

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/231273333>

# Role of Iron-Based Catalyst and Hydrogen Transfer in Direct Coal Liquefaction

ARTICLE in ENERGY & FUELS · FEBRUARY 2008

Impact Factor: 2.79 · DOI: 10.1021/ef7006062

---

CITATIONS

17

---

READS

73

4 AUTHORS, INCLUDING:



Xian Li

Huazhong University of Science and Techn...

22 PUBLICATIONS 119 CITATIONS

SEE PROFILE



Haoquan Hu

Dalian University of Technology

86 PUBLICATIONS 1,378 CITATIONS

SEE PROFILE

# Role of Iron-Based Catalyst and Hydrogen Transfer in Direct Coal Liquefaction

Xian Li, Shuxun Hu, Lijun Jin, and Haoquan Hu\*

*Institute of Coal Chemical Engineering, Dalian University of Technology,  
129 Street, Dalian 116012, P.R. China*

*Received October 13, 2007. Revised Manuscript Received December 26, 2007*

The aim of this research is to understand the major function of iron-based catalysts on direct coal liquefaction (DCL). Pyrolysis and direct liquefaction of Shenhua bituminous coal were carried out to investigate the effect of three solvents (wash-oil from coal-tar, cycle-oil from coal liquefaction, and tetralin) in a N<sub>2</sub> or a H<sub>2</sub> atmosphere and with or without catalyst. The hydrogen content in the solvent and liquid product and the H<sub>2</sub> consumption for every run were calculated to understand the hydrogen transfer approach in DCL. The results showed that the iron-based catalyst promotes the coal pyrolysis, and the dominating function of the catalyst in DCL is to promote the formation of activated hydrogen and to accelerate the secondary distribution of H in the reaction system including the gas, liquid, and solid phases. The major transfer approach of the activated hydrogen is from molecular hydrogen to solvent and then from solvent to coal, and the solvent takes on the role of a “bridge” in the hydrogen transfer approach.

## Introduction

Direct coal liquefaction (DCL) is an advantageous approach for the clean and effective utilization of coal but is also a complex combination of physical and chemical processes which include the removing of extractable material from coal, cracking of larger molecules, and stabilizing the produced free radicals by hydrogen.<sup>1,2</sup> The efficiency of DCL depends on coal characteristics, reaction conditions, catalyst, solvent, atmosphere, and so on.

The catalyst plays an important role in DCL. Iron-based catalysts have been studied widely by researchers,<sup>3–6</sup> but there are various viewpoints on the role and the catalytic mechanism of iron-based catalysts in DCL.<sup>7–10</sup> Generally, the role of the catalyst includes promotion of coal pyrolysis and formation of

activated hydrogen in DCL. The first role has been confirmed by many researchers,<sup>11,12</sup> but most researchers consider that the latter is the major role of the catalyst.<sup>13–16</sup> According to conventional theory on DCL, catalysts promote hydrogen transfer from molecular hydrogen to solvent and then from solvent to coal; that is, the solvent acts as a shuttle for transferring hydrogen from molecular hydrogen to coal, and the activated hydrogen coming from hydrogen donation solvents can cleave some of the strong C–C bonds of coal.<sup>2,17</sup> But other researchers suggested that, in the presence of catalyst and pressurized hydrogen, the main hydrogen transfer occurs directly from molecular hydrogen to coal rather than via hydrogen donation solvents<sup>18–21</sup> and that the major role of the solvent is to provide good solubility to coal rather than as a “hydrogen

\* To whom correspondence should be addressed. Telephone: +86-411-88993966. Fax: +86-411-88993966. E-mail: hhu@chem.dlut.edu.cn.

(1) Huang, H.; Wang, K.; Wang, S.; Klein, T. M.; Calkins, H. W. Kinetics of Coal Liquefaction at Very Short Reaction. *Energy Fuels* **1996**, *10*, 641–648.

(2) Cronauer, D. C.; Jewell, D. M.; Shah, Y. T.; Modi, R. J. Mechanism and Kinetics of Selected Hydrogen Transfer Reactions Typical of Coal Liquefaction. *Ind. Eng. Chem. Fundam.* **1979**, *18*, 153–162.

(3) Hirano, K.; Kouzu, M.; Okada, T.; Kobayashi, M.; Ikenaga, N.; Suzuki, T. Catalytic activity of iron compounds for coal liquefaction. *Fuel* **1999**, *78*, 1867–1873.

(4) Hu, H.; Bai, J.; Zhu, H.; Wang, Y.; Guo, S.; Chen, G. Catalytic Liquefaction of Coal with Highly Dispersed Fe<sub>2</sub>S<sub>3</sub> Impregnated in-Situ. *Energy Fuels* **2001**, *15*, 830–834.

(5) Zhu, J.; Yang, J.; Liu, Z.; Dadyburjor, D. B.; Zhong, B.; Li, B. Improvement and characterization of an impregnated iron-based catalyst for direct coal liquefaction. *Fuel Process. Technol.* **2001**, *72*, 199–214.

(6) Liu, Z.; Yang, J.; Zondlo, J. W.; Stiller, A. H.; Dadyburjor, D. B. In situ impregnated iron-based catalysts for direct coal liquefaction. *Fuel* **1996**, *75*, 51–57.

(7) Ikenaga, N.; Taniguchi, H.; Watanabe, A.; Suzuki, T. Sulfiding behavior of iron based coal liquefaction catalyst. *Fuel* **2000**, *79*, 273–283.

(8) Wang, Z.; Shui, H.; Zhang, D.; Gao, J. A Comparison of FeS, FeS+S and solid superacid catalytic properties for coal hydro-liquefaction. *Fuel* **2007**, *86*, 835–842.

(9) Zhang, L.; Yang, J.; Zhou, J.; Liu, Z.; Li, B.; Hu, T.; Dong, B. Properties and liquefaction activities of ferrous sulfate based catalyst impregnated on two Chinese bituminous coal. *Fuel* **2002**, *81*, 951–958.

(10) Wang, L.; Chen, P. Mechanism study of iron-based catalysts in co-liquefaction of coal with waste plastics. *Fuel* **2002**, *81*, 811–815.

(11) Borah, D.; Barua, M.; Baruah, M. K. Dependence of pyrite concentration on kinetics and thermodynamics of coal pyrolysis in non-isothermal systems. *Fuel Process. Technol.* **2005**, *86*, 977–993.

(12) Bai, J.; Wang, Y.; Hu, H.; Guo, S.; Chen, G. Pyrolysis kinetic of coal in-situ impregnated with Fe<sub>2</sub>S<sub>3</sub>. *J. Fuel Chem. Technol.* **2001**, *29*, 39–43.

(13) Wei, X. Y.; Ogata, E.; Zong, Z. M.; Niki, E. Effect of hydrogen pressure, sulfur and FeS<sub>2</sub> on diphenylmethane hydrocracking. *Energy Fuels* **1992**, *6*, 868–869.

(14) Wei, X. Y.; Ogata, E.; Zong, Z. M.; Niki, E. Effects of iron catalyst precursors, sulfur, hydrogen pressure and solvent type on the hydrocracking of di(1-naphthyl)methane. *Fuel* **1993**, *72* (11), 1547–1552.

(15) Kabe, T.; Saito, M.; Qian, W.; Ishihara, A. Elucidation of hydrogen mobility in coal using a tritium pulse tracer method. Hydrogen exchange reaction of coal with tritiated gaseous hydrogen. *Fuel* **2000**, *79*, 311–316.

(16) Ishihara, A.; Nishigori, D.; Saito, M.; Sturisna, I. P.; Qian, W.; Kabe, T. Elucidation of Hydrogen Mobility in Functional Groups of Coals Using Tritium Tracer Methods. *Energy Fuels* **2002**, *16*, 32–39.

(17) McMillen, D. F.; Malhotra, R.; Chang, S. J.; Ogier, W. C.; Nigenda, S. E.; Fleming, R. H. Mechanisms of hydrogen transfer and bond scission of strongly bonded coal structures in donor-solvent systems. *Fuel* **1987**, *66*, 1611–1620.

(18) Vernon, L. W. Free radical chemistry of coal liquefaction: role of molecular hydrogen. *Fuel* **1980**, *59* (2), 102–106.

(19) Skowronski, R. P.; Ratto, J. J.; Goldberg, I. B.; Heredy, L. A. Hydrogen incorporation during coal liquefaction. *Fuel* **1984**, *63* (4), 440–448.

**Table 1. Proximate, Ultimate, and Petrographical Analyses of Shenhua Coal Sample**

proximate analysis (wt %)			ultimate analysis (wt %, daf)					petrographical analysis (wt %, d)			
$M_{ad}$	$A_d$	$V_{daf}$	C	H	N	S	O <sup>a</sup>	vitrinite	inertinite	exinite	mineral
9.34	5.52	38.24	80.13	4.88	1.06	0.42	13.51	62.8	34.0	1.8	1.4

<sup>a</sup> By difference.

shuttle".<sup>22</sup> Tritium tracer methods were also used to elucidate the hydrogen transfer mechanism in DCL.<sup>23,24</sup> But as for the complex mechanism and various factors in DCL, no consistent viewpoint for the role of the catalyst and the hydrogen transfer mechanism in DCL has been obtained.

In this study, pyrolysis and direct liquefaction of Shenhua bituminous coal were carried out. The effect of solvents with different hydrogen donation capabilities, including wash-oil from coal-tar fraction, cycle-oil from coal liquefaction, and tetralin, on DCL in a N<sub>2</sub> or H<sub>2</sub> atmosphere with or without an iron-based catalyst was investigated to explore the role of the iron-based catalyst. The total hydrogen content in the solvent and liquid product was measured by ultimate analysis, and the H<sub>2</sub> consumption in each run was calculated on the basis of the H<sub>2</sub> mass change before and after reaction in the autoclave to understand the hydrogen transfer mechanism.

### Experimental Section

**Materials.** A Shenhua coal sample was ground to a particle size of less than 100 mesh and dried under vacuum at 100 °C for 10 h. The proximate, ultimate, and petrographical analysis results of the sample are shown in Table 1. Cycle-oil was obtained from 1 t/d pilot plant of DCL in the Beijing Institute of Coal Chemical Engineering (BICCE). Wash-oil is from the coking factory of the Anshan Iron & Steel Group. The nanosized iron catalyst dispersed on the Shenhua coal sample (Fe, about 6 wt %) was offered by BICCE.

**Experimental Procedures.** Coal liquefaction experiments were carried out in a 500 mL autoclave with a magnetic stirrer. In each run, a coal sample, solvent, sulfur, and catalyst were added to the reactor with the required proportion. The added catalyst was 1 wt % Fe of coal, and the molar ratio of sulfur to Fe was 2:1. The solvent, namely, cycle-oil, wash-oil, or tetralin, was added to the reactor in a solvent to coal ratio of 3:1. The initial hydrogen pressure was adjusted to 5.0 MPa, and the stirring rate of the magnetic stirrer was 400 rpm. After that, the reactor was heated to 430 °C and held for 30 min. Upon completion of the experiment, the reactor was taken out from the furnace and cooled to below 200 °C within 15 min with a fan. The experimental details have been described in our previous work.<sup>25</sup>

Coal pyrolysis was performed in a thermogravimetric analyzer (Mettler Toledo TGA/SDTA851<sup>o</sup>), with a coal sample of 20 mg in a N<sub>2</sub> carrier gas with a flow rate of 60 mL/min from room temperature to a final temperature of 900 °C at a heating rate of 5 °C/min.

(20) Ohe, S.; Ito, H.; Makabe, M.; Ouchi, K. Reaction mechanism of coal liquefaction. 1. Two-ring solvent system. *Fuel* **1985**, 64 (7), 902–905.

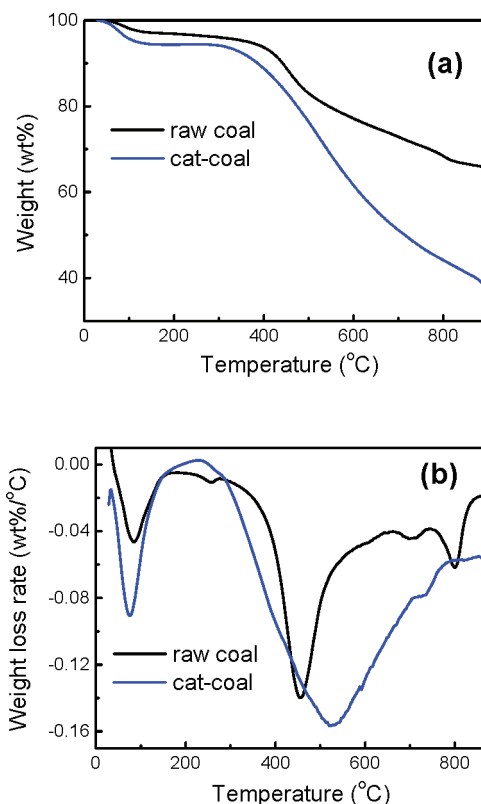
(21) Ouchi, K.; Makabe, M. Hydrogen transfer in the hydrogenation of model compounds. *Fuel* **1988**, 67 (11), 1536–1541.

(22) Wei, X. Y.; Ogata, E.; Zong, Z. M.; Zhou, S.; Qin, Z.; Liu, J.; Shen, K.; Li, H. Advances in the study of hydrogen transfer to model compounds for coal liquefaction. *Fuel Process. Technol.* **2000**, 62, 103–107.

(23) Ishihara, A.; Morita, S.; Kabe, T. Elucidation of hydrogen transfer mechanisms in coal liquefaction using a tritium tracer method: Effects of solvents on hydrogen exchange reactions of coals with tritiated molecular hydrogen. *Fuel* **1995**, 74, 63–69.

(24) Godo, M.; Saito, M.; Ishihara, A.; Kabe, T. Elucidation of coal liquefaction mechanisms using a tritium tracer method: hydrogen exchange reaction of solvents with tritiated molecular hydrogen in the presence and absence of H<sub>2</sub>S. *Fuel* **1998**, 77, 947–952.

(25) Li, X.; Hu, H.; Zhu, S.; Hu, S.; Wu, B.; Meng, M. Kinetics of coal liquefaction during heating-up and isothermal stages. *Fuel* **2008**, 87, 508–513.



**Figure 1.** TG (a) and DTG (b) curves of raw coal and cat-coal.

**Product Separation and Analyses.** The gaseous product was collected and analyzed by gas chromatography. The liquid and solid products from the reactor were separated into liquid product (*n*-hexane soluble, including solvent, water, and oil produced in the liquefaction process), asphaltene (toluene soluble but *n*-hexane insoluble), preasphaltene (tetrahydrofuran (THF) soluble but toluene insoluble), and residue (THF insoluble) by Soxhlet extraction with *n*-hexane, toluene, and THF, respectively. The conversion was defined as the percentage of coal into preasphaltene, asphaltene, oil, and gas during the liquefaction.

### Results and Discussion

**Effect of Iron-Based Catalyst on Coal Pyrolysis.** Thermogravimetry (TG) (weight loss) and differential TG (DTG) (weight loss rate) curves of raw coal and coal with 1 wt % Fe catalyst (cat-coal, without sulfur) are presented in Figure 1. It can be seen that cat-coal has a higher weight loss than raw coal at the same temperature, 61% in contrast to 34% at 900 °C. Clearly, the iron-based catalyst promotes coal pyrolysis markedly. The pyrolysis activation energy and the pre-exponential factor of raw coal and cat-coal were calculated by the integral method.<sup>26</sup> The overall pyrolysis process was considered as a first-order reaction.<sup>27,28</sup> To obtain a fine

(26) Liu, Q.; Hu, H.; Zhou, Q.; Zhu, S.; Chen, G. Effect of inorganic matter on reactivity and kinetics of coal pyrolysis. *Fuel* **2004**, 83, 713–718.

(27) Ulloa, C.; Gordon, A. L.; Garcia, X. Distribution of activation energy model applied to the rapid pyrolysis of coal blends. *J. Anal. Appl. Pyrolysis* **2004**, 71, 465–483.

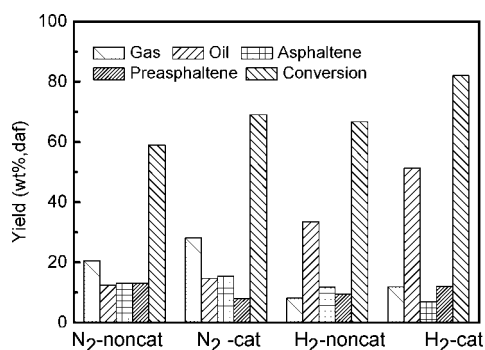
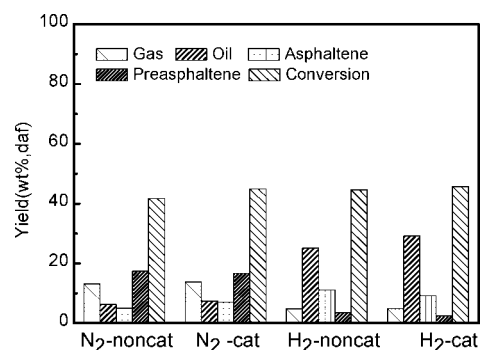
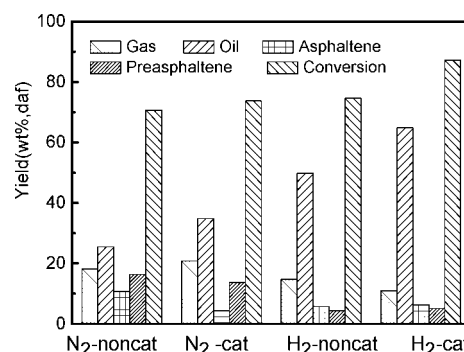
**Table 2.** Kinetic Parameters of Coal Pyrolysis by the Integral Method

sample	<i>T</i> , °C	<i>E</i> , kJ·mol <sup>-1</sup>	<i>A</i> , s <sup>-1</sup>	<i>R</i>
raw coal	280–380	137.1	$7.7 \times 10^8$	-0.977
	380–430	325.0	$3.1 \times 10^{22}$	-0.982
	430–466	461.9	$1.1 \times 10^{31}$	-0.979
	466–510	407.0	$4.1 \times 10^{25}$	-0.975
	510–600	231.4	$9.2 \times 10^{11}$	-0.965
cat-coal	280–380	157.4	$1.37 \times 10^{11}$	-0.980
	380–430	308.9	$6.46 \times 10^{21}$	-0.975
	430–500	237.5	$4.56 \times 10^{14}$	-0.984
	500–600	204.5	$5.47 \times 10^{10}$	-0.977

correlation of the calculated result, the choice of the temperature range for raw coal and cat-coal is not accordant completely. The calculated results are shown in Table 2. The results show that in the presence of catalyst the activation energy of coal pyrolysis obviously reduces, for example, from 430 to 500 °C the activation energy reduces by about 200 kJ mol<sup>-1</sup>; however, at a temperature below 380 °C, the effect of the catalyst on pyrolysis is little.

**Role of Iron-Based Catalyst in DCL.** Figure 2 shows the results of coal liquefaction in a N<sub>2</sub> or a H<sub>2</sub> atmosphere with cycle-oil as solvent. The results in a N<sub>2</sub> atmosphere show that the catalyst promotes the increase in gas yield and conversion from 21% and 59% to 28% and 69%, respectively, but not in oil yield, whereas in a H<sub>2</sub> atmosphere, the catalyst obviously promotes the increase of oil yield and conversion from 33% and 67% to 51% and 82%, respectively. Compared with that in a N<sub>2</sub> atmosphere, the oil yield increases and the gas yield decreases greatly in a H<sub>2</sub> atmosphere.

The results of coal liquefaction in N<sub>2</sub> or H<sub>2</sub> with wash-oil and tetralin as solvent are shown in Figures 3 and 4, respectively, which exhibit a similar tendency as the results with cycle-oil

**Figure 2.** Results of DCL with cycle-oil as solvent. (N<sub>2</sub>- or H<sub>2</sub>-cat or noncat represent a different atmosphere and with or without catalyst).**Figure 3.** Results of DCL with wash-oil as solvent. (N<sub>2</sub>- or H<sub>2</sub>-cat or noncat represent a different atmosphere and with or without catalyst).**Figure 4.** Results of DCL with tetralin as solvent. (N<sub>2</sub>- or H<sub>2</sub>-cat or noncat represent a different atmosphere and with or without catalyst).

as the solvent. The differences of conversion and oil yield among the three solvents mainly come from the different hydrogen donating and dissolving capabilities of the solvent. It is well-known that tetralin is a good hydrogen donating and dissolving solvent for coal liquefaction, so the free radicals produced in coal pyrolysis can be stabilized by activated hydrogen easily in the liquefaction with tetralin as the solvent; the resultant conversion and oil yield are highest among the three solvents at the same liquefaction condition. Wash-oil, the worst hydrogen donation solvent among the three solvents, has the lowest conversion and oil yield at the same liquefaction condition.

The hydrogen content in solvent and liquid products for every run before and after liquefaction was measured by ultimate analysis, and the H<sub>2</sub> consumption of every run was also calculated. The H<sub>2</sub> consumption during DCL was defined as the hydrogen mass change before and after reaction in an autoclave, which is calculated by the following formula:<sup>29</sup>

$$\eta_{H_2} = \frac{M_{H_2} - M_{H_2}'}{M_{daf,coal}} \times 100\% \quad (1)$$

where

$$M_{H_2} = \frac{2.016V}{22.41} \times \frac{P_1 + 0.1013}{0.1013} \times \frac{273.15}{T_1 + 273.15} \quad (2)$$

$$M_{H_2}' = \frac{2.016V}{22.41} \times \frac{P_2 + 0.1013}{0.1013} \times \frac{273.15}{T_2 + 273.15} \times R_{H_2} \quad (3)$$

where  $\eta_{H_2}$  is the H<sub>2</sub> consumption, wt % daf;  $M_{daf,coal}$  is the weight of original coal in a daf basis, g;  $V$  is the volume of the reactor, L;  $P_1$  and  $P_2$  are the pressure in the reactor before and after reaction, respectively, MPa;  $T_1$  and  $T_2$  are the temperature in the reactor before and after reaction, respectively, °C; and  $R_{H_2}$  is the hydrogen content in the gas after reaction.

The hydrogen content in the solvent and liquid product and the H<sub>2</sub> consumption for every run are shown in Table 3. The results of hydrogen content show that the effect of the catalyst on the runs with cycle-oil is more obvious than on those with wash-oil or tetralin as solvent. The wash-oil, the fraction of coal tar from the coking process, has a very small amount of activated hydrogen which can easily be dissociated comparatively whether with or without catalyst. On the contrary, much activated hydrogen can easily be dissociated from the strong hydrogen donation solvent, tetralin, whether with or without catalyst.

(28) Ma, X.; Nagaishi, H.; Yoshida, T.; Xu, G.; Harada, M. Kinetics of rapid coal devolatilization measured using a spot heater apparatus. *Fuel Process. Technol.* **2003**, *85*, 43–49.

(29) Zhu, X.; Li, R.; Zheng, J.; Liu, C. The coal liquefaction research of highly dispersed solid acid catalysts. *Coal Convers.* **2001**, *24*, 51–61.



**Table 3. Hydrogen Content and H<sub>2</sub> Consumption<sup>a</sup>**

		liquid product and solvent			
	original solvent	N <sub>2</sub> -noncat	N <sub>2</sub> -cat	H <sub>2</sub> -noncat	H <sub>2</sub> -cat
Hydrogen Content (wt %)					
WO	7.25	7.23	7.27	7.38	7.24
HS	10.75	9.16	8.68	9.78	10.02
TL	9.09	8.25	8.25	8.22	8.36
H <sub>2</sub> Consumption (wt %, daf Coal)					
WO		−0.51 <sup>b</sup>	−2.78	1.68	1.81
HS		−1.79	−4.32	1.81	2.10
TL		−0.90	−1.81	1.70	1.97

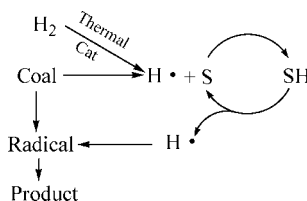
<sup>a</sup> WO, wash-oil; HS, cycle-oil; TL, tetralin. <sup>b</sup> Minus datum means some H<sub>2</sub> formed during the process.

While the cycle-oil is the mixture of aromatic compounds, the existence of the catalyst will be helpful for dissociating activated hydrogen from solvent. So, the catalytic effect on coal liquefaction with wash-oil or tetralin as solvents is less obvious than that with cycle-oil. When cycle-oil is the solvent, the lowest hydrogen content (8.68%) is in the run with a N<sub>2</sub> atmosphere and the catalyst. This is because the catalyst promotes the transfer of hydrogen from solvent to atmosphere and free radicals, and the reducing of hydrogen content in the solvent results in the lowest hydrogen content of liquid product. Also, the highest hydrogen content (10.02%) is in the run with H<sub>2</sub> and catalyst. This is because the catalyst promotes the transfer of hydrogen from H<sub>2</sub> to solvent. The results of H<sub>2</sub> consumption show that some molecular hydrogen forms for the runs with a N<sub>2</sub> atmosphere, and the yield of H<sub>2</sub> for the runs with catalyst is higher than those without catalyst. The H<sub>2</sub> produced in the DCL process with a N<sub>2</sub> atmosphere is mainly from the combination of activated hydrogen produced from the solvent. This means that the catalyst can promote the formation of activated hydrogen from the solvent. On the other hand, in the runs with a H<sub>2</sub> atmosphere, high H<sub>2</sub> consumption and high hydrogen content in the liquid product was the result. From these results it can be concluded that the catalyst accelerates the secondary distribution of hydrogen in the whole reaction system including the gas, liquid, and solid phases, which is the major role of the catalyst in the DCL process, although it also promotes coal pyrolysis.

**Hydrogen Transfer Approach in DCL.** The results of runs with wash-oil as solvent in Figure 3 show that the effect of the catalyst in DCL is not obvious, especially for the runs in a N<sub>2</sub> atmosphere, but the effect of the atmosphere is evident. Compared with that in a N<sub>2</sub> atmosphere, the oil yield increases from 6.2% to 25.1%, and the gas yield reduces from 13.1% to 4.8% for the runs in a H<sub>2</sub> atmosphere without catalysts. From these results, it can be deduced that part of the H<sub>2</sub> joining in the liquefaction reaction is not affected by the catalyst, which is the so-called thermal liquefaction.<sup>30,31</sup> Thermal liquefaction is not the major reaction approach in DCL but cannot be ignored.

(30) Sharma, R. K.; Yang, J.; Zondlo, J. W.; Dadyburjor, D. B. Effect of process conditions on co-liquefaction kinetics of waste tire and coal. *Catal. Today* **1998**, *40*, 307–320.

(31) Ding, W.; Liang, J.; Anderson, L. L. Kinetics of Thermal and Catalytic Coal Liquefaction with Plastic-Derived Liquids as Solvent. *Ind. Eng. Chem. Res.* **1997**, *36*, 1444–1452.

**Figure 5.** Scheme of the main hydrogen transfer approach (S: solvent).

The experimental results also show that the effects of the catalyst and H<sub>2</sub> are most obvious in the runs with the strongest hydrogen donation solvent, tetralin. It is thought that the main sources of activated hydrogen in DCL include thermal and catalytic cracking of coal itself, solvent, and H<sub>2</sub>, and the high oil yield and conversion are the results of the mutual effect of catalyst, strong hydrogen donation solvent, and H<sub>2</sub>.

For further understanding of the role of the solvent, another run with catalyst and H<sub>2</sub> but without solvent was carried out, and the result shows that the oil yield is below 1 wt % daf. This indicates that the “bridge” function of the solvent for hydrogen transfer from molecular hydrogen to free radical is an important part for the hydrogen transfer process besides its good solubility to coal. A strong hydrogen donation solvent can promote hydrogen transfer in the whole reaction system. Figure 5 summarizes the whole hydrogen transfer approach in the Shenhua DCL process. In the process, the activated hydrogen produced from H<sub>2</sub> first is transferred to a solvent, which becomes a H-rich solvent (SH). Then, the activated hydrogen from the H-rich solvent stabilizes the free radicals produced in coal pyrolysis to form liquid products, and the H-rich solvent becomes a H-poor solvent (S). The main function of a strong hydrogen donation solvent in the DCL process is donating and transferring activated hydrogen.

## Conclusions

The iron-based catalyst can promote coal pyrolysis and reduce the pyrolysis activation energy obviously. The major role of the iron-based catalyst in DCL is to promote the formation of activated hydrogen and accelerate the secondary distribution of H in the whole reaction system including the gas, liquid, and solid phases.

At the reaction condition adopted in this paper, the main sources of activated hydrogen in the Shenhua DCL process include thermal and catalytic cracking of coal itself, solvent, and H<sub>2</sub>, and the major transfer approach of hydrogen is from molecular hydrogen to solvent and then to coal; the solvent takes on a “bridge” role in the hydrogen transfer process. The high oil yield of DCL comes from the mutual effect of catalyst, strong donation hydrogen solvent, and H<sub>2</sub>.

**Acknowledgment.** This research was performed with the support of the National Basic Research Project (973 Project) of China (No. 2004CB217603) and the Key Program in Major Research Plan for the West of China, the National Natural Science Foundation of China (No. 90410018).

EF7006062