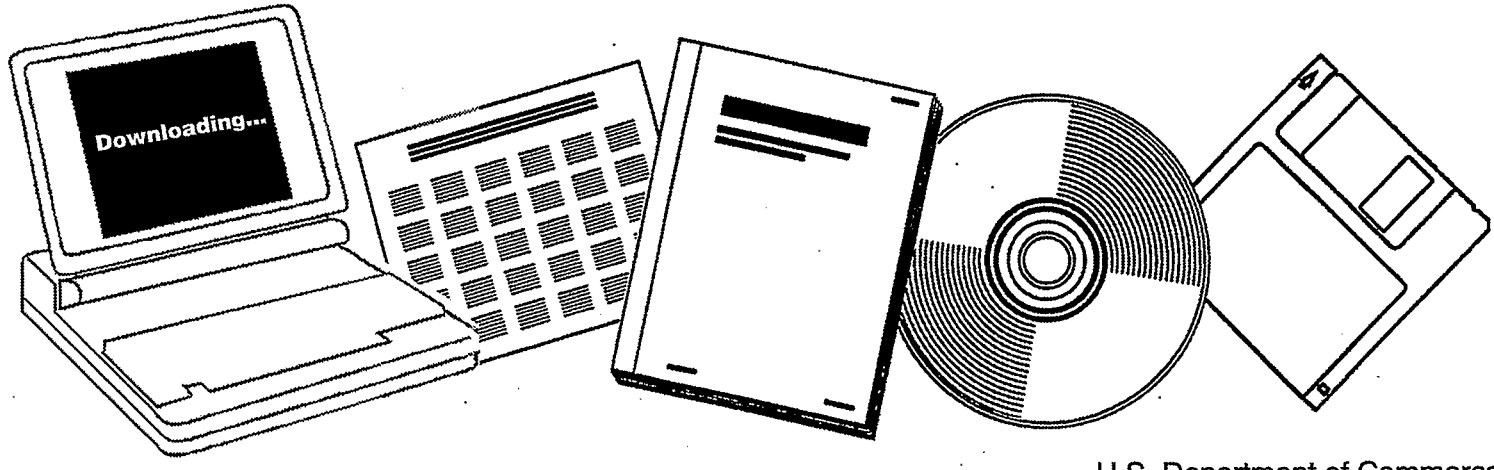
FTIR STUDIES OF HYDROCARBON SYNTHESIS ON PD/ZSM5 CATALYSTS. QUARTERLY PROGRESS REPORT, AUGUST 15, 1985

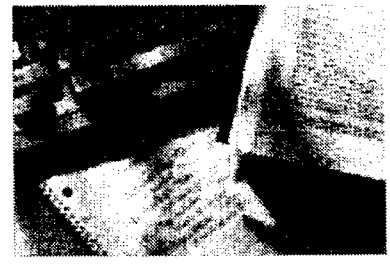
NOTRE DAME UNIV., IN. DEPT. OF CHEMICAL ENGINEERING

15 AUG 1985



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 provides 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

DOE/PC/70788--T2

DE85 016646

DEPARTMENT OF ENERGY

Quarterly Progress Report

August 15, 1985

Project 84PC70788-2

FTIR Studies of Hydrocarbon Synthesis on Pd/ZSM5 Catalysts

directed by

Eduardo E. Wolf
Professor
Department of Chemical Engineering
University of Notre Dame

DISCLAIMER

Brief summary of progress

During the last quarter several objectives were attained:

1) Pd/ZSM5 catalysts are capable of methanol and hydrocarbon synthesis
2) The temperature and pressure dependence of the reaction rates were established. The reaction rate increases with temperature and pressure, and is independent of residence time.
3) Methanol yield reaches a maximum as pressure increases, and it decreases as temperature increases.
4) Ir spectra are dominated by the linear and bridge bonded forms of CO, as well as by bands at 1550- 1400 cm^{-1}.

Summary of progress

Results demonstrating the first two objectives indicated above are displayed in figs. 1-3 in terms of reaction rates versus the corresponding operating variable. Figures 4-6 show the effect of the same variables in the product distribution. Methanol production follows a trend characteristic of a reaction intermediate, which suggest that the catalyst is apparently operating via a bifunctional mechanism.

A typical IR spectrum at low pressure (50 psi), shown in fig. 7, indicate that the prevailing bands are those corresponding to gas phase CO, a band at 1932 due to linearly adsorbed CO, and non identified bands at 1712, 1523, 1442, and 1404 cm^{-1}. As pressure increases, the gas phase CO bands become very large and overtake the linearly adsorbed CO band. The effect of pressure and temperature in the low frequency bands are shown in figs 8-9. While pressure does not affect significantly these bands, temperature changes their relative proportions.

Current work is addressing at the chemical identification of the observed bands, as well as their correlation with the activity and selectivity patterns to establish the reaction pathway.

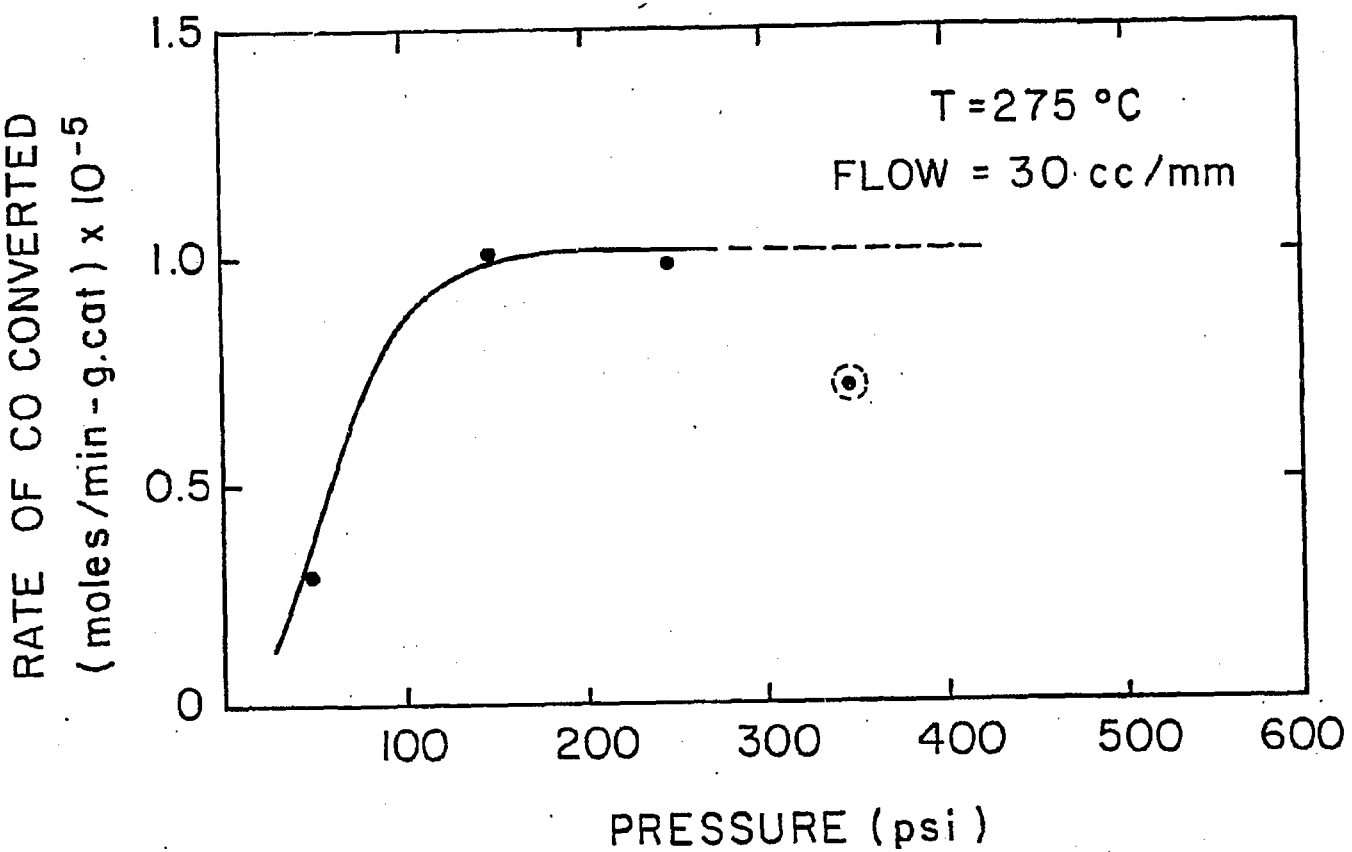

RATE OF CO CONVERTED
(moles/min - g.cat) x 10-5
1.5
1.0
0.5
0
T = 275 °C
FLOW = 30 cc/mm
100
200
300
400
500
600
PRESSURE (psi)

Figure 1

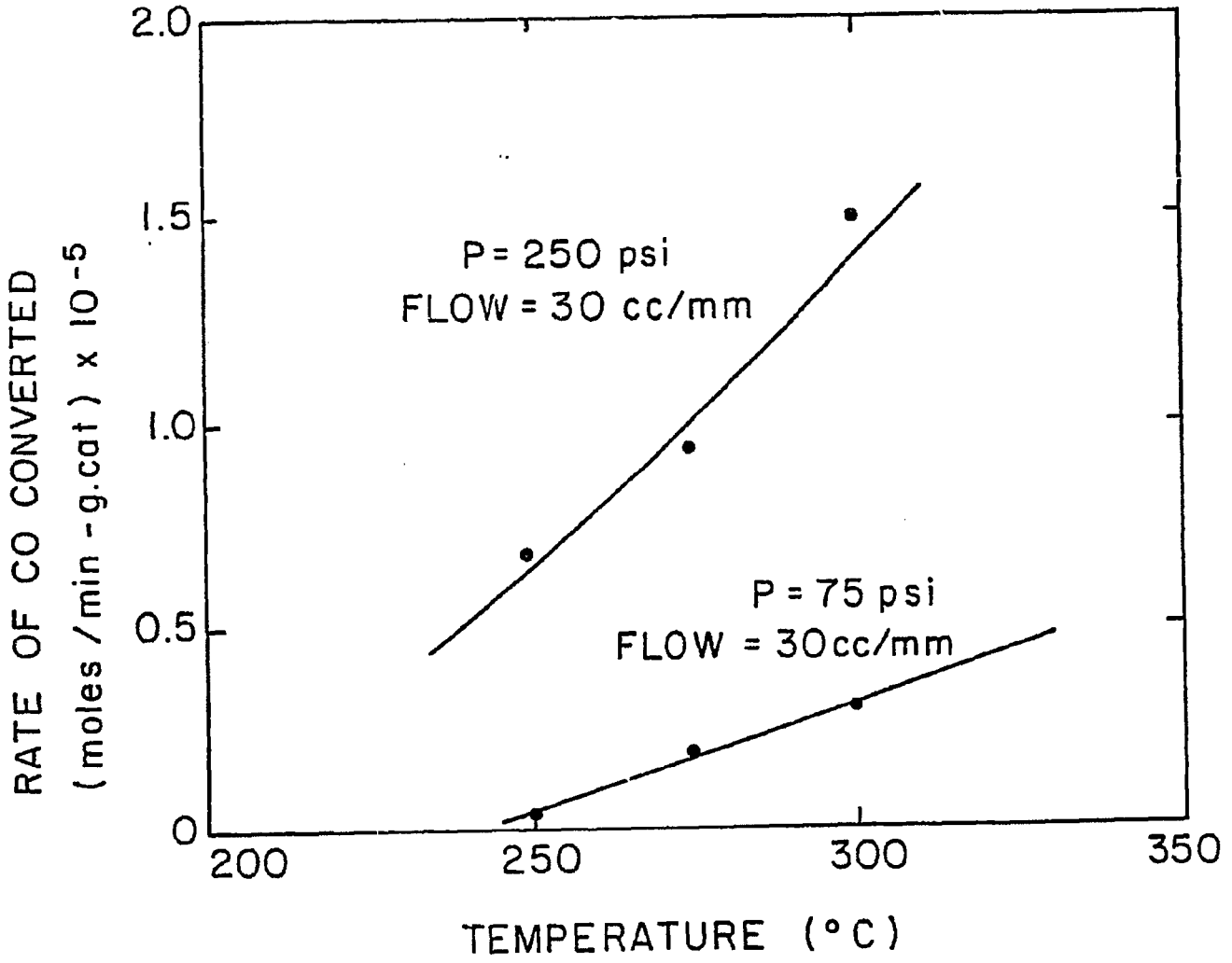

2.0
1.5
1.0
0.5
0
200
250
300
350
RATE OF CO CONVERTED
(moles /min - g.cat) x 10-5
TEMPERATURE (°C)
P = 250 psi
FLOW = 30 cc/mm
P = 75 psi
FLOW = 30cc/mm

Figure 2

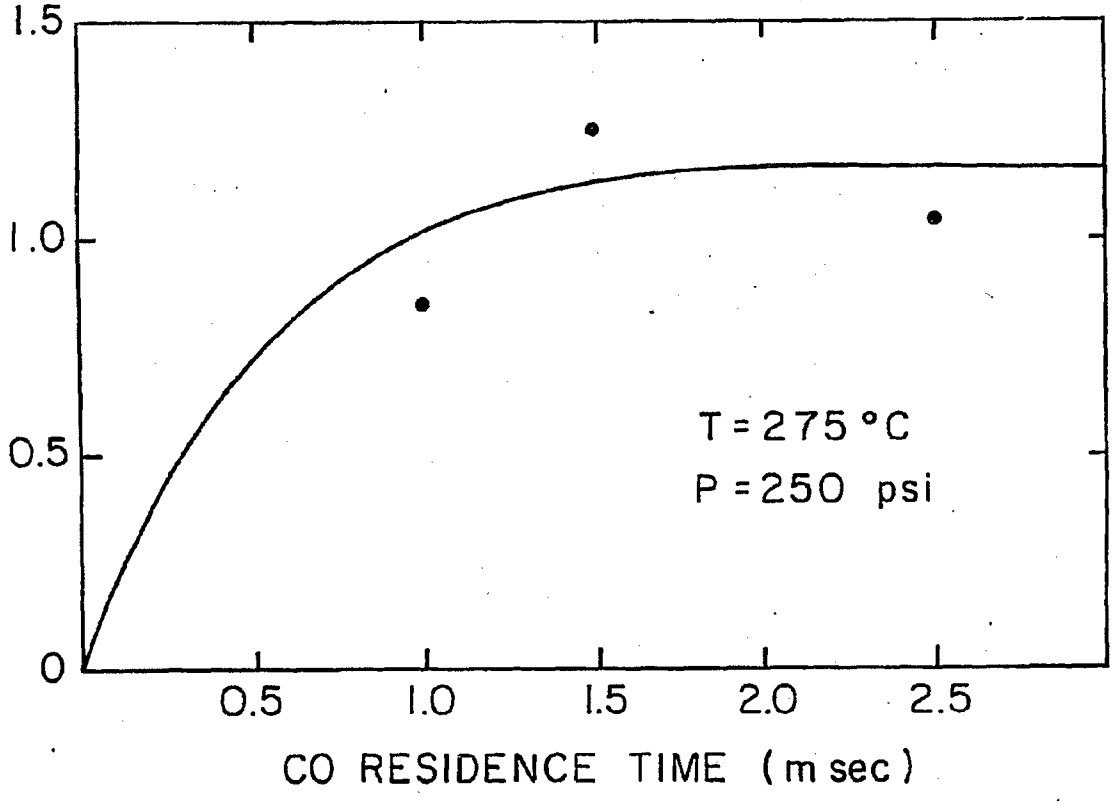


Figure 3

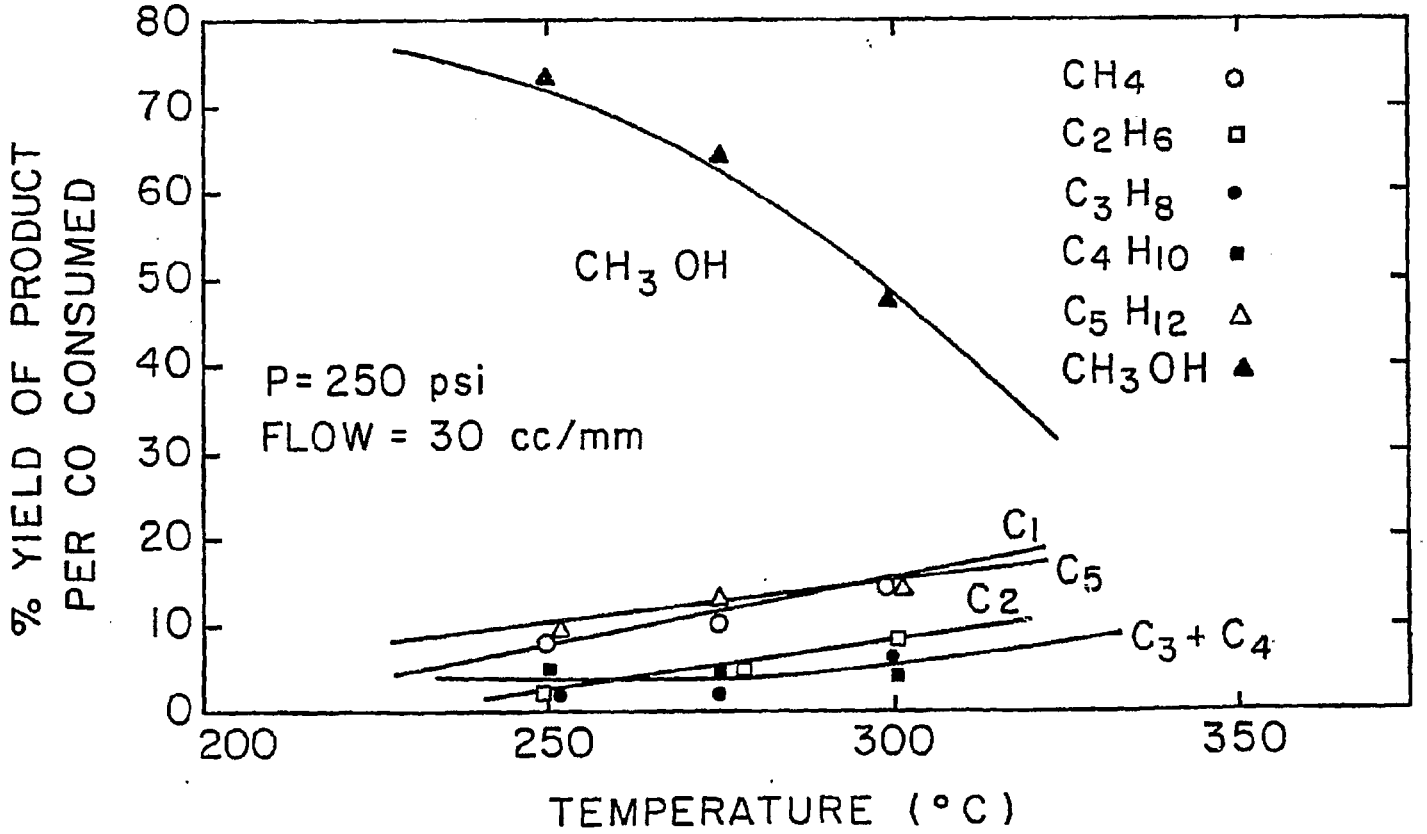

% YIELD OF PRODUCT PER CO CONSUMED
80
70
60
50
40
30
20
10
0
200
250
300
350
TEMPERATURE (°C)
CH4
C2 H6
C3 H8
C4 H10
C5 H12
CH3OH
CH3 OH
P= 250 psi
FLOW = 30 cc/mm
C1
C5
C2
C3 + C4

Figure 4

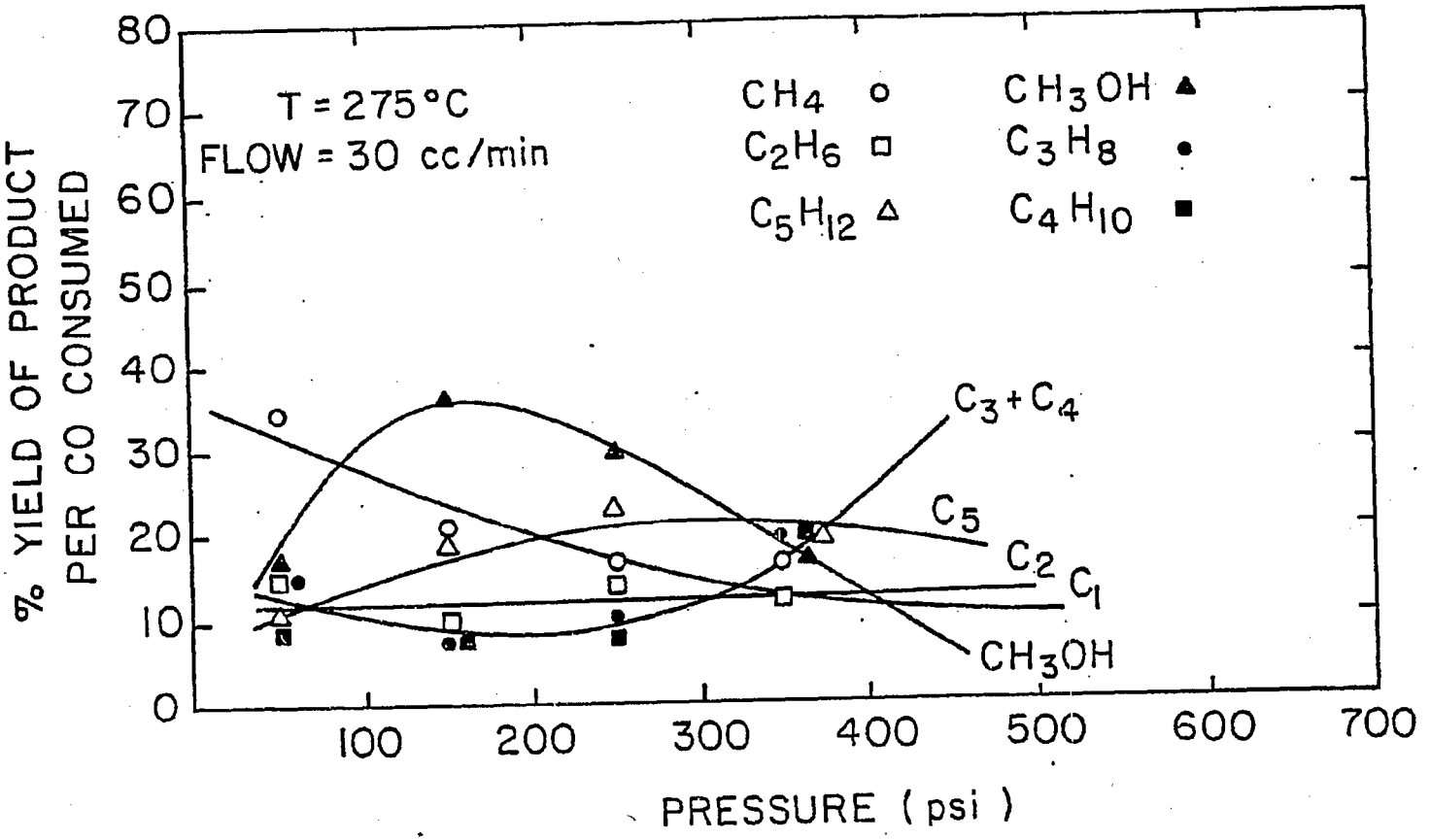

T = 275°C
FLOW = 30 cc/min
CH4
CH3OH
C2H6
C3H8
C5H12
C4H10
C3+C4
C5
C2
C1
CH3OH
% YIELD OF PRODUCT PER CO CONSUMED
PRESSURE (psi)
0
10
20
30
40
50
60
70
80
100
200
300
400
500
600
700

Figure 5

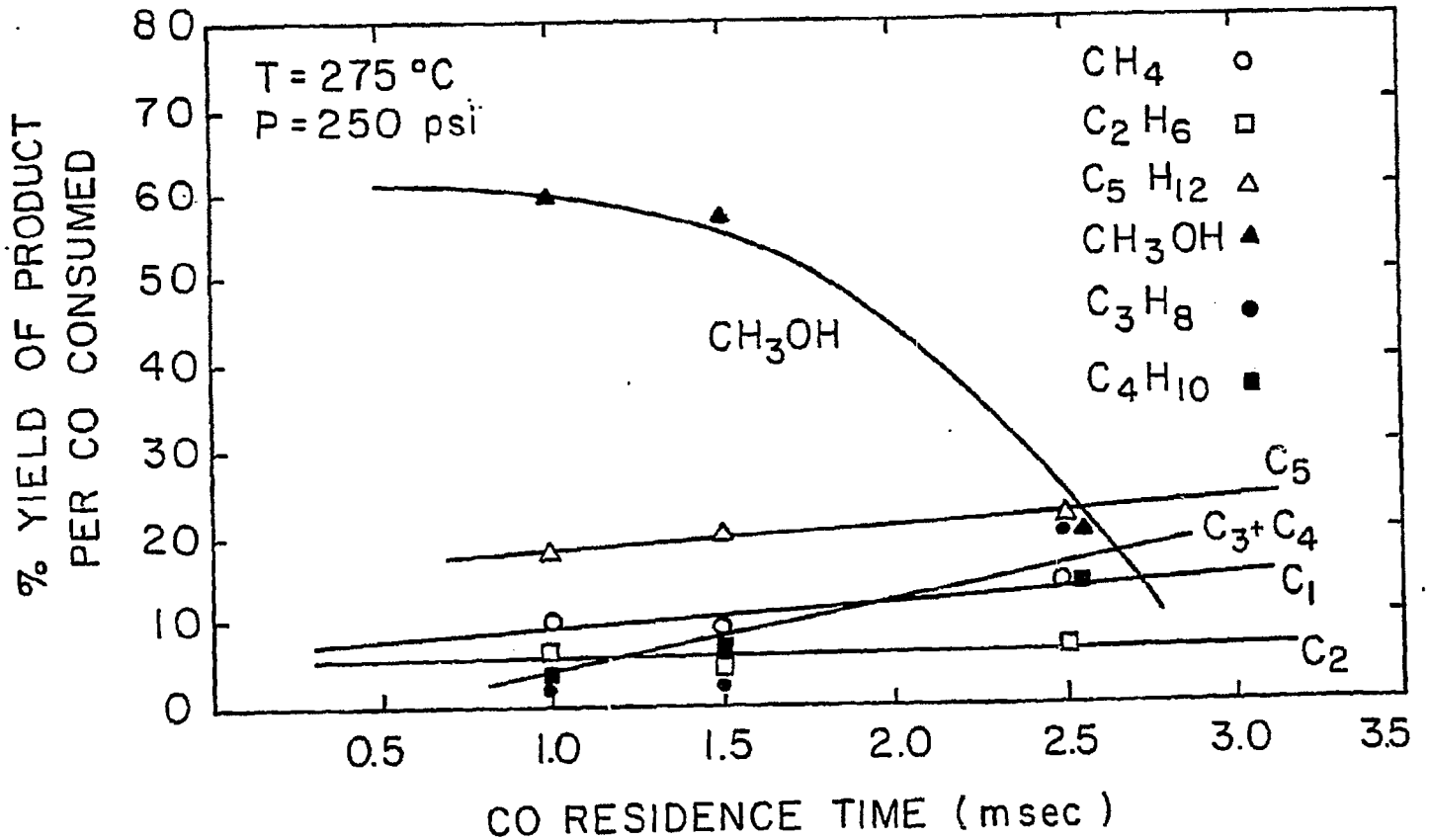
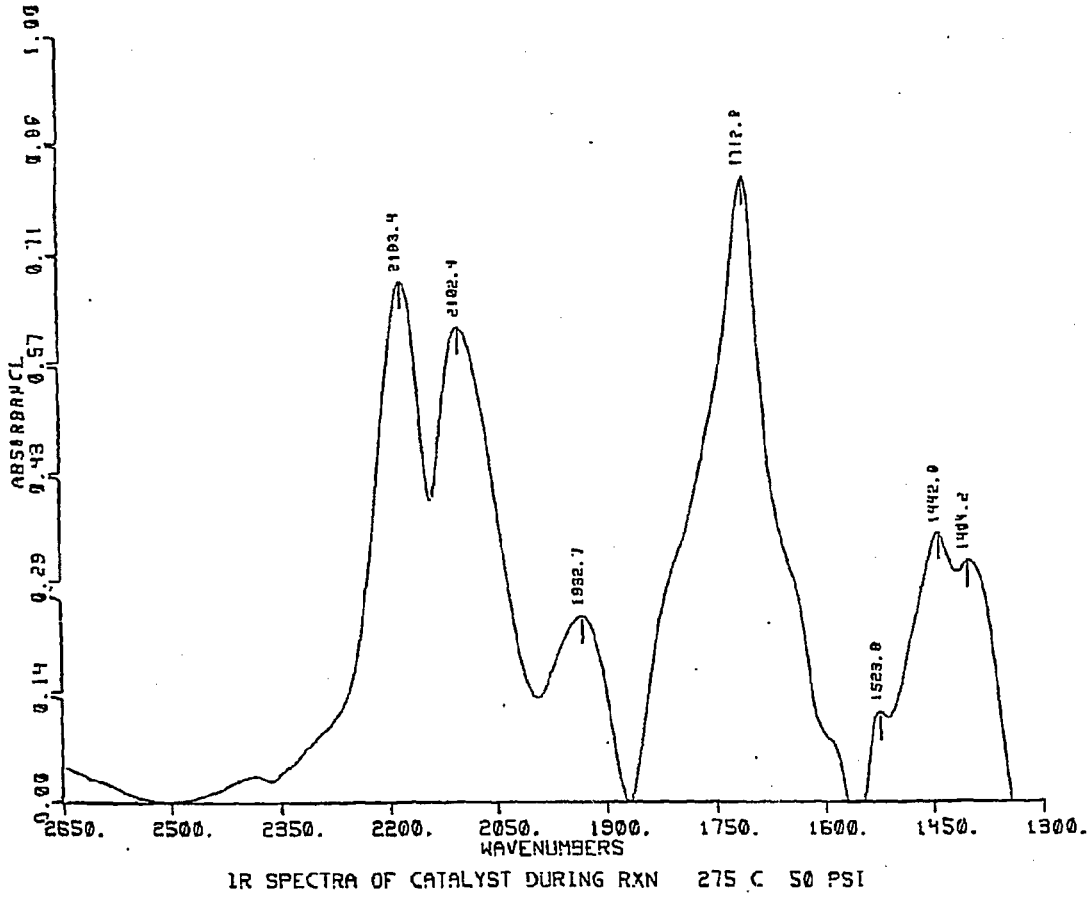

% YIELD OF PRODUCT PER CO CONSUMED
80
70
60
50
40
30
20
10
0
T = 275 °C
P = 250 psi
CH4
C2 H6
C5 H12
CH3OH
C3 H8
C4H10
CH3OH
C5
C3+ C4
C1
C2
0.5
1.0
1.5
2.0
2.5
3.0
3.5
CO RESIDENCE TIME (msec)

Figure 6

Figure 7



IR SPECTRA OF CATALYST DURING RXN 275 C 50 PSI

IR SPECTRA OF CATALYST WAFER
UNDER REACTION CONDITIONS

Figure 8

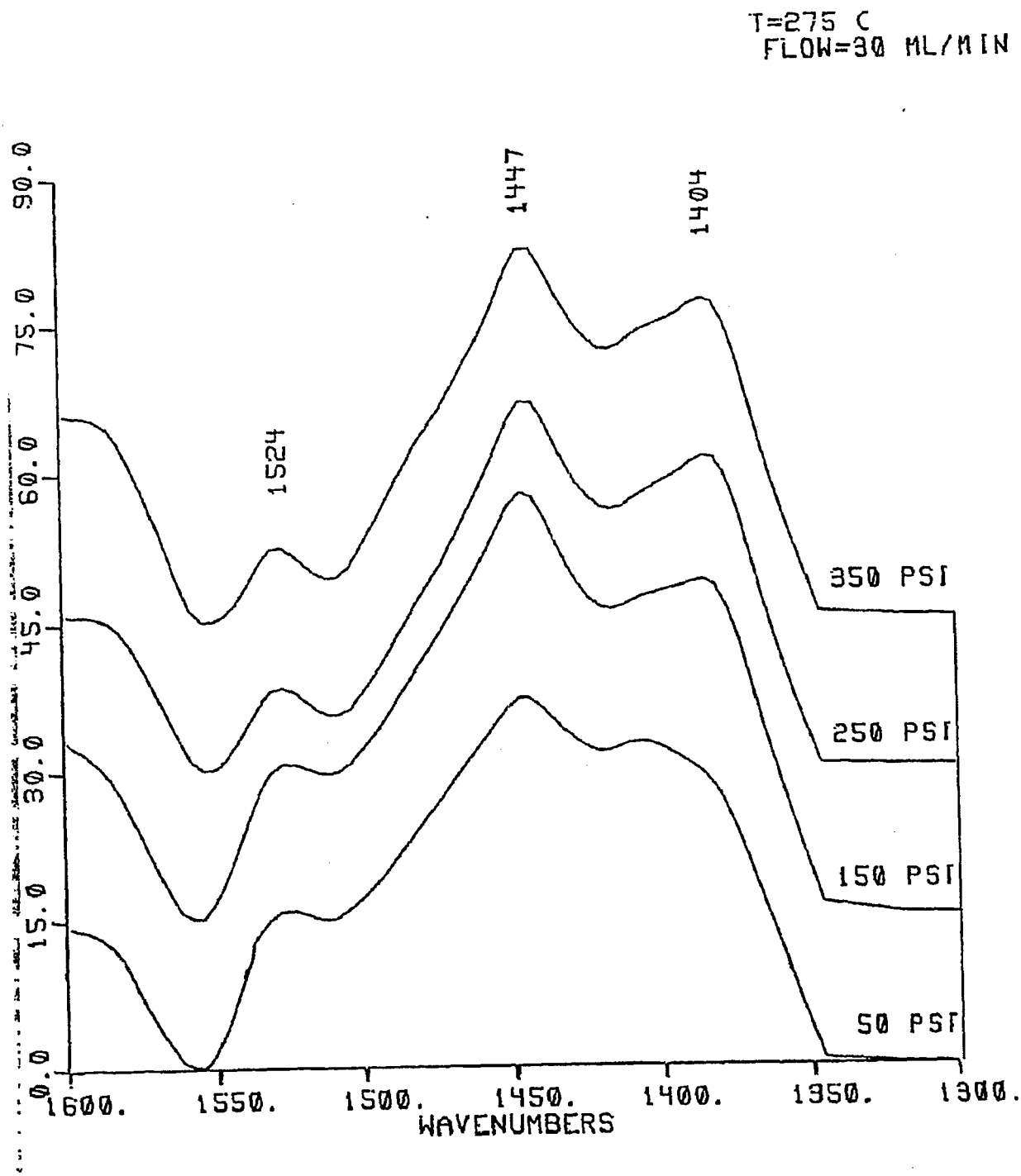
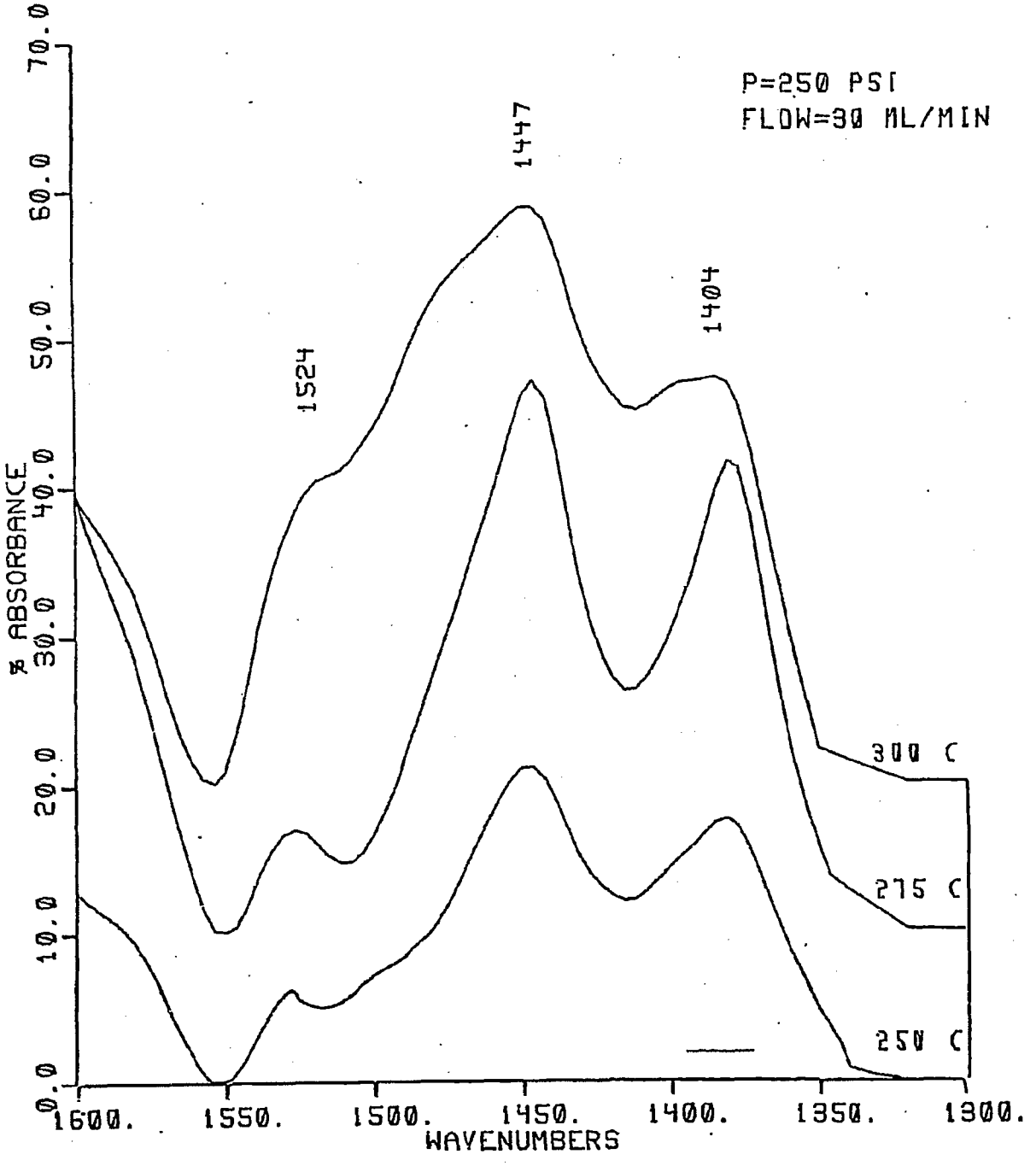


Figure 9

IR SPECTRA OF CATALYST WAFER
UNDER REACTION CONDITIONS



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