TRIFUNCTIONAL CATALYSTS FOR CONVERSION OF SYNGAS TO ALCOHOLS. FIRST QUARTERLY REPORT, SEPTEMBER 1-NOVEMBER 30, 1984

DELAWARE UNIV., NEWARK. DEPT. OF CHEMICAL ENGINEERING

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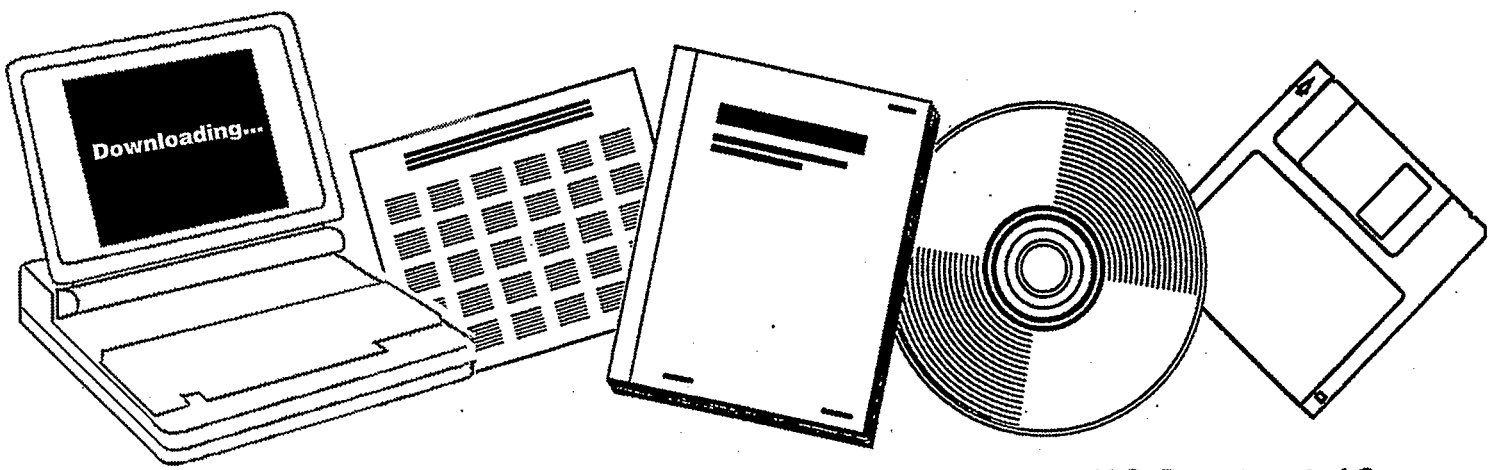

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TRIFUNCTIONAL CATALYSTS FOR CONVERSION OF SYNGAS TO ALCOHOLS

First Quarterly Report for Period
September 1, 1984 to November 30, 1984

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ABSTRACT

The proposed program has been actively initiated, beginning September 1, 1984, as authorized by DOE. In addition to the coprincipal investigators, two key individuals have joined the project: Dr. Sudhakar Chakka, an experienced Post Doctoral Fellow and Mr. Nazeer A. Bhore, a well qualified graduate student who has selected this project for his Ph.D. thesis. Suitable laboratory space has been assigned in the new Spencer Laboratory. Each of the tasks have been addressed and are discussed briefly in this report. Work has started on catalyst preparation and planning for near-term characterization. Considerable effort has been expended in design of the system for testing syngas conversion, including the option of activation of a previously constructed system.

A literature review is underway including current publications, to ensure advantage is being taken of the intensive research effort underway worldwide.

OBJECTIVES:

Task 1. Preparation of Catalyst Samples
2. Testing Catalysts for Snygas Conversion
3. Measurement of Surface Composition and Structure
4. Determination of Nature of Surface Complexes
5. Reaction Mechanism Determination by Isotopic Tracers and Kinetics
6. Design, Prepare and Test Optimized Catalysts

Task 1. Preparation of Catalyst Samples

Catalyst selection is based on the concept of providing scientific information so as to relate performance to structure, especially the electronic (oxidation) state of the metal, as influenced by support and modifiers.

Initial catalysts to be prepared are 3% $Rh-Al_2O_3$, unmodified and modified by potassium, or manganese, or an aromatic amine, or sulfur, or lanthanum.

Variation in preparative techniques will be investigated, e.g. ion exchange, impregnation or coprecipitation so as to chemically bind the rhodium in such a manner to prevent or minimize reduction to metal.

A gamma alumina has been obtained from Air Products derived from Catapal^{r} substrate, 2.4mm extrudate 71.8 vol % porosity, 280 m^2/gm area.

Appropriate chemicals have been ordered.

Task 2. Testing Catalysts for Syngas Conversions

Considerable effort has been expended to plan the high-pressure equipment for reaction measurements and in-situ infrared spectral measurements.

An elaborate system was previously constructed by Dean Runkle as a masters thesis project. A process flow sheet and legend are attached (Fig. C2 and C3 from the thesis). This apparatus was not previously operated. It was designed primarily as an infrared spectral flow reactor for CO hydrogenation. It is being reviewed for its suitability with appropriate renovations for the present project.

A simpler apparatus has been designed as shown in the attached figure labelled "Syngas reactor and in-situ infrared cell system." Some of the items, such as mass flow meters, have longer term delivery. These were provided for in the proposal budget and have been ordered.

There are some chromatographic instruments which will become available, since one student is completing a doctoral research project. These will be utilized in order to provide most effective use of instrument funds.

Task 3. Determination of Surface Composition and Structure

Discussions have been held with Dr. Brian Strohmeier, Instrumentalist, concerning the best form for sample preparation including catalyst pretreatment and expectation of results, especially for the ESCA as well as other instrumental facilities.

Chemisorption measurements will be important and the Catalysis Center facilities have been reviewed in terms of adequacy and availability.

Task 4. Determination of Nature Surface Complexes

The use of high-pressure infrared cells will form a substantial part of this project with in-situ measurements. Fortunately, there are cells available and these have been examined. In addition, a different cell design (Prof. A. Bell, Berkeley) and also one from Shell Amsterdam have been acquired for possible use.

Task 5. Reaction Mechanism Determination by Isotopic Tracers and Kinetics

The existing literature on use of isotopic tracers, including research at the Catalysis Center has been examined critically.

Experiments are planned as outlined in the proposal. There is a question as to the pressure to be utilized in order to obtain meaningful results.

Task 6. Design, Prepare and Test Optimized Catalysts

Data from previous tasks are needed to carry out this task.

PERSONNEL

In addition to the coprincipal investigators, Dr. Sudhakar Chakka joined the project on Nov. 1 as Postdoctoral Fellow. He has just completed a two-year appointment with Professor M. A. Vannice at Pennsylvania State University, working on CO hydrogenation reactions, including synthesis, characterization and activity measurements on supported Pd catalysts.

Mr. Nazeer Bhore, graduate student in chemical engineering, has selected this project for his Ph.D. thesis topic. He comes with a B.S. degree in Chemical Engineering, University of Bombay, where he was first in his class.

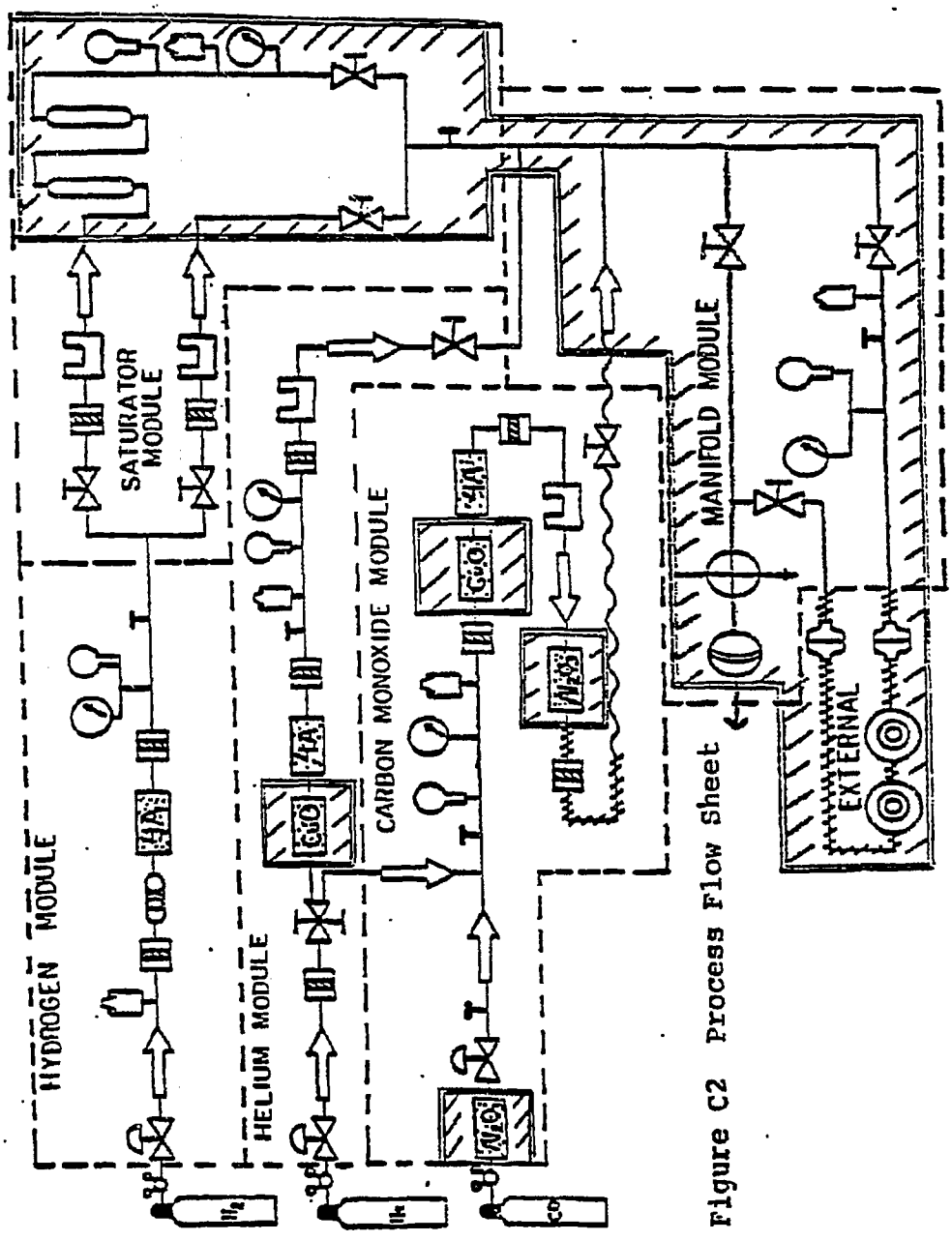
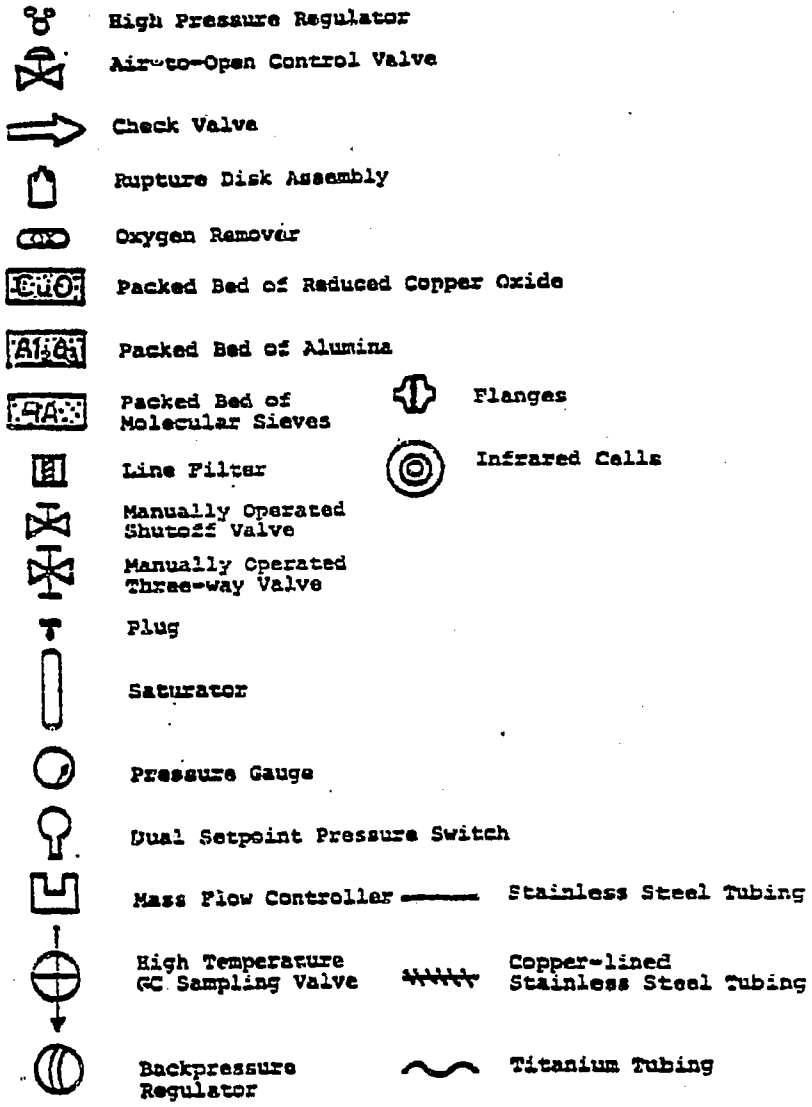
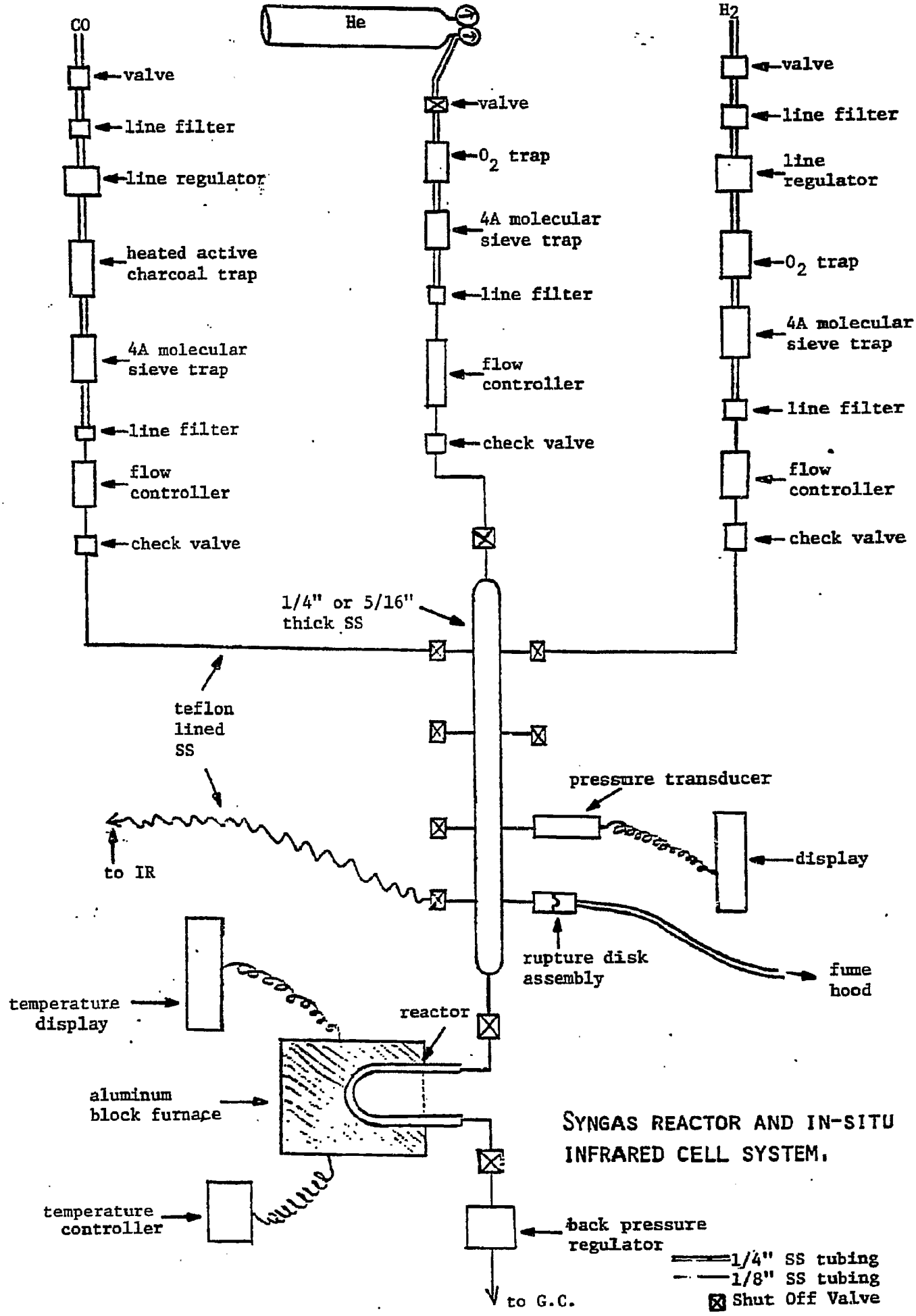


Figure C2 Process Flow Sheet

Figure C3

Legend to Process Flow Sheet





SYNGAS REACTOR AND IN-SITU INFRARED CELL SYSTEM.

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