B.3 Combustor

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Introduction

Regeneration of the reduced metal oxide completes the chemical looping cycle and is as critically important to the chemical looping process as reduction of the metal oxide. Furthermore, the combustor is a necessity for evaluating a complete process analysis of any chemical looping process. In the combustor, reduced metal oxide reacts with oxygen in the air to regenerate it to its original oxidation state. The reduced form of ITCMO and IACMO used in the chemical looping partial oxidation processes are $FeTiO_3$ and $FeAl_2O_4$. Upon oxidation in the combustor, they are regenerated to Fe_2O_3 and TiO_2 (Iron-titanium complex metal oxide), and Fe_2O_3 and Al_2O_3 (Iron-aluminum complex metal oxide), respectively. The oxidation reaction is highly exothermic, and that heat can be transferred to the metal oxide particles to increase its temperature. By operating the combustor at a higher temperature than the reducer, the metal oxide oxygen carrier particles perform a dual function of donating oxygen and transferring heat.

A fluidized bed reactor is used for the combustor. Air and particles flow co-currently upwards, where thermal equilibrium between the two is established. The heat from the oxygen-depleted, high-temperature gas exiting the combustor is recovered.

Model Setup

An Aspen Plus® model for the combustor is constructed to identify the air flow rate necessary to obtain the maximum adiabatic temperature. The large shift towards the products in the equilibrium of the oxidation reaction of the reduced oxygen carrier particles assures that a single RGIBBS reactor can be used to accurately simulate the combustor.

Components and Physical Properties

The stream class is MIXCISLD. The selected databanks are COMBUST, INORGANIC, SOLIDS, PURE32, and AQUEOUS. Table B.12 provides the components list. The physical properties of the solid compounds are calculated based on the Barin equation, which is discussed in Section 6.4.1. The original coefficients for CPSXP2 (a-h), retrieved from the INORGANIC databank, are given in Table B.13.

Table B.12 List of components

Type: Solid	
Hematite (Fe_2O_3)	Iron-dialuminum tetraoxide ($FeAl_2O_4$)
Magnetite (Fe_3O_4)	Iron monosulfide (FeS)
Wuestite ($Fe_{0.947}O$)	Pyrrhotite ($Fe_{0.877}S$)
Iron (Fe)	Silicon carbide (SiC)
Aluminum oxide: alpha-Corundum (Al_2O_3)	
Type: Conventional	
Carbon monoxide (CO)	Nitrogen (N_2)
Carbon dioxide (CO_2)	Nitric oxide (NO)
Hydrogen (H_2)	Sulfur (S)
Water (H_2O)	Hydrogen sulfide (H_2S)
Oxygen (O_2)	Sulfur dioxide (SO_2)

Table B.13 Original parameters for CPSXP2

Component	FE3O4
Temperature unit	°C
T1	576.85
T2	1596.85
Property unit	J/kmol
a	-9.7E+08
b	527383.9
c	-50171.2
d	-35.9673
e	-6.02E-05
f	6.13E-09
g	-4.3E+10
h	5.47E+09

Operating Conditions

The reduced metal oxide, $FeAl_2O_4$, flow rate is fixed at 1 kmol/hr. It enters the combustor at 700 °C, which operates at a pressure of 6 bar. The air flow rate is varied between 0.5 kmol/hr and 1.5 kmol/hr and enters the combustor at a temperature of 600 °C.

Results and Discussion

Because the combustor is highly exothermic, there is a significant temperature rise in the outlet stream when operated adiabatically. When the $FeAl_2O_4$ flow rate is fixed while increasing the air flow rate from 0.5 to 1.5 kmol/hr, the outlet temperature of the combustor initially increases, reaches a peak, and then decreases. In the region where the outlet temperature of the combustor increases with increasing air flow rate, the air is deficient in oxygen and cannot completely oxidize the reduced metal oxide. Increasing the air flow rate increases the extent of the oxidation conversion of the reduced metal oxide, which increases the exit temperature. In the region where the outlet temperature of the combustor decreases with increasing air flow rate, the air is in excess and thus, an increase in the air flow rate increases the heat demand of the excess air, leading to a decrease in temperature. The temperature peak can be found at an air flow rate of 1.2 kmol/hr. At 1,034.7 °C, the oxygen in air is at the stoichiometric value necessary to fully oxidize all of the reduced metal oxide particles. The specific temperature variation as a function of the air flow rate is given in Table B.14.

Table B.14 Temperature variation as a function of air flow rate

AIR FLOW	T
KMOL/HR	°C
0.5	863.5
0.55	877.8
0.6	891.7
0.65	905.3
0.7	918.6
0.75	931.6
0.8	944.3
0.85	956.8
0.9	969.0
0.95	980.9
1	992.7
1.05	1004.1
1.1	1015.4
1.15	1026.4
1.2	1034.7
1.25	1031.6
1.3	1028.5
1.35	1025.5
1.4	1022.5
1.45	1019.6
1.5	1016.7

Conclusions

The chemical looping combustor reactor can be simulated using an RGIBBS reactor module. The extent of oxidation conversion of the reduced metal oxide to Fe_2O_3 can be gauged by observing the temperature variation of the outlet stream of the combustor. When the air flow rate is greater than that corresponding to the temperature peak, the reduced metal oxide particles are fully regenerated. There is an important balance that exists with the excess air because it reduces the outlet temperature of the combustor but is also necessary to ensure complete combustion. Determining the appropriate amount of excess air is dependent upon both experimental results necessary for complete re-oxidation of the reduced metal oxide particles and the energy requirement of the reducer to ensure autothermal operation.

Appendix

The Aspen Plus file of the combustor simulation is given in the file titled, “B.3 Combustor.”