B.2 Solid Feed Reducer

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Introduction

Powder River Basin (PRB) coal, a sub-bituminous coal, is used as the feedstock in this simulation model of a chemical looping reducer reactor processing a non-conventional solid for syngas production. An iron-aluminum composite metal oxide (IACMO) is used as the oxygen carrier. A cocurrent moving bed reactor using PRB coal as feedstock is simulated under the assumption that chemical and phase equilibrium is achieved in the reducer reactor. Reaction (B.2.1) is the primary reaction for syngas production where the carbon in coal is converted to carbon monoxide, CO. In Reaction (B.2.1), coal is represented by pure carbon, C. Because coal has a naturally low hydrogen content, with a hydrogen:carbon mole ratio between 0.3 and 0.7, steam is also injected into the reducer in order to adjust the H_2:CO ratio of the syngas product via the water-gas shift reaction, Reaction (B.2.2). With this model, the effect of IACMO flow rate and the addition of steam into the reducer is studied.

$$C+Fe_2O_3+2Al_2O_3 \rightarrow CO+2FeAl_2O_4 \tag{B.2.1}$$

$$H_2O+CO \leftrightarrow H_2+CO_2 \tag{B.2.2}$$

When there is an insufficient amount of IACMO, all of the carbon in coal cannot be oxidized, resulting in unreacted carbon in the reducer. To prevent carbon deposition, there is a minimum threshold IACMO:coal ratio below which unreacted carbon will be present. With an excess amount of IACMO, full oxidation can occur through Reaction (B.2.3) and Reaction (B.2.4).

$$CO+Fe_2O_3+2Al_2O_3 \rightarrow CO_2+2FeAl_2O_4 \tag{B.2.3}$$

$$H_2+Fe_2O_3+2Al_2O_3 \rightarrow H_2O+2FeAl_2O_4 \tag{B.2.4}$$

Model Setup

A single RGIBBS module can be used to simulate a cocurrent moving bed reducer reactor. The key variables affecting the syngas quality are reaction temperature, pressure, IACMO flow rate, and steam flow rate. In this model, the reducer reactor is operated under isothermal and isobaric conditions. Based on the enthalpy of the reactant and product streams, the heat duty of the reactor is then calculated. The RYIELD reactor in conjunction with a calculator block decomposes the coal into its constituent components based on the ultimate analysis of the coal. The RGIBBS reactor is the reactor that represents the cocurrent moving bed reducer. In reality, the RYIELD reactor does not exist, but it is necessary to accurately model components that have variable compositions. If the modeling of non-conventional solids is an unfamiliar topic, it is suggested to read the Aspen Plus® user guide titled, “Getting Started Modeling Processes with Solids.”

Components and Physical Properties

Table B.7 provides the specified components and physical property parameters used in the simulation. The stream class is MIXCINC. The selected databanks are COMBUST, INORGANIC, SOLIDS, AQUEOUS, and PURE32. The physical properties of the solid compounds are calculated based on the Barin equation, as discussed in Section 6.4.1. The model retrieves the coefficients for the solid phase heat capacity from the INORGANIC databank. The original coefficients for Fe_3O_4 is given in Table B.8.

Table B.7 List of components

Type: Solid	
Hematite (Fe_2O_3)	Iron-dialuminum tetraoxide ($FeAl_2O_4$)
Magnetite (Fe_3O_4)	Carbon-graphite (C)
Ferrous oxide (FeO)	Iron monosulfide (FeS)
Iron (Fe)	Iron disulfide: Pyrite (FeS_2)
Aluminum oxide: alpha-Corundum (Al_2O_3)	
Type: Conventional	
Methane (CH_4)	Nitric oxide (NO)
Ethane (C_2H_6)	Nitrogen dioxide (NO_2)
Propane (C_3H_8)	Sulfur (S)
n-Butane (C_4H_{10}-1)	Hydrogen sulfide (H_2S)
Carbon monoxide (CO)	Sulfur dioxide (SO_2)
Carbon dioxide (CO_2)	Chlorine (Cl_2)
Hydrogen (H_2)	Hydrogen chloride (HCl)
Water (H_2O)	Argon (Ar)
Oxygen (O_2)	Hydrogen cyanide (HCN)
Nitrogen (N_2)	Ammonia (NH_3)
Type: Nonconventional	
Coal	Ash

Table B.8 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 inlet feed to the reducer reactor for the base case simulation of the reducer using PRB coal is given in Table B.9. The RGIBBS reactor operates isothermally at 1000 °C and a pressure of 10 bar.

Table B.9 Inlet flow rate to RGIBBS reducer reactor

Species	Carbon*	H_2O (steam)	Fe_2O_3	Al_2O_3
Flow Rate (kmol/hr)	1	0	0.9	2.4
Temperature (°C)	25	600	1000	1000
Pressure (bar)	1.01325	10	10	10

*Coal flow rate is defined by 1 kmol/hr carbon into reducer

Results and Discussion

The operating range where syngas generation is favored over CO_2 or C formation is controlled initially through the IACMO:C molar ratio. By fixing the flow rate of carbon at 1 kmol/hr, a sensitivity block, IACMO, is set-up where the IACMO flow rate is varied from 0.5 to 5. Table B.10 provides the results of the product distribution, and thus the syngas purity, at varying IACMO:C mole ratios. In Table B.10, the species C in the rightmost column represents the unconverted carbon. When the IACMO flow rate is less than 2 kmol/hr, a fraction of the carbon in coal is not gasified and remains as unconverted carbon. The presence of unconverted carbon not only compromises the syngas conversion but also leads to undesirable CO_2 formation when carried over into the combustor. To avoid unreacted carbon formation, the IACMO flow rate must be greater than 2.

Table B.10 Product distribution as a function of IACMO:carbon molar ratio

IACMO	CO	H_2	CO_2	H_2O	H_2:CO	C
KMOL/HR	KMOL/HR	KMOL/HR	KMOL/HR	KMOL/HR		KMOL/HR
0.5	0.577	0.646	0.018	0.034	1.12	0.375
0.75	0.638	0.647	0.021	0.036	1.01	0.313
1	0.698	0.648	0.024	0.038	0.928	0.251
1.25	0.759	0.648	0.027	0.039	0.855	0.188
1.5	0.819	0.649	0.030	0.040	0.792	0.125
1.75	0.880	0.650	0.033	0.042	0.738	0.063
2	0.940	0.650	0.036	0.043	0.692	0
2.25	0.925	0.641	0.062	0.074	0.693	0
2.5	0.901	0.618	0.092	0.108	0.686	0
2.75	0.873	0.589	0.123	0.142	0.675	0
3	0.842	0.558	0.155	0.176	0.663	0
3.25	0.809	0.526	0.188	0.210	0.650	0
3.3	0.803	0.520	0.195	0.217	0.647	0
3.5	0.776	0.494	0.223	0.244	0.637	0
3.75	0.741	0.462	0.258	0.276	0.624	0
4	0.706	0.431	0.294	0.308	0.611	0
4.25	0.669	0.400	0.330	0.339	0.598	0
4.5	0.632	0.370	0.368	0.370	0.585	0
4.75	0.594	0.340	0.406	0.400	0.573	0
5	0.555	0.311	0.445	0.429	0.561	0

Another variable that could be modified to control the syngas quality is the steam flow rate into the reducer, which is achieved using the Steam sensitivity block. The CO produced is shifted to H_2 formation through Reaction (B.2.2), thereby increasing the H_2:CO ratio in the syngas. At a carbon flow rate of 1 kmol/hr and IACMO flow rate of 3.3 kmol/hr, the steam injection rate was varied from 0.1 to 1 kmol/hr in the sensitivity block. Table B.11 provides the results of the effect of steam on product distribution where it is clearly shown that the H_2:CO ratio increases with increasing steam injection.

Table B.11 Effect of steam on product distribution

STEAM	CO	H_2	CO_2	H_2O	H_2:CO	C
KMOL/HR	KMOL/HR	KMOL/HR	KMOL/HR	KMOL/HR		KMOL/HR
0	0.803	0.520	0.195	0.217	0.647	0
0.1	0.770	0.554	0.229	0.283	0.720	0
0.2	0.740	0.585	0.259	0.352	0.792	0
0.3	0.712	0.614	0.287	0.425	0.862	0
0.4	0.687	0.640	0.312	0.499	0.931	0
0.5	0.664	0.663	0.335	0.576	0.999	0
0.6	0.642	0.685	0.357	0.654	1.07	0
0.7	0.623	0.705	0.377	0.734	1.13	0
0.8	0.604	0.724	0.395	0.815	1.20	0
0.9	0.587	0.742	0.413	0.898	1.26	0
1	0.570	0.758	0.429	0.981	1.33	0

Conclusions

A single stage RGIBBS reactor was used to simulate the cocurrent moving bed gasification reducer using solid fuel (PRB coal) in Aspen Plus®. Based on the minimization of the Gibbs free energy, the products at equilibrium are calculated based on the given conditions in the RGIBBS reactor. The operating conditions under which partial oxidation for syngas production is favored over full oxidation with no unreacted carbon produced can be identified using a sensitivity analysis. The formation of unreacted carbon is present at a low IACMO:C flow ratio and eventually produces CO_2 and H_2O at a high IACMO:C flow ratio. In between the two lies the optimal IACMO:C ratio. The H_2:CO ratio in the syngas can be increased by increasing the steam flow into the reducer at the expense of increased CO_2 formation in the syngas.

Appendix

The Aspen Plus file of the reducer with solid feed simulation is given in the file titled, "B.2 Reducer with Solid Feed."