



DE85004577

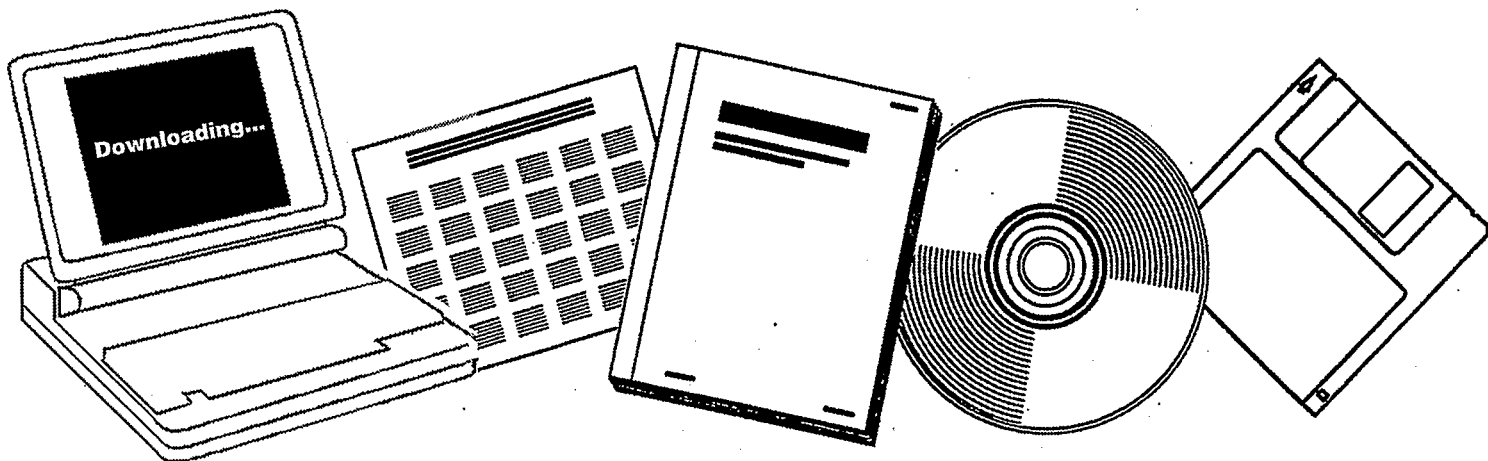
NTIS

One Source. One Search. One Solution.

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

DELAWARE UNIV., NEWARK. DEPT. OF
CHEMICAL ENGINEERING

12 DEC 1984



U.S. Department of Commerce
National Technical Information Service

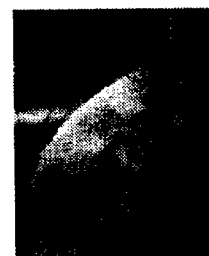
One Source. One Search. One Solution.

NTIS



Providing Permanent, Easy Access to U.S. Government Information

National Technical Information Service is the nation's largest repository and disseminator of government-initiated scientific, technical, engineering, and related business information. The NTIS collection includes almost 3,000,000 information products in a variety of formats: electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.



Search the NTIS Database from 1990 forward

NTIS has upgraded its bibliographic database system and has made all entries since 1990 searchable on www.ntis.gov. You now have access to information on more than 600,000 government research information products from this web site.

Link to Full Text Documents at Government Web Sites

Because many Government agencies have their most recent reports available on their own web site, we have added links directly to these reports. When available, you will see a link on the right side of the bibliographic screen.

Download Publications (1997 - Present)

NTIS can now provide the full text of reports as downloadable PDF files. This means that when an agency stops maintaining a report on the web, NTIS will offer a downloadable version. There is a nominal fee for each download for most publications.

For more information visit our website:

www.ntis.gov



U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161

NOTICE
PORTIONS OF THIS REPORT ARE ILLEGIBLE.

It has been reproduced from the best available copy to permit the broadest possible availability.

**TRIFUNCTIONAL CATALYSTS
FOR CONVERSION OF SYNGAS TO ALCOHOLS**

DOE/PC/70780--1

DE85 004577-

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

K. B. Bischoff, William Manogue and G. Alex Mills
Coprincipal Investigators
Center for Catalytic Science and Technology
Department of Chemical Engineering
University of Delaware
Newark, Delaware 19716

Date Published:
December 12, 1984

Prepared for
Fossil Energy
Department of Energy
Washington, D.C.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Under Contract No. DE-~~AC22-79-ET14830~~

FG22-84PC70780

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees takes any responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

TABLE OF CONTENTS

	<u>Page</u>
I. Abstract	1
II. Objectives	2
III. Tasks 1-6	3
IV. Personnel	6

ABSTRACT

The proposed program has been actively initiated, beginning September 1, 1984, as authorized by DOE. In addition to the principal investigators, two key individuals have joined the project: Dr. Sudhakar Chakka, an experienced Post Doctoral Fellow and Mr. Nazeer A. Bhole, 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 Isoopic 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-Al₂O₃, 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 m²/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 Bhole, 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.

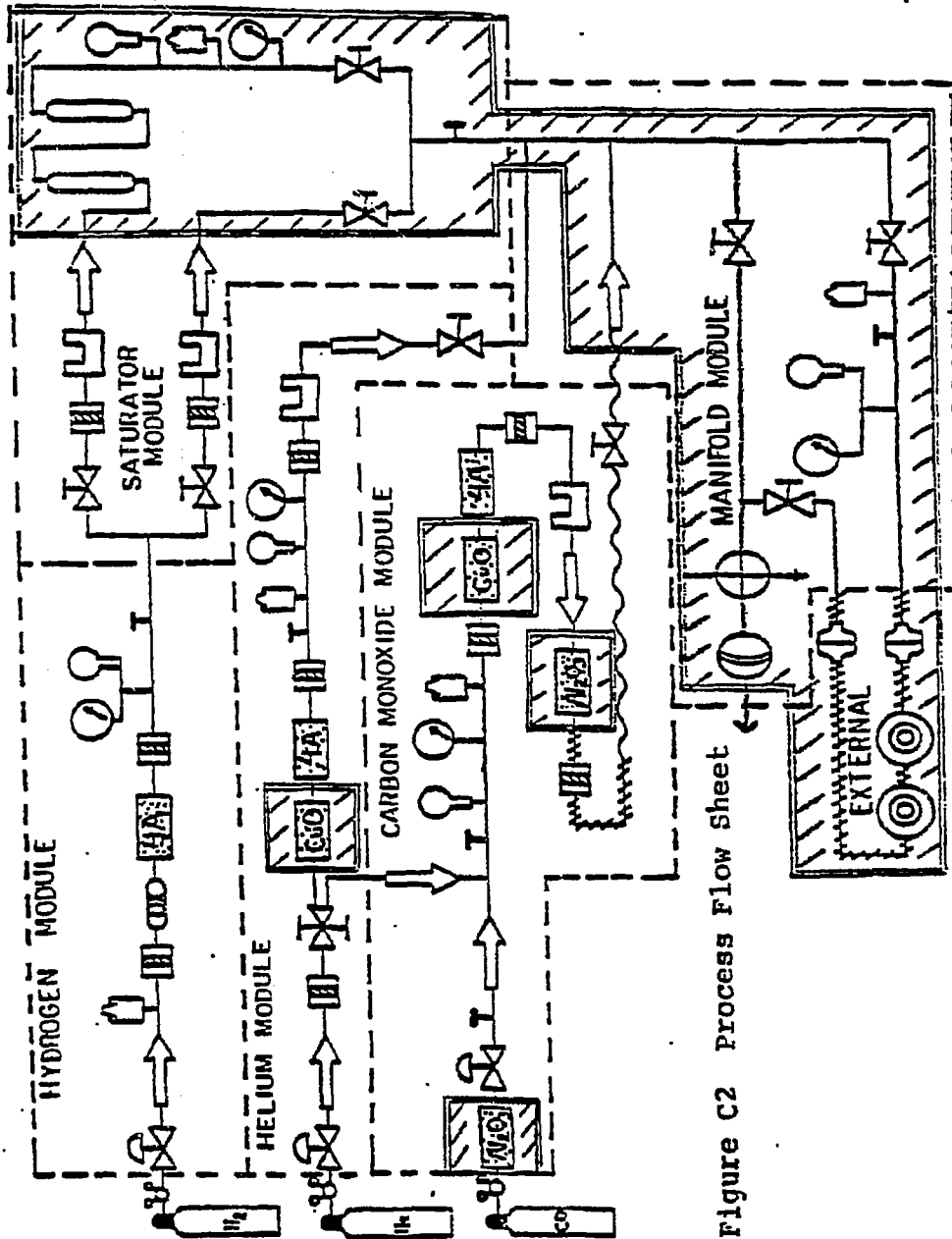























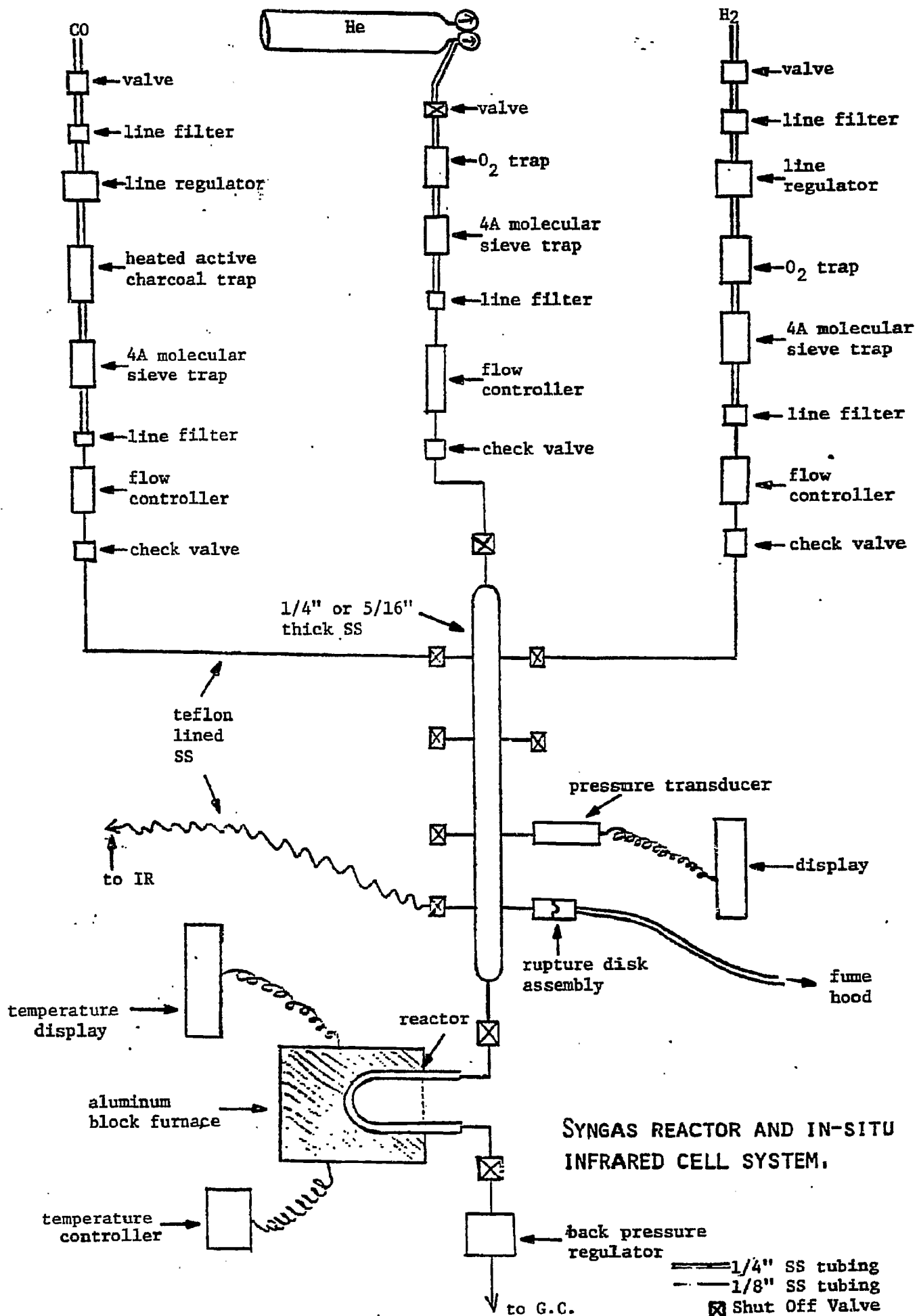


Figure C2 Process Flow Sheet

Figure C3

Legend to Process Flow Sheet

	High Pressure Regulator	
	Air-to-Open Control Valve	
	Check Valve	
	Rupture Disk Assembly	
	Oxygen Remover	
	Packed Bed of Reduced Copper Oxide	
	Packed Bed of Alumina	
	Packed Bed of Molecular Sieves	
	Line Filter	 Flanges
	Manually Operated Shutoff Valve	 Infrared Cells
	Manually Operated Three-way Valve	
	Plug	
	Saturator	
	Pressure Gauge	
	Dual Setpoint Pressure Switch	
	Mass Flow Controller	 Stainless Steel Tubing
	High Temperature GC Sampling Valve	 Copper-lined Stainless Steel Tubing
	Backpressure Regulator	 Titanium Tubing



SYNGAS REACTOR AND IN-SITU INFRARED CELL SYSTEM,

SATISFACTION GUARANTEED

NTIS strives to provide quality products, reliable service, and fast delivery. Please contact us for a replacement within 30 days if the item you receive is defective or if we have made an error in filling your order.

▲ **E-mail: info@ntis.gov**

▲ **Phone: 1-888-584-8332 or (703)605-6050**

Reproduced by NTIS

National Technical Information Service
Springfield, VA 22161

This report was printed specifically for your order from nearly 3 million titles available in our collection.

For economy and efficiency, NTIS does not maintain stock of its vast collection of technical reports. Rather, most documents are custom reproduced for each order. Documents that are not in electronic format are reproduced from master archival copies and are the best possible reproductions available.

Occasionally, older master materials may reproduce portions of documents that are not fully legible. If you have questions concerning this document or any order you have placed with NTIS, please call our Customer Service Department at (703) 605-6050.

About NTIS

NTIS collects scientific, technical, engineering, and related business information – then organizes, maintains, and disseminates that information in a variety of formats – including electronic download, online access, CD-ROM, magnetic tape, diskette, multimedia, microfiche and paper.

The NTIS collection of nearly 3 million titles includes reports describing research conducted or sponsored by federal agencies and their contractors; statistical and business information; U.S. military publications; multimedia training products; computer software and electronic databases developed by federal agencies; and technical reports prepared by research organizations worldwide.

For more information about NTIS, visit our Web site at <http://www.ntis.gov>.

NTIS

**Ensuring Permanent, Easy Access to
U.S. Government Information Assets**



U.S. DEPARTMENT OF COMMERCE
Technology Administration
National Technical Information Service
Springfield, VA 22161 (703) 605-6000
