D1.10

Executive Summary

With increasing energy demands in the U.S., efficient and environmentally acceptable use of our nation's most abundant fossil fuel resource, coal, has become even more crucial. Coal is the most important fuel for electric power generation since it provides 52% of the U.S. electricity and over 87% of the Ohio electric needs [www.americancoalcouncil.org, www.ohiocoal.com]. Advanced technologies that utilize the vast coal reserves in the U.S. and particularly in Ohio in a clean and efficient way will definitely be of increasing significance. Recently, hydrogen production through integrated gasification combined-cycle (IGCC) has emerged as a highly promising technology. The commercialization of these joint power and hydrogen plants needs significant improvements in some of the steps following gasification to produce H_2 more efficiently and economically. As highlighted in a recent USDOE document (www.fe.doe.gov), among them is the water-gas shift reaction, which remains as a technology that would benefit from innovative approaches such as development of highly active, stable, and Cr-free catalysts. The availability of a highly effective catalytic system will play a critical role in the advancement of coal-based electric power generation technologies. However, the design of such a system remains a challenging task. Generally, high-temperature water-gas shift (HT-WGS) reaction is performed over Fe-Cr catalysts. In fact, these catalytic systems are designed to be used primarily for synthesis gas produced from natural gas and do not meet the challenges presented by using coal as the starting fossil fuel. Not surprisingly, sulfur poisoning becomes a much more serious problem for coal-derived syngas. Furthermore, use of Cr poses additional complications due to harmful effects of Cr6+ on human health. Therefore, the development of highly active, sulfur-tolerant, and Cr-free HT-WGS catalysts will bring about the successful use of coal-derived syngas for hydrogen production, resulting in enhanced use of vast Ohio coal reserves. This technology will also provide a missing link between coal use and fuel cell technology, which clearly will play a very important role for the energy needs and the economic development of both the state of Ohio and the nation. As the second year of this project, we are proposing to build upon the foundation which was initiated during the last year that we were part of Consortium III. Our reaction and characterization studies in the first year have already demonstrated the proposed research is on solid ground for continuation. It is found that aluminum is a potential chromium replacement in Fe-based HT-WGS catalysts. In addition, Cu-promoted Fe-Al catalysts exhibit a significant improvement in WGS activity, suggesting that Fe-Al-Cu catalysts are promising candidates for the water-gas shift reaction of coal-derived synthesis gas. If funded, our main focus will be to continue working on high-temperature water-gas shift (HT-WGS) reaction over our best-performing Fe-Al-Cu catalysts designed specifically for coal-derived synthesis gas resulting from coal gasification. Work performed in the second year of the proposed project will be continuation of catalyst development to further improve catalytic activity and stability, in-depth catalyst characterization studies including post-reaction, detailed kinetic studies, and economic analysis of the proposed process and its feasibility for hydrogen production from coal. It is realized that, without efficient sulfur removal, syngas produced from coal gasification contains considerable amounts of H_2S (0.2-1%), leading to sulfur poisoning. Investigation of sulfur tolerance and inhibition effects of other constituents found in coal gas (i.e., COS, CO_2, CH4) will also be conducted.