

Chapter 1

Introduction

This project was initiated in October 1991 as a joint project between West Virginia University and Union Carbide Technical Center. The project has two main tasks. Task 1 focuses on catalyst evaluation and reaction engineering. Task 2 includes process synthesis studies and engine performance tests on alcohols and mixtures of alcohols with petroleum-based fuels.

During the initial phase of the project, the Task 1 group installed and successfully operated two automated reactor systems and three types of reactors for catalyst testing. Over 100 catalysts were tested and evaluated for higher alcohol synthesis. The Task 1 group issued a topical report on higher alcohol synthesis from catalysts obtained by vapor phase thermolysis. Transition metal-based catalysts were prepared and evaluated. Reactor simulation models were developed as part of Task 1. The Task 1 coordinators were Ed Kugler and Dady Dadyburjor. Other Task 1 investigators were Jeff Peterson, Mike Close, Ray Yang, and Walter Hart of Union Carbide.

The Task 2 group developed a computational framework to evaluate the economics of syngas to alcohols processes. A topical report was prepared on the economics of seven base cases for alcohol fuels production. Lurgi, Shell, and Texaco gasification technologies were included, as well as a natural gas case for baseline comparisons. Task 2 included a test program using a single-cylinder variable compression engine to evaluate emissions from mixed alcohol/gasoline blended fuels. The Task 2 coordinator was Joe Shaeiwitz. Other investigators were Richard Turton, Tom Torries, Mridul Gautam, Reda Bata, Wallace Whiting and Manuk Colakyan of Union Carbide.

Carl Irwin, Alan Martin, and Duane Dombeck of Union Carbide were responsible for overall project management and coordination.

This Final Report consists of 20 chapters. Chapters two through six are based on peer reviewed publications resulting from Task 1 research. Chapters 7 through thirteen plus Appendices A through H are from the Topical Report on comparative process economics prepared by the Task 2 group. Chapters 15 through 17 are published in Proceedings of the Pittsburgh Coal Conference. Chapter 18 is a refereed conference paper Chapters 19 and 20 are currently submitted for publication. Results, discussion, and conclusions are included with the particular chapter to which they apply. Similarly, reference and bibliography sections are retained with the applicable chapters.

In addition to extensive research results reported in refereed publications and conference presentations, the project supported approximately six Masters Degree students, one Ph.D. student and four post-doctoral students. These students are now all employed in academic or high-level technical positions in industry.