DOE/PC/94066--T5

Isobutanol-Methanol Mixtures from Synthesis Gas

Quarterly Technical Progress Report

Period Covered: 1 October to 31 December 1995

Contractor

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RESTRICTED DOCUMENT

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EXECUTIVE SUMMARY

A series of $Cu_{0.5}CeMe(II)O_x$ catalysts (Me refers to Group II alkali earth elements) have been prepared by coprecipitating the corresponding metal nitrates with potassium carbonate. The bulk composition of the catalyst has been determined by atomic absorption (AA) analysis.

High-pressure isobutanol synthesis studies have been carried out over a standard BASF Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst. At a CO conversion level of 32 %, the isobutanol carbon selectivity is about 5 %; whereas that of methanol is 40.2 %. A 100% selectivity sum has now been obtained as a result of using response factors measured by our laboratory.

The reactions of ethanol and acetic acid over a number of catalysts have been investigated using a temperature programmed surface reaction (TPSR) technique. Ethanol and acetone are the only desorption products observed over Cs-promoted $Cu/ZnO/Al_2O_3$ catalysts. Surface acetate ion is believed to be the precursor for acetone formation. Over calcined hydrotalcites, i.e, MgO/Al_2O_3, ethylene is formed instead of acetone. The amount of ethylene formed decreases as Mg/Al ratio increases, suggesting a role of aluminum ions in ethanol dehydration reactions.

1. CONTRACT OBJECTIVES AND TASKS

The contract objectives are:

1. To design a catalytic material for the synthesis of isobutanol with a productivity of 200 g isoalcohols/g-cat-h and a molar isobutanol-to-methanol ratio near unity

2. To develop structure-function rules for the design of catalysts for the selective conversion of synthesis gas to isoalcohols

The research program has been grouped into five specific tasks and a set of project management and reporting activities. The abbreviated designations for these tasks are:

- Project Work Plan *(Task 1)*

- Catalyst Synthesis *(Task 2)*

- Catalyst Evaluation in Laboratory Scale Reactors *(Task 3)*

- Identification of Reaction Intermediates *(Task 4)*

- Bench-Scale Catalyst Evaluation at Air Products and Chemicals *(Task 5)*

2. SUMMARY OF ACTIVITIES

Activities during this period have focused on:

- Prepare a series of $Cu_{0.5}Ce_2Me(II)O_x$ catalysts, where Me(II) stands for Group IIA alkali earth elements

- Conduct high-pressure isobutanol synthesis reactions using a standard APCI-supplied Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst manufactured by BASF and supplied by Air Products and Chemicals Inc.

- Study ethanol TPSR over $ZrO_2/MnO/ZnO$, MgO/Al_2O_3, and Cs-modified $Cu/ZnO/Al_2O_3$ catalysts

3. STATUS, ACCOMPLISHMENTS, AND RESULTS

Task 1: Management Plan

No activities were carried out during this reporting period.

Task 2: Catalyst synthesis

Samples were prepared by coprecipitation of 1.2 M mixed metal nitrate solutions with potassium carbonate at 65 °C and a constant pH of 9 under vigorous agitation in a stirred batch reactor. The precipitates were filtered, washed with deionized water at 60 °C, and then dried at 80 - 90 °C for 9 h. The resulting materials were calcined at 450 °C for 4 h. The bulk compositions of the catalysts are shown in Table 1. The atomic ratios of Ce/Cu and Ce/Me(II) were determined by atomic absorption (AA) spectroscopy. Here, Me(II) represents Group IIA alkali earth elements.

Table 1. Catalyst Composition

Sample	Formula	Ce/Cu	Ce/Me(II)
MG1-1O	$Cu_{0.5}Ce_2MgO_x$	3.76	1.70
MG1-2O	$Cu_{0.5}Ce_2CaO_x$	3.86	1.52
MG1-3O	$Cu_{0.5}Ce_2SrO_x$	3.58	1.44
MG1-4O	$Cu_{0.5}Ce_2BaO_x$	3.79	1.50

Only the surface area of $Cu_{0.5}Ce_2MgO_x$ (34 m^2/g) was measured, by dinitrogen physisorption BET methods. No power X-ray diffraction (XRD) analysis has been performed during this reporting period.

Task 3: Catalyst Evaluation in Laboratory Scale Reactors

3.1. Design of Recirculation Reactor Module

Design and specifications for a recirculating reactor unit (RRU3) dedicated to this project have been completed and most parts have been ordered during this reporting period. The construction of RRU3 is underway and about 70 % complete.

3.2. Isobutanol Synthesis at High Pressures in the CMRU

Certification of the CMRU using the Cs-promoted Cu/ZnO catalyst provided by APCI was completed with run CMRU-4. CMRU-3 was conducted with a 2.4 g catalyst charge over a GHSV range of 625-2500 scm^3/h·g·cat. and temperatures 300 - 360 °C. Decreasing the GHSV resulted in the expected increase of CO conversion from 10% at 2500 scm^3/h-g-cat to 22% at 1250 scm^3/h·g cat, the latter conversion being the maximum attainable at 300 °C.

Additionally, the longer contact times at lower GHSV gave rise to increased isobutanol selectivities. As temperature increased, CO conversion to methanol became thermodynamically unfavorable while isobutanol selectivity increased. At GHSV = 625 scm^3/h-g-cat and T = 354 ° C, conversion was only about 5.2%; however, the highest isobutanol-to-methanol ratio of 0.062 was achieved.

Since CMRU-3 resulted in mostly methanol selectivity with very little higher alcohol made, a new batch of the BASF Cs-promoted Cu/ZnO/Al$_2$O$_3$ catalyst from APCI was used for CMRU-4. At this time APCI is also running this catalyst in their fixed bed reactor (the data we currently have was taken from a backmix reactor).

One of the primary goals of CMRU-3 was to determine whether inability to attain a 100 % selectivities sum was caused by alcohols condensation in the lines or by erroneous calculation methods. To this end, we introduced liquid butanol in helium in order to determine: 1) the butanol response factor needed to confirm alcohol selectivity calculations, and 2) the butanol partial pressure at which it begins to condense in the transfer lines. The liquid butanol feed experiment also served to certify the new high pressure syringe pump.

The gas chromatograph FID area was measured at each butanol flow rate, as shown in Figure 1 below:
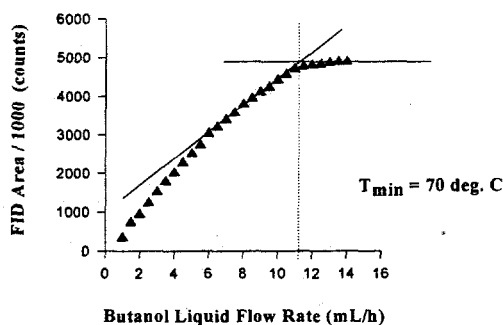
Figure 1: Increasing butanol flow rate resulted in condensation at
$P_{butanol}$ = 0.13 atm, corresponding to T_{sat} = 70 °C.

The gas chromatograph area attained a constant value at a butanol flow rate of approximately 11 ml/h, corresponding to a butanol partial pressure (and vapor pressure) of 0.13 atm. This saturation pressure is indicative of butanol condensation at 70 °C, and implies that a 70 °C cold spot exists in the system. By running the experiment again at 50 psi, we will determine whether the cold spot is present on the high- or low-pressure side of the back pressure regulator.

In order to measure a butanol response factor, data were extracted from the low butanol concentration region of the plot in Figure 1. The measured value was 48.55 area counts/ppm compared with the APCI reported value of 82.12 area counts/ppm. Thus, we have previously underestimated our butanol and other alcohol selectivities by a factor of 1.6, causing the < 100 % mass balance. The high methanol selectivities obtained in both CMRU-3 and CMRU-4 prompted us to measure the methanol response factor. Indeed, we measured 34 area counts/ppm whereas the value used to calculate the original CMRU-3 and CMRU-4 data was 55 area counts/ppm.

CMRU-4 was conducted with the same charge of 2.4 g catalyst used in CMRU-3. Table 1 shows that measured methanol response factor resulted in a 101 % selectivity sum. Additionally, the isobutanol selectivity of CMRU-4 increased by a factor of ten because we previously misread the isobutanol selectivity from the spreadsheet.

Table 1: Comparison of CMRU-3 and CMRU-4

	CMRU-3	CMRU-4
Temperature (C)	325	323
Pressure (psi)	750	750
GHSV (scc/h g cat.)	1250	1250
CO Conversion (%)	0.17	0.32
MeOH Selectivity (%C)	47.92	74.7
i-BuOH Selectivity (%C)	0.49	4.9
CO2 Selectivity (%C)	13.14	24.4
Σ Selectivities (%)	65.43	101
MeOH/i-BuOH	97.80	15

The CMRU-4 data (calculated with the correct methanol response factor) now certifies the unit as operationally sound.

APCI is also running this catalyst in a fixed-bed reactor at this time. Their results to date show that isobutanol selectivity declines rapidly after a few hours with the Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst. With the unit certification complete, we have proceeded to study the Exxon-patented alkali promoted $Cu_{0.5}MgCe_2O_x$ catalysts, one of the two classes of materials selected for emphasis in the project.

Task 4: Identification of Reaction Intermediates

Activities in this task during this reporting period have focused on the study of surface reactions of ethanol and other oxygenated compound over Cs-promoted $Cu/ZnO/Al_2O_3$, $ZrO_2/MnO/ZnO$ and MgO/Al_2O_3 catalysts using a temperature programmed surface reaction
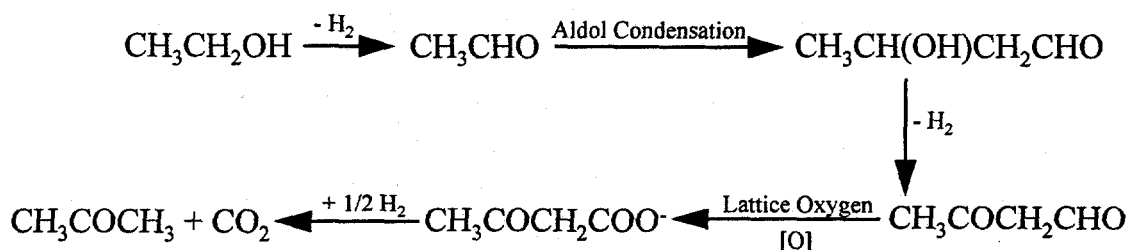
(TPSR) techniques. Because of the transient nature of TPSR, in which both temperature and surface adsorbate coverage vary with time, information can be obtained that is unavailable from steady-state measurement.

All transfer lines after the thermostated saturator in the TPSR unit were kept at 60-70 °C with heating tape in order to minimize the adsorption of reactants and products on the tranfer line walls. Ethanol and other oxygenates were introduced by passing helium through the saturator containing the compound of interest at room temperature. Pulse injection of ethanol diluted in He through a 0.93 mL sample loop into the reactor yielded a sharp and reproducible peak containing 2.5 μmol of ethanol. For example, the half peak width of ethanol mass 45 fragment is only about 3 s. The amount of ethanol determined from the peak area is in consistent with that injected through the sample loop.

The TPSR unit was certified by the reduction of a BASF Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst. In this experiment, 80-140 mesh, 0.150 g of catalyst was charged into a 1.0 cm-i.d. U-shape reactor. Smaller particle sizes could create large pressure drops within the catalyst bed; larger particle sizes can cause intraparticle diffusion, resulting in the changes in desorption peak temperature or the curve shape. A thermocouple well was located in the middle of the catalyst bed supported on a fine quartz frit. The catalyst was first purged with pure He for 10 min at room temperature, followed by the introduction of 5 % H_2 balanced in helium. The reduction was performed at a heating rate of 10 °C/min to 350 °C, and stayed at this temperature for 30 min. A mass spectrometer downstream measured the change of gas composition in the helium stream as a function of temperature. As depicted in Figure 2, H_2, H_2O and CO_2 were detected. Reduction took place at *ca.* 180 °C, and a symmetric CO_2 peak was observed. The left shoulders of H_2 and H_2O peaks can be explained by the effect of surface or bulk carbonates formed during contact with air or remaining from incomplete decomposition during synthesis. At low temperatures, copper reduction is limited by the decomposition of surface carbonates. At *ca.* 260 °C, the rate of CO_2 formation reached maximum. Reduction of Cu^{2+} is no longer limited by surface carbonate decomposition at temperatures greater than 260 °C. The amount of H_2 consumed was 9.3 X 10^{-4} mol, whereas H_2O and CO_2 produced were 1.3 X 10^{-3} mol and 1.6 X 10^{-4} mol, respectively. The amount of CO_2 produced is much less than that of H_2 consumed, indicating that only a small fraction, perhaps only the top few layers of copper exist in the form of copper carbonates. The fact that water produced is in excess of hydrogen consumed may be attributed to dehydroxylation of the catalyst surface. From the atomic absorption (AA) analysis of copper content and the amount of hydrogen consumed, we may conclude that *ca.* 85 % Cu^{2+} was reduced to Cu^0. It is also possible that part of Cu^{2+} might be only partially reduced to Cu^+, which is suspected to play a role in the formation of methanol from synthesis gas.

Cs-promoted $Cu/ZnO/Al_2O_3$ catalysts have been reported to be active and selective for higher alcohol synthesis from CO/H_2 [Smith, K.J., Himmelfard, P.B., Simmons, G.W., and Klier, K., *Ind. Eng. Chem. Res.*, **30**, 61 (1991)]. As discussed in our previously quarterly report, a number of products such as acetaldehyde, acetone, isobutyraldehyde, methyl ethyl ketone, *etc.* have been observed with the initial partial pressures of methanol and ethanol at 60 Torr and 30 Torr, respectively in a gradient recirculating batch reactor at 250 °C and 1 atm. Acetaldehyde is

readily formed over this catalyst. The aldol condensation of acetaldehyde to higher oxygenates on basic sites is proposed to be rate-limiting.

In a typical TPSR study of ethanol over a Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst, ethanol was preadsorbed by passing a mixture of ethanol and helium through the catalyst for 10 min at 35 °C, followed by pure helium purging for 30 min to flush out the gas-phase and weakly adsorbed surface ethanol. The sample was then heated up to about 400 °C at a rate of 30 °C/min in a helium flow of 100 $cc^{-3}min^{-1}$. At higher helium flow rates, concentrations of desorbed components are small and less accurately measured. Also, impurities can be more important at higher flow rates. However, higher carrier gas flows can minimize product readsorption on the catalyst downstream and the time lag between desorption and detection. An optimum flow rate must be high enough so that desorption peak shapes are unchanged by a change in flow rate. The low sensitivity at higher flow rates can be compensated by increasing heating rate. But higher heating rates result in the shift of peak maximum to higher temperatures.

As shown in Figure 3, TPSR measurements of ethanol over the Cs-promoted $Cu/ZnO/Al_2O_3$ are characterized by two desorption peaks, with a peak maximum at 100-110 °C for ethanol and one at about 300 °C for acetone. No other products were detected in the 1-100 amu mass range. The additional small peak observed for mass fragments 43 and 44 at *ca.* 170 °C might be attributed to acetaldehyde, which is a very reactive intermediate. CO_2 was responsible for mass fragments 44 and 28 at about 320 °C. Interestingly, replacement of pure He by 5 % H_2 balanced in helium as a carrier gas enhanced acetone peak intensity. The role of H_2 might be to prevent further condensation reactions of acetone on the catalyst surface .

The formation of acetone can be explained by the decarboxylation of surface acetate ions which result from the oxidation of acetaldehyde by lattice oxygen:

$$CH_3CH_2OH \xrightarrow{-H_2} CH_3CHO \xrightarrow[\text{[O]}]{\text{Lattice Oxygen}} CH_3COO^-$$

$$\Big\downarrow -1/2\,[O]$$

$$1/2\ CH_3COCH_3 + 1/2\ CO_2$$

Lattice oxygen may come from reducible metal oxide of the catalyst. The decomposition of metal acetate leads to the formation of acetone [Fieser, L.F., and Fieser, M., *Organic Chemistry*, 1973]. However, acetone could also result from the aldol condensation of acetaldehyde:

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$$CH_3CH_2OH \xrightarrow{-H_2} CH_3CHO \xrightarrow{\text{Aldol Condensation}} CH_3CH(OH)CH_2CHO$$

$$\Big\downarrow {-H_2}$$

$$CH_3COCH_3 + CO_2 \xleftarrow{+1/2\ H_2} CH_3COCH_2COO^- \xleftarrow[\text{[O]}]{\text{Lattice Oxygen}} CH_3COCH_2CHO$$

Yet no intermediate species such as $CH_3CH(OH)CH_2CHO$ and CH_3COCH_2CHO were observed to support this mechanism. The results of Figure 4 show that the amount of acetone produced is about 10 % of ethanol desorbed. This indicates that only a small fraction of adsorbed ethanol can be held strong enough to undergo surface reactions before desorption.

The TPSR results of acetic acid over a Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst, depicted in Fig. 5, show that there are two acetone peaks with one at *ca.* 270 $^\circ$C and the other at 300 $^\circ$C, indicating that surface acetate ions are the precursors of acetone. These two distinct peaks might be caused by the decomposition of different forms of metal acetates. The acetone formed could undergo secondary reactions on the surface basic sites, resulting a acetone-to-CO_2 ratio less than unity.

Surprisingly, the TPSR of ethanol over a $ZrO_2/MnO/ZnO$ catalyst yielded only ethanol with peak maximum at about 140 $^\circ$C. However, ethanol desorption peak observed over this catalyst (50 $^\circ$C - 280 $^\circ$C) is broader than that over the Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst (50 $^\circ$C - 200 $^\circ$C), indicating the presence of stronger adsorption sites on the former catalyst. The lack of acetone in the product stream is surprising since the $ZrO_2/MnO/ZnO$ catalyst could also provide lattice oxygen necessary for the formation of acetate ions from acetaldehyde. This can be explained by the fact that acetaldehyde, *i.e.*, the precursor for acetate ions, was not formed over this catalyst during the reaction. This further addresses the role of Cu metal plays in the dehydrogenation reactions of ethanol to acetaldehyde.

Hydrotalcites, or magnesium-aluminum hydroxycarbonates, are potential base catalysts and catalyst supports upon calcination since the high surface area is stable to steam treatment [Schaper, H., Berg-Slot, J.J., and Stork, W.H.J., *Appl. Catal.*, **54**, 79 (1989)]. Interestingly, calcined hydrotalcites have also been used as a novel support for Pt clusters in the catalytic aromatics of n-hexane, yielding comparable results to those obtained over zeolite L supported Pt catalysts [Davis, R.J., Derouane, E.G., *Nature*, **349**, 313 (1991)]. These materials have also been reported to be active for typical base-catalyzed reactions including aldol condensation [Reichle, W.T., *J. Catal.*, **94**, 547 (1985)]. Davis and co-workers have found that the basicity of hydrotalcite is, however, weaker than that of MgO [Mckenzie, A.L., Fishel, C.T., and Davis, R.J., *J. Catal.*, **138**, 547 (1992)], which might prevent further aldol condensation of reaction products to yield coke over strong basic sites of MgO.

The TPSR results of ethanol over MgO/Al_2O_3 with Mg/Al ratio ranging from 1.5 to 10 were shown in Figure 6, 7. Broad ethanol desorption peak were observed in the temperature

range of 60-400 °C over these three catalysts, indicating the variation in strength of surface adsorption sites. The amount of ethanol desorbed increased in the order of MgAl(5) > MgAl(1.5) > MgAl(10). Here, MgAl(x) represents a MgO/Al$_2$O$_3$ catalyst with a magnesium-to-aluminum ratio of x. Ethylene, which resulted from the dehydration of surface ethanol, was formed at 380 °C. Less ethylene was produced over MgAl(10) than over MgAl(1.5) or MgAl(5) catalysts, suggesting the role of aluminum ion or acid site plays in the dehydration reaction of ethanol to ethylene.

Task 5: Bench Scale Testing at Air Products and Chemicals

Cs-Modified Catalyst Testing

During this reporting period, a sample of the Cs-promoted BASF catalyst (sample number 13465-26), previously used as the catalyst for the isobutanol plant trial and sent to UC-Berkeley for testing was evaluated in APCI fixed-bed reactor. The series of data measured in the standard CSTR unit was to be used as the baseline for the performance of this catalyst in the reactor setup at Berkeley. Since the reactor at Berkeley is a PFR (plug flow reactor), it was decided to run some baseline tests in the PFR which had been previously set up at ACPI.

The PFR is described in a recent topic report sent to the DOE for approval. It consists of a copper-lined reactor heated by an aluminum heating block. (The reactor is in series with the 50 ml. CSTR which was not used for this set of experiments and shares the same analytical system which has been described previously.) This reactor is quasi-isothermal. In order to limit the heat generation, the catalyst was diluted with quartz chips in the ratio of 1:5 by weight. All data are reported relative to the active catalyst only. Only one thermocouple at the outlet of bed exists. Therefore, the degree of isothermality was not established for these preliminary experiments.

Data for the initial runs are summarized in Table 2. The initial three runs (14047-49 to 53) were characterized by initially reasonable values for methanol and isobutanol productivity judging from the ratio of isobutanol to methanol from the CSTR runs. This was followed by a rapid decrease in the isobutanol productivity within the first 24 h. The level of isobutanol was in fact lower than that expected for an unpromoted methanol catalyst (See 14047-56, for example.) The methanol productivity also showed a decrease in productivity, although the methanol reaction is at very near equilibrium so that decreases in productivity of the catalyst may not be apparent.

Catalyst poisoning was suspected. The apparatus was taken apart and cleaned. Carbon traps were replaced. The quartz powder and glass wool used in the apparatus were washed with acid to remove any possible trace contaminants. A standard methanol run is now being done to establish a baseline and to show that poisons are not present. The catalyst (S3-86) pellets were grounded and screened before use. The results of this run are in Table 2. The run appears normal. Catalyst activity is high after 117 h. The isobutanol productivity, although low, shows little fall-off with time. We conclude that the apparatus is now free of poisons.

4. PARTICIPATING PROJECT PERSONNEL

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Sub-Contractor Manager
Air Products and Chemicals

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Principal Investigator

Table 2. Initial Results of Isobutanol Experiments

Run	Catalyst	Temp. °C	Press. psig	GHSV hr⁻¹	Time on Stream h	Methanol Productivity (gm./kg-hr)	Isobutanol Productivity (gm./kg-hr)	Ratio IBOH/MEOH
1404749	Cs-promoted S3-68/quartz	300	768	5040	6.67*	*	*	0.11
"	"	"	761	5040	77	93	0.19	0.002
1404751	"	300	869	5004	4.65*	*	*	0.015
"	"	"	927	"	23.3	246	2.92	0.012
1404753	"	300	872	5008	4.28*	*	*	0.08
"	"	"	853	"	23.4	128	1.05	0.008
1404756	S3-86 acid-washed quartz	250	763	5008	17.7	339	6.55	-
"	"	"	770	"	117	361	5.15	-

* Short time sample-material balance could not be checked because of the large flow of N_2 in the system from changeover after reduction. The partial pressure of the syngas components is also suspected at this time. Ration of isobutanol to methanol (IBOH/MEOH) is correct. Procedures have been changed so that this should not be a problem any longer.

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Fig. 1. TPR of a Cs-promoted $Cu/ZnO/Al_2O_3$ catalyst
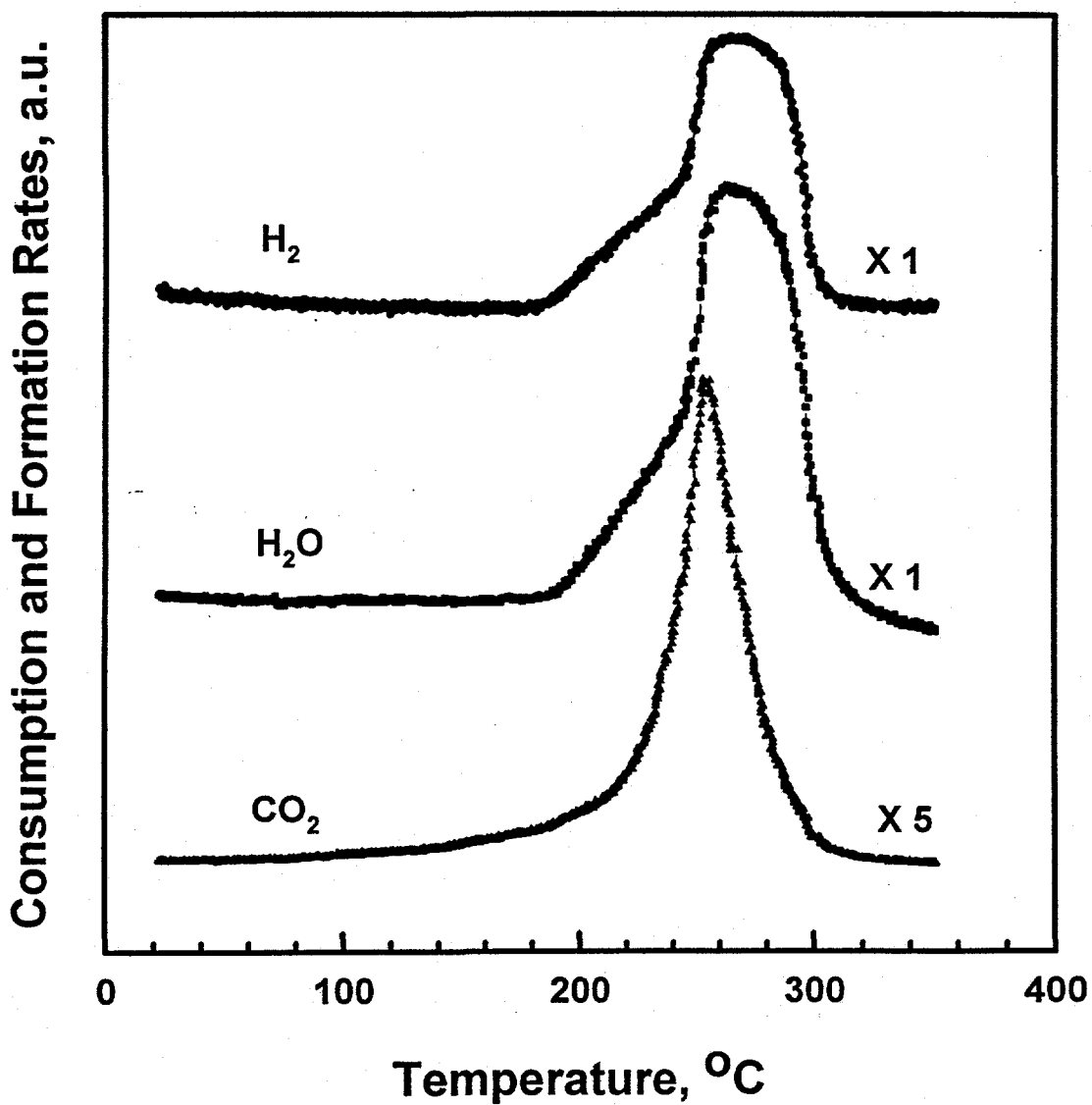5 % H_2 + 95 % He, heating rate: 10 $^\circ$C/min

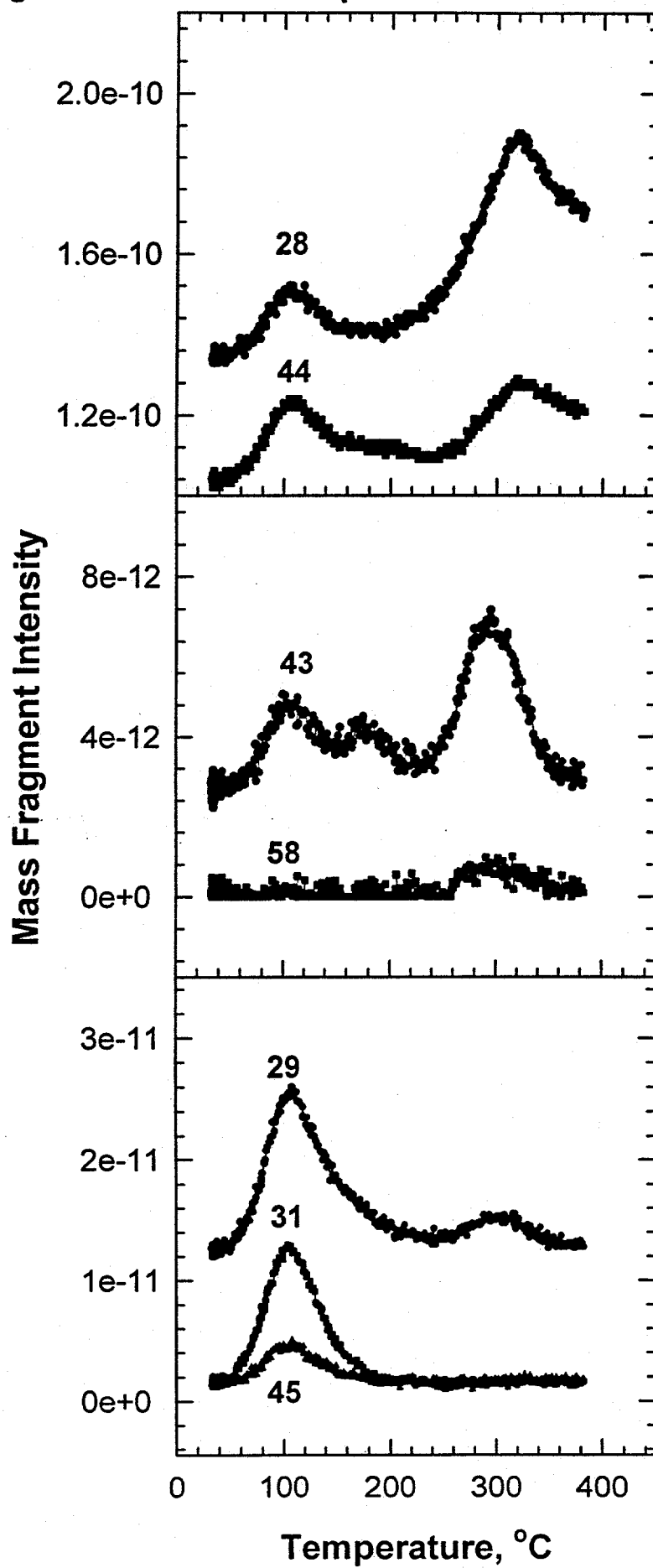# Fig. 2. Ethanol TPSR in pure He stream over a BASF catalyst
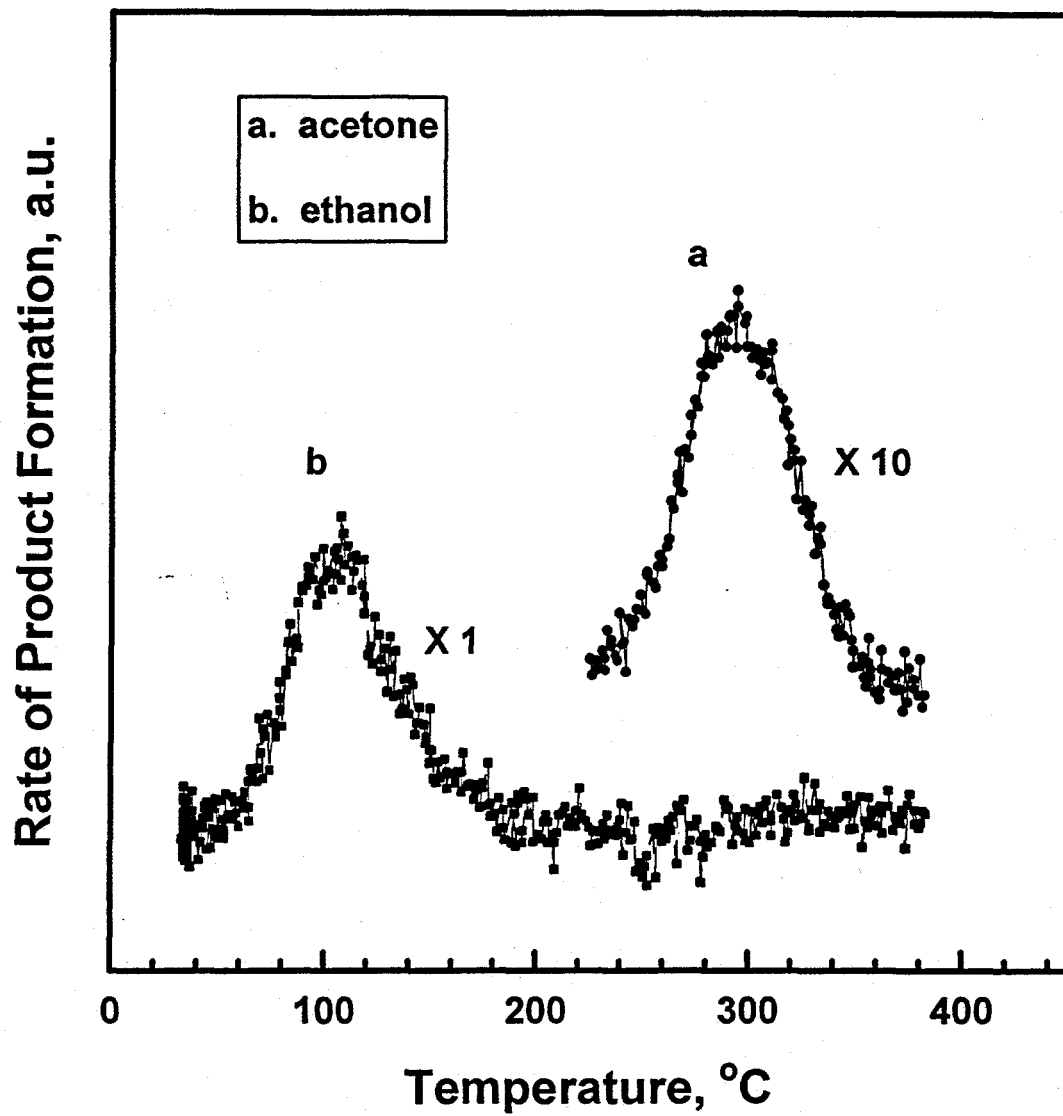
Fig. 3. Ethanol TPSR in pure He stream over a BASF catalyst

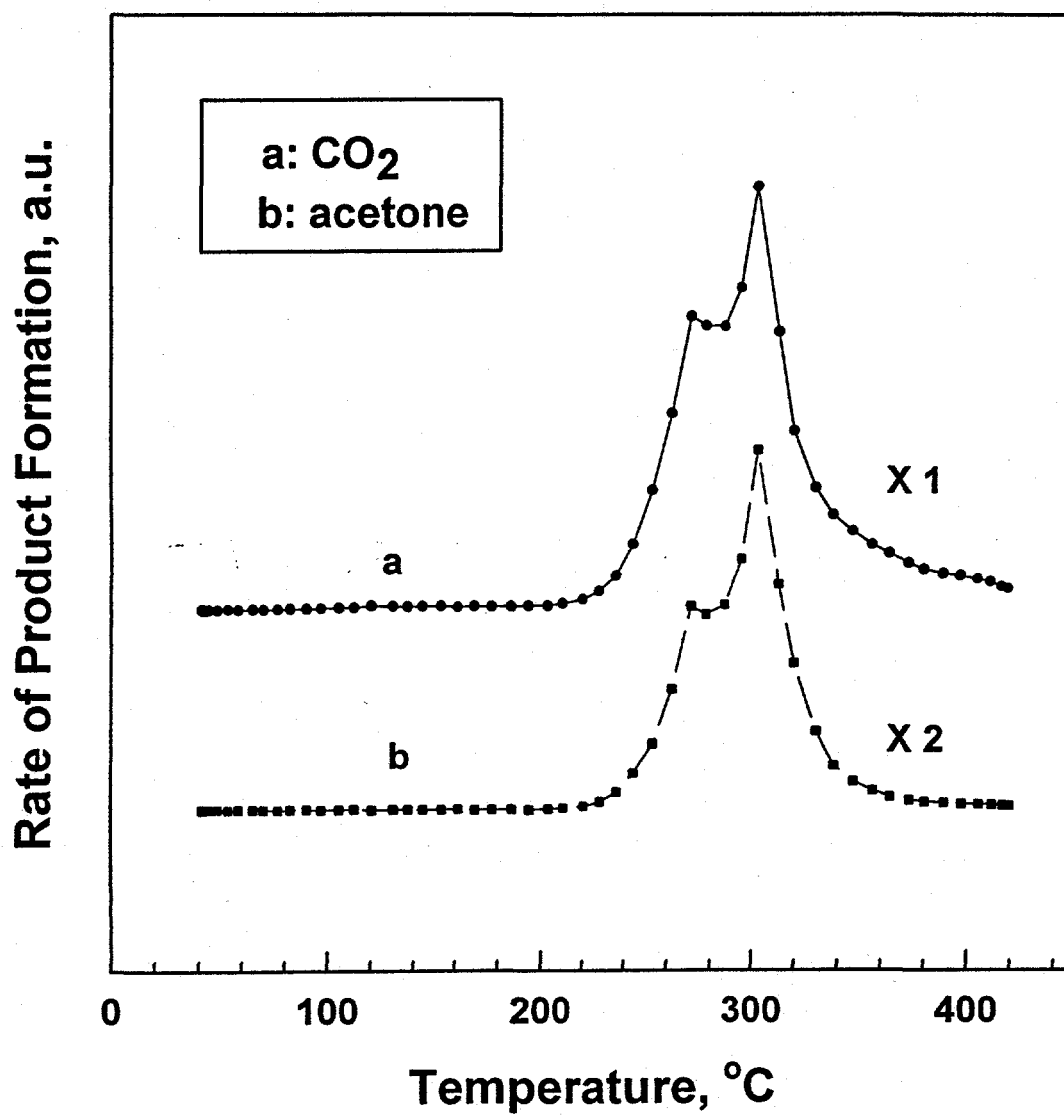## Fig. 4. TPSR of acetic acid over a BASF catalyst

a: CO_2
b: acetone

X 1

a

X 2

b

Rate of Product Formation, a.u.

Temperature, °C

Fig. 5. TPSR of ethanol over MgO/Al$_2$O$_3$

Fig. 6. TPSR of ethanol over MgO/Al$_2$O$_3$

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U.S. DEPARTMENT OF ENERGY
MILESTONE SCHEDULE □ PLAN ☒ REPORT

1. TITLE: ISOBUTANOL METHANOL MIXTURE FROM SYNGAS

2. REPORTING PERIOD: Oct 1, 1995 - Dec 31, 1995

3. IDENTIFICATION NUMBER: DE - AC22 - PC94PC066

4. PARTICIPANT NAME AND ADDRESS: Department of Chemical Engineering, University of California - Berkeley

5. START DATE: Oct 1994

6. COMPLETION DATE: Sept 1997

Duration: 94 — 95 — 96 — 97

Months: O N D | J F M A M J J A S O N D | Q2 Q3 Q4 | Q1 Q2 Q3 Q4

7. ELEMENT CODE	8. REPORTING ELEMENT	10. PERCENT COMPLETE a Plan	b Actual
Task 3	Complete design, construction and start-up of packed bed reactor module	100	100
Task 2	Prepare Cu-based catalyst compositions and characterize structure, surface area, and effectiveness of several synthetic approaches	100	100
Task 2	Choose four promising materials for catalyst evaluation	100	100
Task 3	Construct recirculating reactor module / Establish reaction pathways and rate-determining steps	70	60
Tasks 2 & 3	Identify catalyst components necessary to catalyze rate-determining steps that have been determined	55	40
Tasks 2 & 3	Identify synthetic techniques to increase the reactivity and accessibility of such required sites	75	40
Task 4	Complete construction and start-up of temperature programmed surface reaction apparatus and design of high-pressure infrared cell	80	100
Task 4	Design and construction of high-pressure infrared cell	40	70
Task 4	Calibrate between UCB and APCI laboratories by testing two selected catalysts in slurry reactors	55	20
Task 2	Determine the density and reactivity of the required sites and implement synthetic methods to improve them	5	0

U.S. DEPARTMENT OF ENERGY
MILESTONE SCHEDULE □ PLAN ☒ REPORT

1. TITLE	2. REPORTING PERIOD	3. IDENTIFICATION NUMBER
ISOBUTANOL METHANOL MIXTURE FROM SYNGAS	Oct 1, 1995 - Dec 31, 1995	DE - AC22 - PC94PC066

4. PARTICIPANT NAME AND ADDRESS — Department of Chemical Engineering, University of California - Berkeley

5. START DATE: Oct 1994

6. COMPLETION DATE: Sept 1997

7. ELEMENT CODE	8. REPORTING ELEMENT	9. DURATION	10. PERCENT COMPLETE (a Plan / b Actual)
Task 4	Identify reaction intermediates by TPSR and high pressure infrared methods		5 / 10
Tasks 3 & 5	Identify catalysts with highest isoalcohol yields (two) and evaluate at conditions resembling envisioned commercial practice.		0 / 0
Task 5	Assess economic viability of these catalytic materials		0 / 0
Task 5	Complete testing of at least two selected catalysts in slurry reactors.		0 / 0
Tasks 3 & 5	Choose two materials for detailed studies of the reaction mechanism and of optimum synthetic protocols		0 / 0
Tasks 3 & 5	Complete mechanistic studies on most promising materials		0 / 0
Tasks 2 & 5	Develop synthetic procedures that can be carried out on a commercial scale. Suggest a range of catalyst compositions for future study.		0 / 0
Task 5	Complete testing of the two selected catalytic materials		0 / 0
Task 5	Assess future research requirements, technical readiness and economic viability of the most promising approach		0 / 0
	Produce final report		0 / 0

Duration timeline: O N D (94) | J F M A M J J A S O N D (95) — Q2 Q3 Q4 (96) Q1 Q2 Q3 Q4 (97)

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    CARBON MONOXIDE;COPPER OXIDES;CERIUM OXIDES;ALKALINE EARTH METAL
    COMPOUNDS;CATALYSTS:T3;CHEMICAL PREPARATION:Q3;CHEMICAL REACTION YIELD;
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