TITLE: **CATALYTIC GASIFICATION OF COAL USING EUTECTIC SALT MIXTURES**

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ABSTRACT

OBJECTIVES

The project, Catalytic Gasification of Coal Using Eutectic Salt Mixtures, is being conducted jointly by Clark Atlanta University (CAU), the University of Tennessee Space Institute (UTSI) and the Georgia Institute of Technology (GT). The aims of the project are to:

- Identify appropriate eutectic salt mixture catalysts for the gasification of Illinois #6 coal;
- Evaluate various impregnation or catalyst addition methods to improve catalyst dispersion;
- Evaluate effects of major process variables (e.g., temperature, system pressure etc) on coal gasification;
- Evaluate the recovery, regeneration and recycle of the spent catalysts in a bench-scale fixed bed reactor; and
- Conduct thorough analysis and modeling of the gasification process to provide a better understanding of the fundamental mechanisms and kinetics of the process.

ACCOMPLISHMENTS TO DATE

Several binary and ternary eutectic catalysts have been identified for the gasification of coal. The eutectic catalysts identified increased gasification rate significantly. The methods of catalyst preparation and addition had significant effect on the catalytic activity and coal gasification. The catalytic activity increased by varying degrees with catalyst loading.

Based on the TGA studies, the 43.5% Li_2CO_3-31.5% Na_2CO_3-25% K_2CO_3(LNK) and 39% Li_2CO_3-38.5% Na_2CO_3-22.5% Rb_2CO_3(LNR) ternary eutectics and the 29% Na_2CO_3-71% K_2CO_3 (NK) binary eutectic were selected for the bench scale fixed-bed studies.

Experiments were carried out to obtain a kinetic expression of the Langmuir-Hinshelwood type for the hetergeneous gasification reaction. The effect of the amount of steam on the water-gas shift reaction was elucidated from the experiments carried at different steam flow rates for the catalyst systems studied. It was found to be in accordance with the thermodynamics of the shift reaction. A simple Langmuir-Hinshelwood model, excluding the effect of hydrogen inhibition provided a reasonably good fit to the experimental data at different temperatures and steam flow rates. The general form of the Langmuir-Hinshelwood expression obtained was:

$$R = K_1 P_{H2O} / (1 + K_2 P_{H2O})$$

Where R is the specific gasification rate (min^{-1}), K_1 is the reaction rate constant, K_2 is the adsorption constant and P_{H2O} is the partial pressure of steam in the bed (kPa)

The ternary catalyst system was a much better eutectic catalyst compared to the binary catalyst system. In general, eutectics with melting point less than the gasification temperature were better substitutes to the single alkali metal salts because they resulted in better catalyst distribution and dispersion in the carbon matrix when in the liquid phase. At 10 wt % of catalyst loading, the activation energy of the ternary catalyst system (LNK) was about half (98kJ/mol) the activation energy for the single catalyst system (K_2CO_3), which was about 170 kJ/ mole. The binary catalyst system (NK) showed an activation energy of about 201 kJ/mol, which was slightly higher compared to the K_2CO_3 catalyst system.

The study of the effects of water-to-char ratio and agitation time on the catalyst recovery showed that these two parameters do not significantly affect the extraction efficiency of the catalyst ions from the gasified char.

The XRD characterization confirmed that there are some new phases such as $NaKCO_3$, $LiNaCO_3$, and most notably $LiKCO_3$ formed during the gasification. This may contribute to the eutectics having higher catalytic activity. It was also found that a new intermediate

specie, $KLiSO_4$ exists in the gasified char. The effect of the different intermediates will be discussed and studied in the future.

PLANS FOR THE COMING YEAR

- The bench scale fixed-bed gasification reactor studies will concentrate on the ternary catalyst system 39% Li_2CO_3-38.5% Na_2CO_3-22.5% Rb_2CO_3.
- Evaluate the recovery, regeneraton and recycle of the spent catalysts. Future work will focus on the effect of temperature on the water extraction efficiency and the regeneration and recycle of the catalysts. Other means of catalyst recovery such as lime or acid extraction may be evaluated in the coming period.
- Characterization of the catalysts, coal/catalyst samples and products will be undertaken to assess catalyst dispersion and the effectiveness of the catalysts and impregnation/addition methods.
- Data analysis and modeling, economic evaluation of the gasification process and project management and reporting will also continue in the future.

ARTICLES, PRESENTATIONS, AND STUDENT SUPPORT

Journal Articles (Prepared and Ready to be Submitted for Publication)

- Yeboah, Y. D., Y. Xu, A. Sheth, A. Godavarty, P. Agrawal, Catalytic Gasification of Coal Using Eutectic Salts: I. Identification of Eutectics.
- Godavarty, A., A. Sheth, Y. D.Yeboah, Y. Xu, P. Agrawal, Catalytic Gasification of Coal Using Eutectic Salts: II. Reaction Kinetics.
- Godavarty, A., A. Agarwal, Distribution and Catalytic Activity of Eutectic Salts in Steam Gasification of Coal.

Conference Presentations/Proceedings and Technical Reports

- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, Semi-annual-Process Report to DOE, April, 1998
- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, Semi-annual-Process Report to DOE, Oct., 1998.
- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, Semi-annual-Process Report to DOE, April, 1999.
- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, "Catalytic Gasification of Coal Using Eutectic Salt Mixtures", presented at 7th Annual Historically Black Colleges and Universities and Other Minority Institutions, Miami, Florida, April, 1999.
- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, "Catalytic Gasification of Coal Using Eutectic Salt Mixtures", DOE University Coal Research Conference, Pittsburgh, PA, June, 1999
- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, Semi-annual-Process Report to DOE, Oct., 1999.

- Yeboah, Y. D., Y. Xu, A. Sheth, P. Agrawal, Semi-annual-Process Report to DOE, April, 2000.

Students Supported under this Grant

- Antron Palmer and Tamara Gray, graduated with BS in Chemical Engineering from Clark Atlanta University (CAU) in May 1999. They are currently working with Milleken Corp. and the US Patent office respectively.
- Pamela Reid is a senior in Chemical Engineering at CAU and is due to graduate in May 2000. She has been accepted for graduate school in Chemical Engineering at Michigan University and Florida A&M University.
- Latanya Funches is a Junior in Chemical engineering at CAU
- Anuradha Godavarty graduated with MS degree in chemical Engineering from The University of Tennessee Space Institute (UTSI) in August 1999. She is currently pursing a Ph.D at Texas A&M University.
- Chandramouli Sastry is a graduate student in chemical Engineering at UTSI.
- Megan Czarny is an undergraduate student in Chemical Engineering at Georgia Institute of Technology (Georgia Tech).