TITLE	NOVEL SLURRY PHASE DIESEL CATALYSTS FOR COAL-DERIVED SYNGAS
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ABSTRACT

OBJECTIVE

The primary objective of this research program is to develop attrition resistant catalysts that exhibit high activities for conversion of coal derived syngas (H_2/CO ratio of ~ 0.7). The specific objective is to develop novel catalysts for synthesis of clean diesel fuels from coal.

ACCOMPLISHMENTS TO DATE

We have continued our work on the characterization of Fe Fischer-Trospch catalysts using x-ray diffraction, Mossbauer spectroscopy and Transmission Electron Microscopy that was initiated in our previous UCR grant. Our results have been summarized in presentations at the International Conference on Electron Microscopy, at the Natural Gas Conversion meeting and the ACS symposium on syngas conversion. Our major finding is that the active state of an Fe Fischer-Tropsch catalyst involves highly dispersed iron carbide particles. However, a Fe catalyst pretreated in CO and converted to iron carbide is not in its most active state. During reaction conditions at high pressure, we see a phase transformation that causes a breakup of the initially formed carbide particles into nanosized particles. These nanosized particles have a high surface area that leads to enhanced activity for Fischer-Tropsch synthesis. These findings have major implications for the design of attrition resistant Fe catalysts for F-T synthesis. It is not sufficient to create a catalyst that is strong initially in its spray dried form, but we need one that can

accommodate the chemical attrition that accompanies phase transformations under synthesis conditions. Consequently, our efforts are directed at novel catalyst morphologies with a porous structure that provides access to the nano-sized carbide particles but at the same time prevents the transport of these carbide particles into the Fischer-Tropsch slurry reaction products. We have also examined the attrition resistance of catalysts previously prepared by Prof. Bukur at TAMU that have been shown to be very active and selective for the production of coal-derived syngas. Our initial tests show that these catalysts may possess adequate attrition resistance, but their irregular particle sizes and shapes may not be desirable for a slurry reactor due to posible unfavorable hydrodynamics. Our SEM analysis also shows that many of the commonly available catalyst supports may not possess the desired spherical particle morphology.

During the past year, Prof. Bukur and his student at Texas A&M have initiated runs on the F-T synthesis reactor so that realistic reactor tests of the catalysts synthesized in this research program can be performed. Prof. Bartholomew and his student at BYU have initiated work on Mossbauer synthesis that will complement the characterization at UNM for the study of phase evolution of the F-T catalysts that are synthesized in this effort.

SIGNIFICANCE TO FOSSIL ENERGY PROGRAMS

The Fischer-Trospch synthesis represents a viable approach to convert natural gas and coal into liquid fuels. Most current interest in this field is directed at natural gas conversion and the catalyst of choice appears to be Cobalt based. However, Fe catalysts have several advantages, they are cheap, can tolerate a wide range of H_2:CO ratios and they provide high reactivities. The disadvantage is that the high iron loadings make these catalysts friable and attrition that takes place during their use in a slurry bubble column reactor make product wax separation very difficult. Hence, the synthesis of novel attrition resistant catalysts is very important for further development of alternative fuel sources to meet our nation's transportation needs.

PLANS FOR THE COMING YEAR

- Continue synthesis of novel attrition resistant catalysts at the bench scale
- Commence testing of the most promising catalysts in fixed bed reactors
- Perform simulated slurry bubble column runs to establish attrition behavior
- Continue characterization studies to improve understanding of support and promoter effects

ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Journal Articles & Conference proceedings

- H. Pham and A. K. Datye, "The Synthesis of Attrition Resistant Slurry Phase Iron Fischer-Tropsch Catalysts", Preprints of the Div. Of Petr. Chem., Amer. Chem. Soc., vol. 44, pg 115-118 (1999).
- Y. Jin, L. Mansker and A. K. Datye, "The Nature of the Active Phase in Iron Fischer-Tropsch Catalysts", Preprints of the Div. Of Petr. Chem., Amer. Chem. Soc., vol. 44, pg 97-99 (1999).
- Y. Jin and A. K. Datye, " Phase Transformations in Iron-Fischer Tropsch Synthesis (FTS) Catalysts", Proc. Intl. Congr. Electron Microscopy, Cancun 1998, vol. II, pg 379 – 380.
- Y. Jin and A. K. Datye, "Characterization of Slurry Bubble Column Iron Fischer-Tropsch Catalysts", "Natural Gas Conversion V, Stud. Surf. Sci. Catal., 199, pg 209-214 (1998).
- N. B. Jackson, L. Evans and A. K. Datye, "Attrition Determining Morphology Changes in Iron Fischer-Tropsch Catalysts," Natural Gas Conversion V, Stud. Surf. Sci. Catal., 199, pg 137-142 (1998).
- H. N. Pham and A. K. Datye, "Measuring the Strength of Slurry Based Heterogeneous Catalysts", Powder Technology, in press.
- H. N. Pham, A. Viergutz, R. J. Gormley and A. K. Datye, "Improving the Attrition Resistance of Slurry Phase Heterogeneous Catalysts", "Powder Technology", submitted.
- H. N. Pham and A. K. Datye, "The Synthesis of Attrition Resistant Slurry Phase Iron Fischer-Tropsch Catalysts", "Catalysis Today", submitted.
- L. D. Mansker, Y. Jin, D. B. Bukur and A. K. Datye, "Characterization of Slurry Phase Iron Catalysts for Fischer-Tropsch Synthesis", Appl. Catal., submitted.

Conference Presentations

- Y. Jin and A. K. Datye, " Phase Transformations in Iron-Fischer Tropsch Synthesis (FTS) Catalysts", presented at the International Congress of Electron Microscopy, Cancun, 1998.
- N. B. Jackson, L. Evans and A. K. Datye, "Attrition Determining Morphology Changes on Iron Fischer-Tropsch Catalysts"" presented at the Proceedings of the 5t^{h} International Natural Gas Conversion Symposium, Italy, 1998.
- Y. Jin and A. K. Datye, "Characterization of Bubble Column Slurry Phase Iron Fischer-Tropsch Catalysts", presented at the Proceedings of the 5t^{h} International Natural Gas Conversion Symposium, Italy, 1998.
- L. D. Mansker and A. K. Datye, "Quantitative Diffraction Methods Applied to the Characterization of Working Iron Fischer-Tropsch Catalysts", presented at the 13th Annual Western States Catalysis Club Meeting, Albuquerque, 1999.
- Y. Jin, L. Mansker and A. K. Datye, "The Nature of the Active Phase in Iron Fischer-Tropsch Catalysts", presented at the 13th Annual Western States Catalysis Club Meeting, Albuquerque, 1999.
- H. N. Pham and A. K. Datye, "The Synthesis of Attrition Resistant Slurry Phase Iron Fischer-Tropsch Catalysts", presented at the 13th Annual Western States Catalysis Club Meeting, Albuquerque, 1999.

- H. Pham and A. K. Datye, "The Synthesis of Attrition Resistant Slurry Phase Iron Fischer-Tropsch Catalysts", presented at the 217th National Meeting, American Chemical Society, Symposium of Syngas Conversion to Fuels and Chemicals, Anaheim, 1999.
- Y. Jin, L. Mansker and A. K. Datye, "The Nature of the Active Phase in Iron Fischer-Tropsch Catalysts", presented at the 217th National Meeting, American Chemical Society, Symposium of Syngas Conversion to Fuels and Chemicals, Anaheim, 1999.

Students Supported under this grant

- Yaming Jin (Ph. D.), student in chemical and nuclear engineering, Univ. of New Mexico
- Linda Mansker (Ph. D.) student in chemical and nuclear engineering, Univ. of New Mexico
- Hien Pham (Ph. D.) student in chemical and nuclear engineering, Univ. of New Mexico
- Magnus Bergroth, undergraduate student in chemical and nuclear engineering. Magnus worked on this project last summer supported by the NSF/REU program. He has since continued working during the semester
- Alec Klinghoffer (Ph. D) student in chemical engineering, Texas A&M university
- J. Xu (Ph. D.) student in chemical engineering at Brigham Young University