

## II. Introduction

The objective of Contract DE-AC22-81PC40077, under which the work described here was performed, was to develop a cost effective catalytic process for converting syngas ( $H_2 + CO$ ) to liquid hydrocarbon fuels (LHF) including gasoline, turbine and diesel fuel. The catalytic process was to use microporous crystalline catalysts - also known as Shape Selective Catalysts (S.S.C.) or "Molecular Sieves" - in combination with metal catalysts (M.C.) from the Group VIII transition metals.

As a result of the upheavals in the petroleum economy during the 1970's, and the simultaneous growing pressure on the available petroleum reserves for use in non-fuel applications, the search for alternatives to petroleum based energy became a major national priority. Against this background, and to draw on Union Carbide's special expertise in the catalytic chemistry of hydrocarbons and in molecular sieve catalysis, the present contract was started in 1981.

The original term of 30 months, from the starting date of March 1981, was extended by agreement, first to 36 months, and again to 42 months. Development work was completed in September 1984.

Most of the first twelve months was occupied by preparatory work. This included:

- Assembly of staff,
- Allocation and remodeling of laboratory facilities,
- Specification, procurement, installation, testing, and calibration of experimental apparatus,
- Design of preliminary test protocols,
- Design, preparation, installation, and debugging of analytical techniques and computer software,
- Shake-down runs from which the final test protocols were derived.

#### Task 1

The objective of Task 1 was to select one or more of the promising microporous molecular sieve crystal catalysts from Union Carbide's product portfolio, as candidates for initial testing in Task 2. To identify the capabilities of these materials for synthesizing the desired higher molecular weight liquid hydrocarbons from light intermediates, they were to be tested without the use of metal components.

Two series of tests were to be carried out on the selected catalysts. One set would employ methanol as the feed and the other would employ propylene.

Work on Task 1 began in June 1981 and was completed in February 1983.

## Task 2

The objective of Task 2, which was the main thrust of the contract, was to develop a catalyst and process for the most cost-effective synthesis of liquid hydrocarbon fuels from syngas.

The catalytic systems contemplated were combinations of one or more SSC's (identified as the best candidates from Task 1 results) with one or more of the MC's of known effectiveness in catalyzing the synthesis of light intermediates from syngas.

The first tests in Task 2 were conducted in June 1982 and the work continued through the remaining term of the contract.

## Task 3

Task 3 was a fundamental study of surface effects and reaction intermediates during the hydrogenation of carbon monoxide on transition metal catalysts. The objective was to support Task 2 efforts in two respects:

First, to characterize the surface structure and chemical intermediates of several important MC catalyst candidates using the most advanced scientific techniques and skills available.

Second, to determine the primary hydrocarbon (or alcohol) products obtained on a few selected MC catalysts.

These findings were to be fed continuously into the work on Task 2.

Because of their expertise in surface studies and in the design and construction of appropriate test apparatus, Task 3 was conducted by Professor G. A. Somorjai, University of California at Berkeley, under a subcontract. The subcontract was started in June 1981 and completed in February 1984.

The Final Technical Report for Task 3 was delivered as Appendix B of the Third Annual Report, for the period March 1983 to February 1984, and will not be repeated here.

#### Task 4

Task 4 comprised the tasks of program management and the preparation of technical reports.