

EFFECT OF MOLYBDENUM SULFIDE CATALYST ON THE MECHANISM OF COAL LIQUEFACTION

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INTRODUCTION

Molybdenum sulfide catalyst has been used to improve liquefaction yield and to refine coal oils for the last 60 to 70 years [1]. It was an important step in coal liquefaction that these catalysts were developed because before that time known catalysts were poisoned by sulfur [1], an element all coals contain. In 1923, M. Pier found selective, oxidic catalysts used in methanol synthesis that were less sensitive to sulfur than the metallic catalyst that was developed from ammonia synthesis [1]. In 1924, M. Pier prepared sulfur resistant coal hydrogenation catalysts: sulfides and oxides of molybdenum, tungsten, and the iron group metals [1].

Weller and Pelipetz [2] used ammonium heptamolybdate (AHM) to liquefy Rock Springs subbituminous B coal (Table 1) and found a remarkable increase in coal conversion when using a catalyst (92.7%) relative to an uncatalyzed reaction (33.7%). Their work shows that both oils and asphaltenes increase in yield. The reaction conditions of 450°C for 1 h at 1000 psig were such that asphaltenes initially produced could easily crack to oils. However, with a change in the oil-to-asphaltene (O/A) ratio from 3.71 for the uncatalyzed reaction to 1.51 for the catalyzed reaction, it appears the catalyst functions mainly to form asphaltenes. With the use of only one coal, there is not enough data to substantiate this trend. Table 2 contains data from Garg and Givens [3] showing AHM catalyst to have virtually no effect on total conversion, but a substantial increase in the O/A ratio from 0.19 to 0.38. At their reaction conditions (825°F for 35 min at 2000 psig), molybdenum catalyst appears to function to hydrogenate asphaltenes to oils. Since these data are in contradiction to those of Weller and Pelipetz, experimental work with more coals is necessary to see how coal rank and structure relate to the mechanism of molybdenum sulfide catalyst behavior in coal liquefaction. If these data are compared to liquefaction work done in our laboratory with molybdenum sulfide catalysts at low severity reaction conditions, the beginning of an understanding of the role molybdenum catalysts play in the coal liquefaction can be developed.

EXPERIMENTAL

Three different catalyst precursors were used. Sulfided ammonium molybdate (SAM) was prepared, as described in several publications [4-6], by bubbling H₂S into a solution of ammonium heptamolybdate. Sulfided tetrahydroquinolinium molybdate (STM) of the chemical formula (THQH)₆Mo₈S₂₂O₅·H₂O (where THQH represents protonated tetrahydroquinoline) was prepared as described by Burgess and Schobert [7]. Ammonium tetrathiomolybdate (ATM) was prepared in a similar manner to SAM, except the addition of NH₄OH provided sufficient additional ammonium ions to drive the reaction to completion [8].

The coal was impregnated in the same manner as reported previously [4-6]. Coal was slurried with catalyst precursor solutions for 2 hours and vacuum freeze dried to less than 1% moisture. Although several molybdenum sulfide precursors were used, previous data have shown that the predominant active catalyst species is MoS₂ [4-9], and relative comparisons can be made about the effect of molybdenum catalysts on coal liquefaction. However, it should be recognized that the degree of dispersion of the catalyst precursors on coal could be different because three different molybdenum sulfide catalyst precursors were used.

Five coals were used. Data on the elemental composition of each coal are contained in Tables 3-8. All reactions were carried out in 25 ml microautoclave (tubing bomb) reactors, and heating was accomplished in a temperature controlled fluidized sandbath. The catalyst loading was 1% expressed as weight of molybdenum (not of molybdenum compound) on a daf basis. The reactor was flushed three times with hydrogen, with the final addition pressurized to 6.9 MPa (cold). The reactor was vertically oscillated 2.5 cm at 200 cycles per minute. Two subbituminous B coals and a hvA bituminous coal used a single stage reaction at 425°C for 10 min and a temperature-staged reaction (350°C for 1 h followed by 425°C for 10 min). The solvent used was naphthalene at a 2/1 solvent-to-coal ratio, and the mass of the coal reacted was 2.5g. A Texas lignite and a hvB bituminous coal used the following reaction conditions: a phenanthrene solvent at a 1/1 solvent-to-coal ratio, with the coal mass 5g, and the reaction temperature was 275°C for 30 min.

For the first three coals (PSOC 1266, 1401, and 1488), the cooled reactor was vented into a glass expansion bulb, and the contents were analyzed by gas chromatography using a Varian model 3700. The contents of the reactor were then rinsed with tetrahydrofuran (THF) into a dried Soxhlet thimble and extracted for about 12 h under nitrogen. The THF was removed by rotary evaporation. The solid residue was dried at 100°C for 12 h before weighing. Conversion was calculated by subtracting the weight of the residue from the weight of the coal and dividing by the dmmf weight of the coal. Liquids were further separated into asphaltenes and oils by adding hexane to the THF-soluble portion. This mixture was refluxed for 12 h under nitrogen, followed by filtration into hexane-solubles and insolubles. The hexane was removed by rotary evaporation, and the samples were dried at 100°C for 1 h before weighing. The oil (hexane-soluble) yield was calculated by difference from the conversion percentages of the gas yield, THF solubles, and the THF insolubles.

For the last two coals (DECS-1 and DECS-6), the work-up procedure was changed slightly. Gas percentages were not determined, so the calculated difference for the oils includes the gas yield as well. Once the pressure was vented from the reactor, the contents of the tubing bomb were rinsed with toluene into a dried, weighed ceramic thimble and Soxhlet extracted for about 12 h under nitrogen. The toluene was removed from the extract by rotary evaporation. Toluene-solubles were further separated into asphaltenes and oils by adding about 400 ml of hexane to the extract. The mixture was stirred for 1 h and asphaltenes were allowed to settle overnight, with solids separated by vacuum filtration. The toluene-insoluble residue was then Soxhlet extracted with THF to separate preasphaltenes from the residue. THF was removed from the extract by rotary evaporation. Preasphaltenes, asphaltenes, and residue were dried overnight under vacuum at 110°C. Conversion was calculated by subtracting the weight of the residue from the weight of the coal and dividing by the daf weight of the coal.

RESULTS AND DISCUSSION

Conversion data for coals PSOC 1266 and 1401 at 425°C for 10 min are contained in Table 3, and conversion data for these two coals at 350°C for 1h followed by 425°C for 10 min are contained in Table 4. These data were obtained by M. Epstein [2]. For the single stage at 425°C, the bituminous coal (PSOC 1266) and the subbituminous coal (PSOC 1401) reacted in a similar manner. When comparing catalyzed experiments to uncatalyzed experiments, the change in total conversion was ~25% for both coals, with oil yields decreasing and asphaltene yields increasing substantially. The O/A for PSOC 1266 was 0.32 for the uncatalyzed experiment and 0.07 for the catalyzed experiment. A similar trend was noticed with PSOC 1401 with an O/A 6.1 for the uncatalyzed experiment and 0.42 for the catalyzed experiment.

Temperature-staging had a substantial effect on conversion of both coals. For PSOC 1266, when comparing catalyzed experiments to uncatalyzed experiments, the change in total conversion was about the same, ~28%, but the increase was substantial for the oil yield, while the asphaltene yield decreased. The O/A changed from 0.22 for the uncatalyzed experiment to 1.33 for the catalyzed experiment. However, for the subbituminous coal PSOC 1401, when comparing catalyzed experiments to uncatalyzed experiments, the conversion increased ~50%, with increases in both oil and asphaltene yields. The greatest increase occurred in the asphaltene yield, with O/A for the uncatalyzed experiments 1.46 and for the catalyzed experiments 0.60.

PSOC 1488 liquefaction data using two different molybdenum sulfide catalyst precursors are located in Tables 5-7. Table 5 contains data at 425°C for 10 min, Table 6 contains data at 350°C for 1 h followed by 425°C for 10 min, and Table 7 contains data for 350°C for 1 h. At 425°C for 10 min, total conversion for the uncatalyzed experiment is low, at 25%. The experiment using SAM has a total conversion of 66%. There is little change in the oil yield (~14%), but there is a large increase in asphaltene production, from 10% for no catalyst to 46% for the SAM-catalyzed experiment. At this temperature, STM-catalyzed experiments showed poor yields, with oil yield about the same (14%) and asphaltene yield at 20%. The O/A ratio reflects this behavior by decreasing from 1.25 for the uncatalyzed experiment to 0.73 for the STM-catalyzed experiment and 0.29 for the SAM-catalyzed experiment.

Temperature-staging also had a significant effect on the catalyzed experiments. When using no catalyst, total conversion was 31%, with low oil yield (12%) and low asphaltene yield (14%). However, when comparing experiments using SAM and STM, total conversion increased to ~80%. The predominant increase for both catalytic experiments was in asphaltene yield, from 14% to 58% for SAM-catalyzed experiments and 50% for STM-catalyzed experiments. Although the STM experiment showed a lower asphaltene yield, a high oil yield (~25%) was observed compared to SAM-catalyzed experiments (~16%). STM seems to be more effective for hydrogenating asphaltenes to oils, as discussed elsewhere [9]. The O/A of the uncatalyzed experiment is 0.84, and similar to the 425°C experiments, the O/A decreased for the STM-catalyzed experiment to 0.52 and to 0.28 for the SAM-catalyzed experiment.

Data for experiments at 350°C for 1 h are located in Table 7. However, although the yields are lower than the temperature-staged experiments, the catalytic experiments showed an increase primarily in the asphaltene yields compared to uncatalyzed experiments, as in the previous results for PSOC 1488. At low severity, an indication of the coal's liquefaction ability can be readily seen, although the liquid yields are not high. The next set of data to be discussed is at even lower severity reaction conditions, but can be used to indicate a trend in how the coal will liquefy at higher reaction conditions.

Liquefaction data at 275°C for 30 min for a Texas subbituminous C coal (DECS-1) and a hvB bituminous coal (DECS-6) are located in Table 8. Conversion for DECS-1 is low at 275°C, but when comparing catalyzed experiments to uncatalyzed experiments, the predominant increase occurs in the preasphaltenes and asphaltenes and not in the oil fraction. The O/A (here A represents the sum of preasphaltenes and asphaltenes) changes from 0.32 for the uncatalyzed experiments to 0.2 for ATM-catalyzed experiments. The bituminous coal has a higher initial conversion (18% versus 6% for uncatalyzed). Although the total conversion increases in the ATM-catalyzed experiments (25%) compared to uncatalyzed experiments for DECS-6, the O/A remains constant at 0.38.

Despite the facts that different reaction conditions and different molybdenum catalyst precursors were used, there are some trends that can be seen in this whole body of work [2-9]. In the Penn State experimental work, two bituminous coals were reacted. PSOC 1266 (temperature-staged reaction) liquefaction yields (Tables 4) increased when comparing catalyzed experiments to uncatalyzed experiments, with the increased conversion being predominantly oils. DECS-6 liquefaction yields (Table 8) increased when comparing catalyzed experiments to uncatalyzed experiments, where liquefaction yield increases were equal between oils and asphaltenes. DECS-6 was reacted at very low severity reaction conditions (275°C), however, and cracking asphaltenes to oils at 275°C may be difficult. If these data are compared to Garg and Given's data (Table 2) [3], in which they used a hvC bituminous coal, a similar trend is noticed. They obtained a very high liquefaction conversion without catalyst (85%), and although in the catalytic experiment the total conversion did not increase much (87%), the O/A increased from 0.19 to 0.38. The molybdenum catalyst appears to function predominantly to hydrogenate asphaltenes to oils because, in all of these cases, initial conversion to asphaltenes even without catalyst is usually high. There was one exception with PSOC 1266 for the 425°C/10 min experiment (Table 3). The O/A ratio decreased when comparing the catalyzed experiment to the uncatalyzed experiment from 0.32 to 0.07. This phenomenon may be because the reaction conditions do not allow enough time for asphaltenes to be hydrogenated to oils. PSOC 1488, a subbituminous coal, (Table 5) at 425°C/10 min shows a similar occurrence. However, for

experiments using STM, reaction yields are very low, and may be due to poisoning of MoS₂ by products of THQ decomposition [9].

Three subbituminous coals were reacted. Liquefaction yields for all three (Tables 3-8) were substantially increased by the use of catalyst. For PSOC 1401, for the temperature-staged experiment, total conversion (Table 4) increased from 42% to 91%, where the increase in conversion was predominantly in the asphaltenes. The O/A ratio changed from 1.46 for the uncatalyzed experiment to 0.60 for the SAM-catalyzed experiment. For PSOC 1488, for all reaction conditions and both catalyst precursors (Tables 5-7), the catalytic experiments showed an increase in total conversion compared to uncatalyzed experiments, where the predominant increase was in the asphaltenes. DECS-1 (Table 8) showed a similar trend. Weller and Pelipetz [2] also show a similar trend (Table 1). The catalyst appears to first function to break apart the macromolecular network, and then, function to hydrogenate some of the asphaltenes to oils if conditions are conducive to do so. So why is the molybdenum catalyst functioning differently in bituminous and subbituminous coals?

Subbituminous coals contain more oxygen and are thought to be more highly crosslinked than bituminous coals. Hirsch describes low-rank coals with an open structure where there are many crosslinks (heteroatoms and hydrocarbon chains) connected to small aromatic systems (3 rings or less) [10]. Bituminous coals (85-91% C) tend to have a liquid structure, where there are fewer crosslinks, larger aromatic systems, and overall more order in structure [10]. Without catalyst or hydrogen donor solvent, little atomic hydrogen is available externally because hydrogen radicals generated from H₂ tend to react with each other before being able to react with radicals as the crosslinks break apart. Since ether, thioether, and some carbon-carbon bonds are relatively weak [11-13], if catalyst provides atomic hydrogen at the milder reaction conditions ($\leq 350^{\circ}\text{C}$ or temperature-staging), radicals can be generated more slowly and capped more efficiently to form asphaltenes. Since subbituminous coals in general contain more crosslinks to break apart, the catalyst functions mainly to provide hydrogen for capping generated radicals. Hence the large asphaltene yields and relatively large conversions for subbituminous coals when using molybdenum catalyst. Bituminous coals contain fewer crosslinks, so the requirement for radical capping with hydrogen supplied via the catalyst is lower relative to subbituminous coals. Therefore, molybdenum catalyst can function to hydrogenate generated asphaltenes to oils.

CONCLUSIONS

When coal liquefies, there are competing reaction mechanisms of coal depolymerization to asphaltenes, repolymerization of generated radicals to char, and the formation of oils from asphaltenes. It appears that molybdenum sulfide catalyst, during temperature-staging and low severity conditions, primarily intervenes in liquefaction for subbituminous coals to provide atomic hydrogen to cap depolymerized coal fragments that form asphaltenes. This is because subbituminous coal contain a relatively high crosslink density compared to higher ranks of coals, and the catalyst remains very busy generating asphaltenes. For bituminous coals, conversions without catalyst tend to be relatively high, so molybdenum catalyst primarily intervenes to provide atomic hydrogen to help crack asphaltenes to oils. Because the crosslink density in bituminous coal is lower than in subbituminous coal, the catalyst is not as involved in capping radicals and can be effective as a hydrogenation vehicle to generate oils. Repolymerization is reduced as the activity in the other processes increases, therefore, less char is produced. For the coals DECS-1,6, work is still in progress to include temperature-staging and to evaluate various methods of dispersing catalyst. These results will be reported at future meetings. Since the sample set is quite small, similar experiments on a larger set of coals would provide more insight into the role rank plays with molybdenum catalyst and low severity coal liquefaction.

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Table 1: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Data from Weller and Pelipetz [7]

Authors	Weller and Pelipetz [7]	
Coal	Rock Springs - Sub B - C-73.9, H-5.0, N-1.5, S-0.8, O-13.6	
Conditions	450°C, 1 hr, 1000 psi H ₂	
Conversion	No Catalyst	AHM^c
Tot Conv (Benzene Insolubles)^a	33.7	92.7
Oils (Hexane Solubles)	10.4	41.1
Asphaltenes (Benzene Sol/Hexane Insol)	2.8	27.2
O/A^b	3.71	1.51

- a) Total conversion.
- b) Oil to asphaltene ratio.
- c) Catalyst is ammonium heptamolybdate.

Table 2: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Data from Garg and Givens [8]

Authors	Garg and Givens [8]	
Coal	Kentucky Elkhorn #2 -hvCb C-77.8 H-5.2, N-1.8, S-1.1, O-7.2	
Conditions	825°F, 35 min, 2000 psig, H ₂ 18.9 MCF/T	
Conversion	No Catalyst	AHM^c
Tot Conv (THF Insolubles)^a	85.3	86.8
Oils (Hexane Solubles)	12.2	21.7
Asphaltenes (THF Sol/Hexane Insol)	65.4	57.9
O/A^b	0.187	0.375

- a) Total conversion.
- b) Oil to asphaltene ratio.
- c) Catalyst is ammonium heptamolybdate.

Table 3: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Epstein [2]

Author	Epstein [2]			
Coals	PSOC 1266-dmmf- hvAb - C-83.2, H-5.0, N-2.1, S-0.5, O-8.6			
	PSOC 1401-dmmf-Sub B - C-74.3 H-5.2, N-1.1, S-0.2, O-19.3			
Conditions	425°C, 10 min, 1000 psi H ₂			
Coal	PSOC 1266		PSOC 1401	
Conversion	No Cat ^d	SAM ^e	No Cat	SAM
Tot Conv (THF Insol)^a	58.1	72.6	42.5	66.7
Oils (Hex Sol)	13.7	4.8	28.8	17.6
Asph (THF. Sol/Hexane Insol)^b	42.8	66.7	4.7	41.8
Gas	1.6	1.1	9.0	7.3
O/A ^c	0.32	0.07	6.1	0.42

- a) Total conversion.
- b) Asphaltenes.
- c) Oil to asphaltene ratio.
- d) No catalyst.
- e) Catalyst is sulfided ammonium molybdate.

Table 4: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Epstein [2]

Author	Epstein [2]			
Coals	PSOC 1266-dmmf- hvAb - C-83.2, H-5.0, N-2.1, S-0.5, O-8.6			
	PSOC 1401-dmmf-Sub B - C-74.3 H-5.2, N-1.1, S-0.2, O-19.3			
Conditions	350°C, 1 h/425°C, 10 min, 1000 psi H ₂			
Coal	PSOC 1266		PSOC 1401	
Conversion	No Cat ^d	SAM ^e	No Cat	SAM
Tot Conv (THF Insol)^a	59.0	77.3	41.9	90.7
Oils (Hex Sol)	10.2	48.8	14.5 g	28.2 g
Asph (THF. Sol/Hexane Insol)^b	47.3	36.8	9.9	46.7
Gas^f	2.5	2.4	17.5	15.8
O/A ^c	0.22	1.33	1.46	0.60

- a) Total conversion.
- b) Asphaltenes.
- c) Oil to asphaltene ratio.
- d) No catalyst.
- e) Catalyst is sulfided ammonium molybdate.
- f) Gas a total of both stages.
- g) Corrected data.

Table 5: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Burgess and Schobert [5,9]

Author	Burgess and Schobert [5,9]		
Coals	PSOC 1488-dmmf-Sub B - C-76.6, H-5.2, N-1.0, S-0.5, O-17.2		
Conditions	425°C, 10 min, 1000 psi H ₂		
Coal	PSOC 1488		
Conversion	No Cat^d	SAM^e	STM^f
Tot Conv (THF Insol)^a	25.4	65.7	42.7
Oils (Hex Sol)	12.0	13.1	14.6
Asph (THF. Sol/Hexane Insol)^b	9.6	45.8	20.0
Gas	3.9	6.8	8.1
O/A^c	1.25	0.29	0.73

- a) Total conversion.
- b) Asphaltenes.
- c) Oil to asphaltene ratio.
- d) No catalyst.
- e) Catalyst is sulfided ammonium molybdate.
- f) Catalyst is sulfided tetrahydroquinolinium molybdate.

Table 6: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Burgess and Schobert [5,9]

Author	Burgess and Schobert [5,9]		
Coals	PSOC 1488-dmmf-Sub B - C-76.6, H-5.2, N-1.0, S-0.5, O-17.2		
Conditions	350°C, 1h/425°C, 10 min, 1000 psi H ₂		
Coal	PSOC 1488		
Conversion	No Cat^d	SAM^e	STM^f
Tot Conv (THF Insol)^a	30.8	78.5	80.1
Oils (Hex Sol)	11.7	16.2	25.2
Asph (THF. Sol/Hexane Insol)^b	13.9	57.7	49.5
Gas	5.2	5.5	5.5
O/A^c	0.84	0.28	0.52

- a) Total conversion.
- b) Asphaltenes.
- c) Oil to asphaltene ratio.
- d) No catalyst.
- e) Catalyst is sulfided ammonium molybdate.
- f) Catalyst is sulfided tetrahydroquinolinium molybdate.

Table 7: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Burgess and Schobert [5,9]

Author	Burgess and Schobert [5,9]		
Coals	PSOC 1488-dmmf-Sub B - C-76.6, H-5.2, N-1.0, S-0.5, O-17.2		
Conditions	350°C, 1h 1000 psi H ₂		
Coal	PSOC 1488		
Conversion	No Cat ^d	SAM ^e	STM ^f
Tot Conv (THF Insol) ^a	18.3	47.8	48.5
Oils (Hex Sol)	6.8	10.2	11.1
Asph (THF. Sol/Hexane Insol) ^b	7.1	33.9	33.8
Gas	4.4	3.8	3.6
O/A ^c	0.96	0.30	0.33

- a) Total conversion.
- b) Asphaltenes.
- c) Oil to asphaltene ratio.
- d) No catalyst.
- e) Catalyst is sulfided ammonium molybdate.
- f) Catalyst is sulfided tetrahydroquinolinium molybdate.

Table 8: Liquefaction Conversion Data Comparing the Use of Molybdenum Catalyst to Using No Catalyst - Data from Davis et al. [6]

Authors	Davis, Schobert, Mitchell, and Artok [6]			
Coals	DECS 1-dmmf - Sub C - C-76.1, H-5.5, N-1.5, S-1.1, O-15.8			
Conditions	DECS 6 -dmmf - hvB b - C-80.8, H-6.1, N-1.6, S-0.5, O-11.0			
Conditions	275°C, 30 min, 1000 psi H ₂			
Coal	DECS - 1		DECS - 6	
Conversion	No Cat ^e	ATM ^f	No Cat	ATM
Tot Conv (THF Insol) ^a	6.6	9.0	17.7	25.0
Oils (Hex Sol) + Gas	1.6	1.5	4.9	6.9
Asph (Tol. Sol/Hexane Insol) ^b	2.2	3.6	2.1	3.0
Preasph.(THF Insol/Tol. Sol) ^c	2.8	3.9	10.7	15.1
O/A (where A=Asph+Preasph) ^d	0.32	0.2	0.38	0.38

- a) Total conversion.
- b) Asphaltenes.
- c) Preasphaltenes.
- d) Oil to asphaltene ratio.
- e) No catalyst.
- f) Catalyst is ammonium tetrathiomolybdate.