C.2 Coal to Electricity Process

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Introduction

Aside from chemical synthesis, chemical looping gasification and reforming can also be used for power generation. Coal for electricity generation via partial oxidation incorporates the coal-to-syngas (CTS) process coupled with an Integrated Gasification Combined Cycle (IGCC). The details of the CTS-IGCC process is given in Section 6.8.3. Coal is gasified to syngas via the CTS process, and the syngas is then combusted to drive a gas turbine followed by heat recuperation in a Heat Recovery Steam Generator (HRSG) to generate high-pressure steam that is used to generate electricity in a Rankine cycle. The first step of this process, which is syngas generation via chemical looping coal gasification, is simulated using Aspen Plus®. The operating conditions of this process are optimized for the maximum production of syngas. Additionally, the compression energy required to pressurize the syngas and spent air to 40 bar is studied.

Process Configuration

The schematic of the chemical looping section of this CTS-IGCC process is shown in Figure C.2.1. Pre-treated Illinois #6 coal is partially oxidized by an iron-aluminum composite metal oxide (IACMO) and steam in the reducer, where it produces syngas, a mixture of CO and H_2. The reduced IACMO oxygen carrier is regenerated with air in the combustor. The syngas produced in the chemical looping reducer is cleaned through a series of downstream processes and then combusted to generate electricity in a combined cycle. Oxygen-depleted air from the combustor outlet, which mainly consists of nitrogen, is mixed with syngas prior to entering the gas turbine to reduce the combustion temperature in order to minimize the formation of nitrous oxides. The chemical looping gasification system operates at 6 bar while the gas turbine operates around 40 bar, so the syngas and spent air streams need to be compressed to the gas turbine operating pressure. The CTS-IGCC couples heat streams and turbomachinery to efficiently generate electricity.

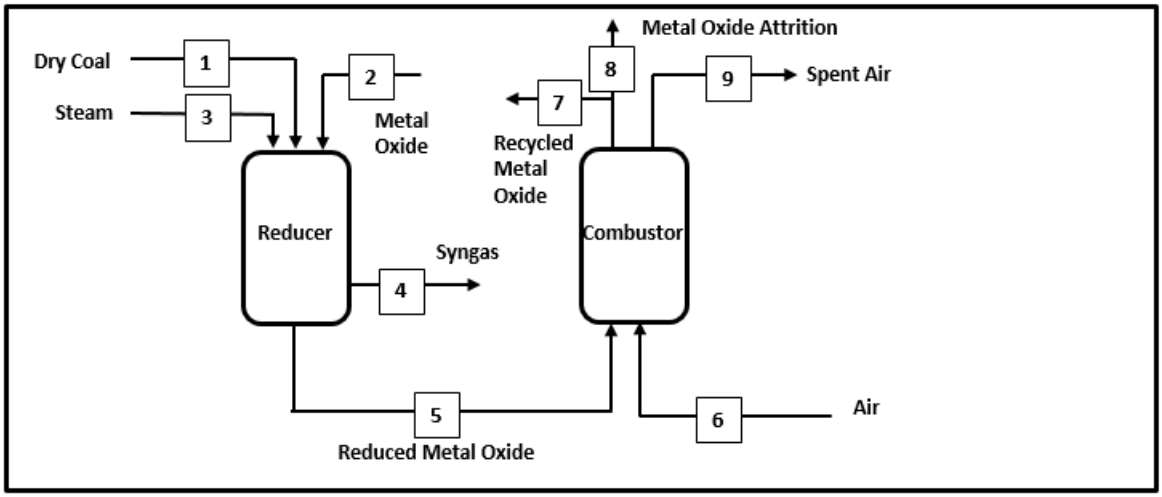

Figure C.2.1 Chemical looping gasification

Components and Physical Properties

The process simulation is completed using Aspen Plus® simulation software. This section lists the definitions and settings used for process modeling. The parameters used in this coal-to-electricity simulation are defined in Table C.7 and Table C.8.

Table C.7 Parameters used in the simulation

Parameter	Setting
Stream Class	MIXCINC
Thermodynamic and Physical data bank (in order)	INORGANIC, SOLIDS, PURE28, AQUEOUS
Method filter	ALL
Base Method	PR-BM (Peng-Robinson Boston-Mathias)
Reactor module type	RGIBBS

Table C.8 List of components

Type: Solid	
Hematite (Fe_2O_3)	Iron-dialuminum tetraoxide ($FeAl_2O_4$)
Magnetite (Fe_3O_4)	Titanium dioxide: Rutile (TiO_2)
Ferrous oxide (FeO)	Iron-titanium trioxide: Ilmenite ($FeTiO_3$)
Wuestite ($Fe_{0.947}O$)	Carbon: graphite (C)
Iron (Fe)	Iron disulfide: Pyrite (FeS_2)
Aluminum oxide: alpha-Corundum (Al_2O_3)	Iron monosulfide (FeS)
	Pyrrhotite ($Fe_{0.877}S$)
Type: Conventional	
Methane (CH_4)	Oxygen (O_2)
Acetylene (C_2H_2)	Nitrogen (N_2)
Ethylene (C_2H_4)	Nitric oxide (NO)
Ethane (C_2H_6)	Sulfur (S)
Propane (C_3H_8)	Hydrogen sulfide (H_2S)
Benzene (C_6H_6)	Sulfur dioxide (SO_2)
Naphthalene ($C_{10}H_8$)	Carbonyl sulfide (COS)
Carbon monoxide (CO)	Chlorine (Cl_2)
Carbon dioxide (CO_2)	Hydrogen chloride (HCl)
Hydrogen (H_2)	Argon (Ar)
Water (H_2O)	Hydrogen cyanide (HCN)
	Ammonia (NH_3)
Type: Nonconventional	
Coal	Ash

Operating Conditions

Parameters for each of the feed streams and reactors are given in Table C.9 and Table C.10, respectively.

Table C.9 Inlet stream specifications

Stream	Coal	Air	Fe_2O_3	Al_2O_3
Flow Rate (kmol/hr)	1	1.764	0.705	5.394
Temperature (°C)	25	25	1,050	1,050
Pressure (bar)	6	1	6	6

Table C.10 Chemical looping reactor operating conditions

Block	Reducer	Combustor
Temperature (°C)	940	1,050
Pressure (bar)	6	6

Results and Discussion

Table C.11 presents the component flow of each stream. Based on the input parameters given in the sections above. Table C.12 provides the results of the compressor energy requirements. For the results given in Table C.11 and C.12, the stream names and unit operation ID refers to those given in the coal-to-electricity simulation file that is provided.

Table C.11 Flow rate of chemical looping gasification species

Stream	AIR	CYCS	DRYCOAL	OC	REDSOUT	SPENTAIR	STEAM	SYNGAS
Flow rate (kmol/hr)								
O2	0.37	0	0.041	0	0	0.018	0	0
N2	1.393	0	0.008	0	0	1.393	0	0.008
C	0	0	1	0	0	0	0	0
H2	0	0	0.42	0	0	0	0	0.733
CO	0	0	0	0	0	0	0	0.86
CO2	0	0	0	0	0	0	0	0.133
CH4	0	0	0	0	0	0	0	0.006
H2O	0	0	0.006	0	0	0	0.5	0.165
S	0	0	0.015	0	0	0	0	0
COS	0	0	0	0	0	0	0	0.001
H2S	0	0	0	0	0	0	0	0.014
NH3	0	0	0	0	0	0	0	0
HCL	0	0	0	0	0	0	0	0.002
CL2	0	0	0.001	0	0	0	0	0
FE2O3	0	0.705	0	0.705	0	0	0	0
FE3O4	0	0	0	0	0	0	0	0
FE0.947O	0	0	0	0	0	0	0	0
FE	0	0	0	0	0	0	0	0
AL2O3	0	5.395	0	5.395	3.984	0	0	0
FEAL2O4	0	0	0	0	1.411	0	0	0
FEO	0	0	0	0	0	0	0	0
FES	0	0	0	0	0	0	0	0
FE0.877S	0	0	0	0	0	0	0	0
FES2	0	0	0	0	0	0	0	0
Total Mole Flow (kmol/hr)	1.764	6.1	1.491	6.1	5.395	1.411	0.5	1.923
Mass Flow (kg/hr)	50.882	662.691	15.024	662.691	651.404	39.595	9.008	35.318
Temperature (°C)	25	1050.1	25	1050	940.5	1050.1	650	940.5
Pressure（bar)	1	6	6	6	6	6	6	6

Table C.12 Operating parameters for the compressors

	Stream Compressed	Stages	Compression Ratio	Work (kW)	Cooling Duty (kW)
COMP1	Syngas	3	1.882	3.200	-2.300
COMP2	Spent Air	3	1.882	2.562	-1.711
COMP3	Air	2	2.449	3.081	-1.263

Conclusions

The CTS-IGCC process was simulated using Aspen Plus®. Illinois #6 coal is partially oxidized in the chemical looping reducer reactor to produce CO and H_2. The syngas is then combusted to produce electricity in a gas turbine followed by heat recovery that generates steam to produce additional electricity in a steam turbine cycle. Operating variables such as temperature, pressure, oxygen carrier flow rate, and oxygen carrier support percentage are all adjusted to maximize syngas production. Energy recovery through heat recuperation turbomachines allow for efficient and economical electricity generation from coal gasification chemical looping.

Appendix

The Aspen Plus file of the CTS-IGCC process is given in the file titled, “C.2 Coal to Electricity.”