WO	1.76 x 10 ⁻⁷⁶	1.70 x 10 ⁻⁶⁴	3.53 x 10 ⁻⁵⁵	9.77 x 10 ⁻⁴⁸	1.18 x 10 ⁻⁴¹
WO ₂	1.82 x 10 ⁻⁵³	5.88 x 10 ⁻⁴⁵	2.43 x 10 ⁻³⁸	4.66 x 10 ⁻³³	9.63 x 10 ⁻²⁹
WO ₃	5.09 x 10 ⁻³³	9.69 x 10 ⁻²⁸	1.24 x 10 ⁻²³	2.36 x 10 ⁻²⁰	1.13 x 10 ⁻¹⁷
W ₂ O ₆	2.34 x 10 ⁻³¹	4.57 x 10 ⁻²⁶	6.15 x 10 ⁻²²	1.22 x 10 ⁻¹⁸	6.08 x 10 ⁻¹⁶
W ₃ O ₈	3.41 x 10 ⁻⁵³	3.35 x 10 ⁻⁴⁴	3.52 x 10 ⁻³⁷	1.44 x 10 ⁻³¹	5.70 x 10 ⁻²⁷
W ₃ O ₉	1.15 x 10 ⁻³⁵	1.56 x 10 ⁻²⁹	9.77 x 10 ⁻²⁵	6.64 x 10 ⁻²¹	9.22 x 10 ⁻¹⁸
W ₄ O ₁₂	4.30 x 10 ⁻⁴¹	3.87 x 10 ⁻³⁴	1.09 x 10 ⁻²⁸	2.47 x 10 ⁻²⁴	9.28 x 10 ⁻²¹
W ₅ O ₁₅	8.09 x 10 ⁻⁵²	2.19 x 10 ⁻⁴³	8.95 x 10 ⁻³⁷	1.73 x 10 ⁻³¹	3.81 x 10 ⁻²⁷
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.55 x 10 ⁻¹³	2.20 x 10 ⁻¹¹	3.50 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.45 x 10 ⁻¹⁵	2.46 x 10 ⁻¹⁴	1.14 x 10 ⁻¹³
$\Sigma P(W)$ (atm)	2.45 x 10 ⁻³¹	2.80 x 10 ⁻²⁶	2.32 x 10 ⁻²²	3.17 x 10 ⁻¹⁹	1.13 x 10 ⁻¹⁶
Ni(1728)	0	0	0	0	0
NiO(c)	0	0	0	0	0
NiWO ₄ (c)	1	1	1	1	1
W(3695)	0	0	0	0	0
WO ₂ (c)	0	0	0	0	0
WO ₃ (1747)	0	0	0	0	0
W ₁₈ O ₄₉ (c)	0	0	0	0	0
W ₂₀ O ₅₈ (c)	0	0	0	0	0
W ₂₅ O ₇₄ (c)	0	0	0	0	0

TABLE 3. (Concluded)

Species	Partial Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
	ZnWO₄(c)				
Zn	2.22 x 10 ⁻²⁶	1.05 x 10 ⁻²¹	4.31 x 10 ⁻¹⁸	3.26 x 10 ⁻¹⁵	7.30 x 10 ⁻¹³
ZnO	2.43 x 10 ⁻²⁶	4.78 x 10 ⁻²²	9.87 x 10 ⁻¹⁹	4.30 x 10 ⁻¹⁶	6.11 x 10 ⁻¹⁴
W	7.03 x 10 ⁻¹⁰⁵	4.68 x 10 ⁻⁸⁹	9.63 x 10 ⁻⁷⁷	6.78 x 10 ⁻⁶⁷	7.62 x 10 ⁻⁵⁹
WO	5.47 x 10 ⁻⁷⁴	2.13 x 10 ⁻⁶²	2.17 x 10 ⁻⁵³	3.36 x 10 ⁻⁴⁶	2.46 x 10 ⁻⁴⁰
WO ₂	5.65 x 10 ⁻⁵¹	7.37 x 10 ⁻⁴³	1.49 x 10 ⁻³⁶	1.60 x 10 ⁻³¹	2.01 x 10 ⁻²⁷
WO ₃	1.59 x 10 ⁻³⁰	1.22 x 10 ⁻²⁵	7.61 x 10 ⁻²²	8.10 x 10 ⁻¹⁹	2.35 x 10 ⁻¹⁶
W ₂ O ₆	2.27 x 10 ⁻²⁶	7.18 x 10 ⁻²²	2.31 x 10 ⁻¹⁸	1.44 x 10 ⁻¹⁵	2.66 x 10 ⁻¹³
W ₃ O ₈	1.03 x 10 ⁻⁴⁵	6.60 x 10 ⁻³⁸	8.11 x 10 ⁻³²	5.84 x 10 ⁻²⁷	5.20 x 10 ⁻²³
W ₃ O ₉	3.48 x 10 ⁻²⁸	3.08 x 10 ⁻²³	2.25 x 10 ⁻¹⁹	2.69 x 10 ⁻¹⁶	8.41 x 10 ⁻¹⁴
W ₄ O ₁₂	4.04 x 10 ⁻³¹	9.57 x 10 ⁻²⁶	1.54 x 10 ⁻²¹	3.43 x 10 ⁻¹⁸	1.77 x 10 ⁻¹⁵
W ₅ O ₁₅	2.37 x 10 ⁻³⁹	6.79 x 10 ⁻³³	7.75 x 10 ⁻²⁸	8.29 x 10 ⁻²⁴	1.52 x 10 ⁻²⁰
O	5.02 x 10 ⁻¹⁷	1.12 x 10 ⁻¹⁴	7.55 x 10 ⁻¹³	2.20 x 10 ⁻¹¹	3.50 x 10 ⁻¹⁰
O ₂	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²	2.00 x 10 ⁻²
O ₃	1.45 x 10 ⁻¹⁷	3.14 x 10 ⁻¹⁶	3.45 x 10 ⁻¹⁵	2.46 x 10 ⁻¹⁴	1.14 x 10 ⁻¹³
$\Sigma P(W)$ (atm)	2.30 x 10 ⁻²⁶	7.49 x 10 ⁻²²	2.54 x 10 ⁻¹⁸	1.71 x 10 ⁻¹⁵	3.52 x 10 ⁻¹³
Zn(693)	0	0	0	0	0
ZnO(2248)	0	0	0	0	0
ZnWO ₄ (c)	1	1	1	1	1
W(3695)	0	0	0	0	0
WO ₂ (c)	0	0	0	0	0
WO ₃ (1747)	0	0	0	0	0
W ₁₈ O ₄₉ (c)	0	0	0	0	0
W ₂₀ O ₅₈ (c)	0	0	0	0	0
W ₂₅ O ₇₄ (c)	0	0	0	0	0

a: Melting point.

b: Mole fraction of condensed phase.

TABLE 4.

TOTAL W-CONTAINING SPECIES PRESSURE OVER $\text{WO}_3(\text{c})$ AND SOME
 $\text{MWO}_4(\text{c})$ IN PRESENCE OF PURE O_2 AT 0.02 ATM TOTAL PRESSURE

Oxide	Total W-containing Species Pressure (atm)				
	700 K	800 K	900 K	1000 K	1100 K
$\text{WO}_3(\text{c})$	4.24×10^{-24}	1.05×10^{-19}	2.91×10^{-16}	1.69×10^{-13}	3.07×10^{-11}
$\text{CoWO}_4(\text{c})$	6.47×10^{-29}	8.74×10^{-25}	1.46×10^{-21}	6.13×10^{-19}	1.02×10^{-16}
$\text{CuWO}_4(\text{c})$	4.24×10^{-24}	1.05×10^{-19}	2.91×10^{-16}	1.69×10^{-13}	3.07×10^{-11}
$\text{FeWO}_4(\text{c})$	4.24×10^{-24}	1.05×10^{-19}	2.91×10^{-16}	1.69×10^{-13}	3.07×10^{-11}
$\text{NiWO}_4(\text{c})$	2.45×10^{-31}	2.80×10^{-26}	2.32×10^{-22}	3.17×10^{-19}	1.13×10^{-16}
$\text{ZnWO}_4(\text{c})$	2.30×10^{-26}	7.49×10^{-22}	2.54×10^{-18}	1.71×10^{-15}	3.52×10^{-13}

APPENDIX B

Final Report by General Electric