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Project Title:

Production of Elemental Sulfur and Methane from H₂S and CO₂
Derived from a Coal Desulfurization Process

by

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ABSTRACT

During the sixth quarter of the project, simulations were carried out to investigate the feasibility of producing elemental sulfur and methane from hydrogen sulfide and carbon dioxide by using the overall reaction of H₂S and CO₂ based on the following equation:

The results indicate that two reaction zones are required to realize the above reaction. The first reaction zone should be composed of multiple stages to recover the elemental sulfur without the equilibrium limitations. With optimum temperatures in each zone, the conversion can be increased significantly. The simulation also indicates less amounts of by-products, such as COS, CS₂ and SO₂. The limitation on the extraction of sulfur is directly related to the sulfur vapor pressure.

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Work Performed

One of the project efforts is to study the feasibility of producing methane from hydrogen sulfide (H₂S) and carbon dioxide (CO₂) besides producing elemental sulfur. Before a bench scale experiment is carried out, some simulation works are needed in order to understand the thermodynamic limits and reaction mechanisms within the reaction system. The overall reaction proposed is^[1]:

The basic idea of this reaction was that a rich gas stream of H₂S and CO₂ passed through a high temperature catalyst bed to form elemental sulfur, methane and water vapor. The reaction has been described to be effective but details of the particulars of this reaction such as thermodynamic analyses and multistage operations have not been found in the literature. The process as envisioned is simple and has obvious operational advantages over the existing sulfur recovery processes such as Claus process since it recovers valuable fuel from H₂S.

Different H₂S decomposition methods have been reviewed by Zaman and Chakma^[2], which included thermal, thermochemical, plasmochemical and other diverse technologies. Methanation with CO and CO₂ is mentioned in some publications^[3-5]. However, detailed research works on Reaction (1) are not available in the literature.

The thermodynamic simulation for the reaction of H₂S and CO₂ were performed by using the JANAF Thermochemical Tables^[6] and the Stanjan method^[7]. The feed was 80 mole % of H₂S and 20 mole % of CO₂. The reaction temperatures ranged from 450°C to 1100°C, and the pressure was kept at 1 atm. Gas components in the reaction system were CH₄, CO,

COS, CO₂, CS₂, H₂, H₂O, H₂S, S₂O and S. Although the sulfur actually formed as a combination of allotropes^[8-9], only the total amount of sulfur was considered due to the fact that this approximation proved to be very close to the total sum of all allotropes. It has been verified in the calculation that above 650°C the error of total amount of produced sulfur caused by using S₂ to stand for sulfur allotropes was not detectable within the double precision numerical significant figures.

As mentioned in the last report, recycle and multiple reaction zones are necessary for Reaction (1) as several possible steps in the attempt of thermochemical approach. It was indicated that following individual reactions were possible for the reaction of H₂S and CO₂ in reaction zones:

The thermodynamic limiting step of the system is the decomposition of H₂S. The initial ratio of H₂S to CO₂ is set to 4 which matches the stoichiometric ratio of Reaction (1). The H₂S decomposition reaction and the water-gas shift reaction are endothermic, therefore, the H₂S mole fraction decreases as the system temperature increases causing more formation

of sulfur and CO. However, the methanation reactions are exothermic, therefore the mole fractions of CO and CO₂ decrease as the system temperature decreases producing more CH₄. These facts require that the system must be divided into at least two reaction zones and at least one product should be removed from the system to prevent re-equilibrium to occur as the system temperature changes. We propose that the sulfur be continuously extracted from the system by means of condensation or adsorption/absorption. At the end of the reaction, the system eventually cools down to room temperature, 25°C. As an example, when the reaction temperature is 900°C (in zone one) the equilibrium component distribution is as following after gradually cooling down to 25°C (in zone two):

(mole fraction in percentage)

Species in the system:	H ₂ S	CO ₂	CH ₄	H ₂	CO	H ₂ O	COS	S ₂	SO ₂ & CS ₂
Initial Composition: (900°C)	80.00	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Final Composition: (900°C)	3.34	3.18	0.02	61.88	15.76	15.97	0.03	0.00*	0.00
Final Composition: (25°C)	5.43	0.00	30.58	2.87	0.00	61.12	0.00	0.00*	0.00

*S₂ has already been removed from the system during the each equilibrium stage and recovered.

The above results strongly support the concept of continuous removal of sulfur. It is clearly shown that the final distribution of the related species matches the stoichiometric relations in Reaction (1).

The significance of the current simulation is that sulfur is removed from the system when the reactions reach an equilibrium at each stage. Then the sulfur is removed and the residues are into the next stage and react. When the new equilibrium reaches, sulfur is removed again. This process continues until the efficiency of sulfur removal becomes very low, i.e., there is no sulfur to be extracted from the system. Thermodynamically, the limitation is controlled by the sulfur vapor pressure of the condensed phase. The final product distributions at various reaction temperatures are shown in Table 1. Table 2 shows the product distribution at 25°C.

The H_2 mole fraction becomes lower in the presence of CO_2 since CO_2 reacts with H_2 to form H_2O and CO . The equilibrium of H_2S decomposition is shifted to favor the formation of elemental sulfur. Now, CO , CO_2 and H_2 can form CH_4 while the system cools down to the room temperature.

Results and Discussion

Simulations were carried out to investigate the effect of major variables on the equilibrium composition of the species in the system. The purpose of this exercise is to find out the optimum reaction temperature and the number of theoretical stages based on the limitation of sulfur vapor pressure.

CH_4 :

When the system reaches its final equilibrium stage, which is limited by the sulfur

vapor pressure, no sulfur can be extracted from the system. The equilibrium mole fraction of CH_4 as a function of temperature from 450 to 1100°C is shown in Figure 1. The high mole fraction of CH_4 is obtained at low reaction temperature since the methanation reaction is exothermic. When the reaction temperature is around 500°C, the mole fraction of CH_4 is 1.5%. As shown in Figure 2, when the reaction temperature in the first zone is 950°C, the system gradually cools down to 25°C, which favors the formation of CH_4 , the mole fraction of CH_4 in the second zone reaches 32%. Higher reaction temperature promotes more H_2S decomposition into H_2 and S_2 . Since sulfur is removed at each equilibrium stage, there is less chance for regeneration of H_2S to occur. High mole fraction of H_2 in the system residue favors the methanation reaction to form CH_4 . Figure 3 shows the effects of reaction temperature and the number of theoretical stages on the equilibrium mole fraction of CH_4 in zone one. Low temperature and large number of stages favor the methanation reaction. The majority of CH_4 is formed in the second reaction zone which acts a methanation reactor.

H_2 :

Figure 4 illustrates the equilibrium mole fraction of H_2 as a function of temperature when the system reaches its final equilibrium, that is, there is no sulfur can be extracted from zone one. Between 450 and 1100°C, higher reaction temperature promotes higher mole fraction of H_2 . When the reaction temperature is around 900°C, the mole fraction of H_2 levels off at 62%. Above 900°C the H_2 mole fraction does not increase significantly. Then the system cools down gradually to the 25°C (Figure 5) without quenching because virtually

no re-equilibrium occurs. Most of the H_2 react with CO and CO_2 to form CH_4 and depleting its mole fraction down to 2.9% for the first zone temperature above $900^\circ C$, and down to almost zero % for the first zone temperature below $900^\circ C$. The effects of the reaction temperature and the number of theoretical stages are shown in Figure 6. The high temperature and large number of stages favor the production of H_2 in the first reaction zone.

CO:

Figure 7 shows the relationship of equilibrium mole fraction of CO with reaction temperature when the system reaches the final equilibrium. Because the water-shift reaction is endothermic, the higher mole fraction of CO is achieved at a high reaction temperature. At $700^\circ C$, the mole fraction of CO in the system reaches 11.4%. Above $700^\circ C$ the CO mole fraction monotonically increases, reaching 17.3% at $1100^\circ C$. Considering that the initial concentration of CO_2 is only 20%, the conversion of CO_2 is high. When system cools down to the $25^\circ C$ (Figure 8) the mole fraction of CO is down to less than 1 ppm. Figures 9 shows the effect of reaction temperature on the equilibrium mole fraction of CO. High temperature and high number of cycles favor the production of CO in the first zone.

H_2S :

Figure 10 shows the final equilibrium mole fraction of H_2S as a function of temperature. The initial concentration of H_2S is set to 80% to match the stoichiometric ratio in Reaction 1. The mole fraction of H_2S continually goes down as the reaction temperature

goes up. At 900°C, the mole fraction of H_2S is only about 3.3%. There is only a small amount of re-equilibrium occurring after cooling down to 25°C. (See Figures 10 and 11.) Figures 12 shows that high temperature and large number of stages favor the H_2S decomposition reaction in the first reaction zone.

CO_2 :

The pattern of the CO_2 mole fraction change is similar to that of H_2S . Figure 13 shows the final mole fraction of CO_2 continually decreasing with the increasing reaction temperature due to the fact that the water-shift reaction is endothermic. When the reaction temperature reaches 900°C, the mole fraction of CO_2 is only about 3.1%. As the system cools down to the 25°C (Figure 14), most of the CO and CO_2 react with H_2 to form CH_4 . Figure 15 also indicates that high temperature and large number of stages favor the water-shift reaction.

H_2O :

Figures 16 and 17 show the equilibrium mole fraction of H_2O as a function of temperature when the system reaches the final equilibrium. The high mole fraction is obtained at high reaction temperature.

COS and CS_2 :

Within the temperature range being investigated, the equilibrium mole fractions of

COS and CS₂ are very small (Figures 19 and 22) when the system reaches its final equilibrium state.

SO₂:

Between the reaction temperature of 450 to 1000°C, the equilibrium mole fraction of SO₂ is always less than 1 ppm (Figures 25-27) when the system reaches its final equilibrium state.

S₂:

Figures 28-29 show the final equilibrium mole fraction of S₂. The sulfur removal efficiency will be discussed in the next report when more reliable data on sulfur vapor pressure is found. The highest number of stages up to 10,000 was used in order to find the final extraction equilibrium point. However, when the number of stages increased over 3000, the calculation reached beyond the significant figures of the computer.

Future Work

Sulfur melting point is 112.8°C and boiling point is 444.6°C^[10] at 1 atm. The vapor pressure of sulfur will affect the condensation efficiency of sulfur. This is a limit or a boundary for extraction of sulfur from the reaction system. The relationship of sulfur vapor pressure with temperature will determine the optimum value of reaction temperature in the first and second zones. It will also aid the experimental decision on how many stages are

really needed to reach a practical equilibrium limit in a bench scale experiment. These questions will be addressed in the next quarter. A bench-scale experiment will also be performed.

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Table 1. Equilibrium Mole Fraction of the Related Species at the Final Stage before Cooling down the Reaction System to 25° C

Reaction Temperature (C)	CH4	CO	COS	CO2	CS2	H2	H2O	H2S	SO2	S2
450	0.0094	0.0142	0.0130	0.1710	0.0002	0.0301	0.0473	0.7149	0.0000	0.0000
500	0.0101	0.0294	0.0117	0.1614	0.0002	0.0586	0.0626	0.6661	0.0000	0.0000
550	0.0084	0.0513	0.0102	0.1468	0.0002	0.1000	0.0789	0.6042	0.0000	0.0000
600	0.0057	0.0760	0.0086	0.1269	0.0001	0.1532	0.0956	0.5339	0.0000	0.0000
650	0.0035	0.1024	0.0071	0.1038	0.0001	0.2138	0.1056	0.4635	0.0000	0.0000
700	0.0035	0.1137	0.0034	0.0633	0.0000	0.3574	0.1229	0.3357	0.0000	0.0000
750	0.0017	0.1294	0.0023	0.0515	0.0000	0.4382	0.1329	0.2439	0.0000	0.0000
800	0.0008	0.1415	0.0015	0.0436	0.0000	0.5028	0.1423	0.1675	0.0000	0.0000
850	0.0003	0.1506	0.0010	0.0386	0.0000	0.5419	0.1511	0.1164	0.0000	0.0000
900	0.0002	0.1576	0.0003	0.0318	0.0000	0.6188	0.1579	0.0334	0.0000	0.0000
950	0.0001	0.1632	0.0002	0.0294	0.0000	0.6224	0.1629	0.0218	0.0000	0.0000
1000	0.0000	0.1674	0.0001	0.0271	0.0000	0.6239	0.1665	0.0148	0.0000	0.0000
1050	0.0000	0.1707	0.0001	0.0253	0.0000	0.6233	0.1701	0.0105	0.0000	0.0000
1100	0.0000	0.1732	0.0000	0.0234	0.0000	0.6262	0.1734	0.0037	0.0000	0.0000

Table 2. Equilibrium Mole Fraction of the Related Species at the Final Stage after Cooling down the Reaction System to 25°C

Reaction Temperature (C)	CH4	CO	COS	CO2	CS2	H2	H2O	H2S	SO2	S2
450	0.0210	0.0000	0.0000	0.1915	0.0000	0.0000	0.0429	0.7447	0.0000	0.0000
500	0.0336	0.0000	0.0000	0.1890	0.0000	0.0000	0.0681	0.7093	0.0000	0.0000
550	0.0500	0.0000	0.0000	0.1845	0.0000	0.0000	0.1004	0.6650	0.0000	0.0000
600	0.0712	0.0000	0.0000	0.1743	0.0000	0.0000	0.1416	0.6130	0.0000	0.0000
650	0.0981	0.0000	0.0000	0.1597	0.0000	0.0000	0.1828	0.5594	0.0000	0.0000
700	0.1586	0.0000	0.0000	0.0820	0.0000	0.0000	0.3156	0.4437	0.0000	0.0000
750	0.2006	0.0000	0.0000	0.0577	0.0000	0.0000	0.3979	0.3438	0.0000	0.0000
800	0.2388	0.0000	0.0000	0.0377	0.0000	0.0000	0.4742	0.2494	0.0000	0.0000
850	0.2653	0.0000	0.0000	0.0262	0.0000	0.0000	0.5288	0.1797	0.0000	0.0000
900	0.3058	0.0000	0.0000	0.0000	0.0000	0.0287	0.6112	0.0543	0.0000	0.0000
950	0.3139	0.0000	0.0000	0.0000	0.0000	0.0235	0.6268	0.0358	0.0000	0.0000
1000	0.3188	0.0000	0.0000	0.0000	0.0000	0.0207	0.6359	0.0245	0.0000	0.0000
1050	0.3225	0.0000	0.0000	0.0000	0.0000	0.0162	0.6439	0.0174	0.0000	0.0000
1100	0.3242	0.0000	0.0000	0.0000	0.0000	0.0210	0.6486	0.0062	0.0000	0.0000

Figure 1. The Effect of Temperature on Equilibrium Mole Fraction of CH_4

Figure 2. The Effect of Reaction Temperature on Equilibrium Mole Fraction of CH₄ after Cooling down the Reaction System to 25°C

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