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**DEACTIVATION BY CARBON OF
IRON CATALYSTS FOR INDIRECT LIQUEFACTION**

Quarterly Technical Progress Report
For Period March 16, 1990 to June 15, 1990

Calvin H. Bartholomew
Brigham Young University
Provo, Utah 84602

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FORWARD

This report summarizes technical progress during the fifteenth quarter (March 16 to June 15, 1990) of a four-year study conducted for the Department of Energy (DOE) under Contract No. DE-FG22-86PC90533. The principal investigator for this work was Dr. Calvin H. Bartholomew; Dr. Sayeed Akhtar was the technical representative for DOE.

Scott Eliason, a Ph.D. candidate contributed to the technical accomplishments and to this report. Dr. Bartholomew was the principal author.

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ABSTRACT

During the fifteenth quarter design of software for a computer-automated reactor system to be used in the kinetic and deactivation studies was continued. Further progress was made towards the completion of the control language, control routines, and software for operating this system. Progress was also made towards testing of the system hardware and software. Two new Fe/K/Al₂O₃ catalysts were prepared and H₂ adsorption data were obtained for these and unpromoted catalysts by two different methods. Kinetic and deactivation data were obtained for CO hydrogenation on K-promoted Fe as a function of time, temperature, and H₂/CO ratio. The PI attended the Spring National AIChE Meeting in Orlando, Florida, March 17-21 where he presented two invited papers and the 7th BES Catalysis and Surface Chemistry Research Conference held March 25-28 where he presented a poster paper. He also hosted the annual ASME Corrosion Meeting April 5-6 at BYU which focused on coal mineral transformations at which he presented a paper. On April 30 Professor Bartholomew presented a short course on Catalysis Deactivation at Catalytica Associates; he also presented a 3-day course on the same subject at Shell R&D in Houston on May 21-23 and visited with Shell personnel on May 24th. On May 7th the Catalysis Laboratory hosted Dr. Lynn Slaugh, distinguished scientist at Shell.

I. OBJECTIVES AND SCOPE

A. Background

Although promoted cobalt and iron catalysts for Fischer-Tropsch (FT) synthesis [1] of gasoline feedstock were first developed more than three decades ago, a major technical problem still limiting the commercial use of these catalysts today is carbon deactivation. Carbon deactivation is especially severe in processes that directly use synthesis gas with an $H_2:CO$ ratio of approximately 1:2 or less. Because these conditions are thermodynamically and kinetically favorable for carbon formation, rapid deactivation and physical disintegration of the catalyst are possible. Indeed, carbon formation is the major cause for loss of catalyst activity in the only presently commercial FT process in South Africa [1]. Thus, there is considerable motivation for understanding the fundamental mechanisms of carbon deactivation in order to find means of mitigating these problems. Models and/or data for predicting rate of carbon formation and its effects are needed so that the deleterious effects on catalysts and processes can be minimized. Data are especially needed for Fe/K catalysts because of their clear cost advantage and commercial significance.

B. Objectives

This report describes recent progress in a fundamental, three-year investigation of carbon formation and its effects on the activity and selectivity of promoted iron catalysts for FT synthesis, the objectives of which are:

1. Determine rates and mechanisms of carbon deactivation of unsupported Fe and Fe/K catalysts during CO hydrogenation over a range of CO concentrations, $CO:H_2$ ratios, and temperatures.
2. Model the rates of deactivation of the same catalysts in fixed-bed reactors.

C. Technical Approach

To accomplish the above objectives, the project will be divided into the following tasks:

1. Determine the kinetics of reaction and of carbon deactivation during CO hydrogenation on Fe and Fe/K catalysts coated on monolith bodies.
2. Determine the reactivities and types of carbon deposited during reaction on the same catalysts from temperature-programmed-surface-reaction spectroscopy (TPSR) and transmission electron microscopy (TEM). Determine the types of iron carbides formed at various temperatures and H_2/CO ratios using x-ray diffraction and Moessbauer spectroscopy.
3. Using a reaction model for FT synthesis developed in this laboratory, the kinetics of reaction and deactivation measured in Task 1, and models of fixed-bed reactors from

other workers, develop mathematical deactivation models which include heat and mass transport contributions for FT synthesis in packed-bed reactors.

The approach for each of these areas of study is described below:

Task 1: Kinetic/Deactivation Studies. While some kinetic data are available for CO hydrogenation on Fe/K [2-4], it is proposed that additional data be obtained with catalysts prepared in this study to confirm the previous work and to extend the range of experimental conditions, e.g. temperature and CO:H₂ ratio. Wash-coated monolithic catalysts will be used to minimize the effects of pore diffusion on the rate of reaction [5,6]. Iron catalysts used in the kinetic studies will be prepared by wash-coating Celcor (Corning Glass Works) monoliths (2.5 cm diam. by 1 cm long) with aqueous slurries containing previously reduced and passivated Fe or Fe/K catalysts. Washcoating procedures have been developed in this laboratory [5-8] which enable thin layers of either supported or unsupported catalysts to be deposited on the walls of monolith channels. These washcoated monolithic catalysts are ideal for kinetic studies because of their low pressure drops and high effectiveness factors [5,6].

Fe and Fe/K catalysts will be prepared according to procedures recently developed in our lab (9,10): (1) decomposition of iron nitrate (or iron and potassium nitrates) at 200°C in inert gas followed by reduction and/or (2) impregnation of the dehydroxylated alumina support with Fe pentacarbonyl/pentane followed by drying and reduction. The latter technique results in Fe/alumina catalysts of high dispersion and extent of reduction. Thus, this latter technique could be used to some advantage in the preparation of Fe/alumina/monolith catalysts for the kinetic/deactivation studies. After drying, the catalysts will be reduced in flowing hydrogen at 400-450 °C, using an established heating schedule that maximizes surface area [10,11]. Hydrogen uptakes of the reduced catalysts will then be measured so that reaction rates can be compared on the basis of catalytic surface area. These measurements will also be based on techniques recently developed in this laboratory [9,11]. Data obtained in this laboratory [9,10,12] indicate that the activities and selectivities of Fe and Fe/K catalysts prepared by our techniques have catalytic properties typical of iron FT catalysts.

Reaction kinetic and deactivation studies will be carried out using a Berty internal recycle reactor system previously described [5, 13]. The Berty CSTR reactor has the advantages of (i) gradientless operation with respect to temperature and reactant concentrations, and (ii) the capability of adjusting the stirring speed to eliminate effects of external mass transport. The combination of the Berty reactor and wash-coated monolithic catalysts will ensure the collection of intrinsic surface reaction rates in the absence of pore-diffusional and external film diffusional disguises [5,13]. The use of the Berty reactor also enables deactivation kinetics to be measured directly and unambiguously for each given set of conditions [7,14]. As part of this task the Berty Reactor System will be computer automated and the analysis will be augmented by the addition of a new H.P. 5890 chromatograph slaved to a micro computer.

Reaction kinetics will be obtained by measuring CO conversion over a range of temperatures and reactant concentrations, e.g. 180-250°C, $P_{\text{CO}} = 10\text{-}50$ kPa, $P_{\text{H}_2} = 10\text{-}50$ kPa, and $\text{H}_2\text{:CO} = 1.1\text{-}3.1$. To ensure the collection of intrinsic kinetic data in the absence of deactivation phenomena, the reactant gasses and argon diluent will be carefully purified of oxygen, sulfur compounds, and iron pentacarbonyl. Deactivation effects due to carbon will be avoided during kinetic measurements by careful choice of operating conditions and by periodically treating the catalyst in pure hydrogen just prior to changing gas composition and temperature. Kinetic data will be obtained over a period of 24 hours at each condition so that both initial and steady-state rates and product distributions are obtained. Product distributions will be measured on-line using heated lines to carry the products to a chromatograph equipped with glass capillary and Chromosorb 102 columns connected to flame ionization and thermal conductivity detectors, respectively, as described previously [15]. The study of Fe and Fe/K catalysts will enable the effects of potassium on the reaction kinetics to be determined.

Deactivation kinetics due to carbon formation will be obtained by measuring CO conversion and product distribution as a function of time for 24-48 hours at a given set of reaction conditions. Temperatures and reactant concentrations will be varied from run to run, e.g. 250-350°C; $P_{\text{CO}} = 10\text{-}50$ kPa; and $\text{H}_2\text{:CO} = 0.5\text{-}2.0$. Again the study of both Fe and Fe/K catalysts will permit effects of potassium on the kinetics of deactivation to be determined.

Task 2: Study of Carbon reactivities and Types. The reactivities of carbon species deposited during CO hydrogenation on Fe and Fe/K catalysts will be determined using temperature-programmed-surface-reaction spectroscopy (TPSR) with hydrogen [7,16]. The data will be obtained using a TPD system featuring a UTI-100C quadrupole mass spectrometer and programmable peak selector [17]. The peak selector enables up to 9 different peaks to be selected simultaneously and will facilitate analysis of methane and C_{2+} hydrocarbons during TPSR of the carbon-deactivated catalysts with hydrogen.

Catalysts will be pretreated in synthesis gas ($\text{H}_2\text{:CO} = 0.5$ to 2.0) at various reaction temperatures (e.g. 250 to 350°C) over a period of 16-24 hours, cooled in He carrier gas to 25°C, and then reacted with H_2 (10% H_2 in He or Ar) while increasing the temperature of the sample at a linear rate of 30°C/min. The use of small, powdered samples (50-100 mg; 80-100 mesh) and low carrier gas flow rates (20-40 cm³/min) will ensure the absence of intra- and interparticle concentration gradients [17-21]. These conditions have been shown in previous TPD studies conducted in this laboratory [17-19] to be optimum for minimizing pore diffusion effects, sample measurement lag times, and concentration gradients [20,21]. Previous studies of carbon-deactivated catalysts with TPSR [7,16,22] have enabled identification of different carbon species having a range of reactivities. Again, it is important to investigate both Fe and Fe/K catalysts since Dwyer [23] found evidence of different forms of carbon on clean iron and potassium-covered iron surfaces.

Different forms of carbon deposited during CO hydrogenation on iron catalysts will be identified by submitting samples from the deactivation rate studies for examination by transmission electron microscopy (TEM). TEM has been used in several previous investigations in this laboratory to identify different forms of carbon--particularly vermicular (filamentous) carbons [24-26]. By submitting samples tested at various temperatures, it will be possible to determine at which temperature vermicular carbon formation occurs.

The role of iron carbides in deactivation during CO hydrogenation will be determined by analyzing spent catalysts from the deactivation runs by x-ray diffraction and Moessbauer spectroscopy. Moessbauer spectroscopy has already proven itself as a useful tool for identifying various iron carbides formed during CO hydrogenation [27-29]. It will be interesting to determine if certain carbides are associated with the more severe conditions of carbon deactivation, i.e. high temperature and low H₂:CO ratio and how potassium affects carbide formation.

Task 3: Mathematical Modeling of Catalyst Deactivation by Carbon. The development of a chemical mathematical model for deactivation of iron catalysts during Fischer-Tropsch synthesis will follow an approach similar to that used previously in this laboratory to model methanation in fixed beds [5,30,31]. The one-dimensional, quasi-steady-state model will feature simultaneous solution of (i) the rate equations for the main reaction and for deactivation [14,32,33]. The kinetics for the main reaction will be calculated according to the model recently developed by Rankin and Bartholomew [34] and will be based on the dissociation of adsorbed carbon monoxide, subsequent hydrogenation of the surface carbide [7,16, 35-37], and provision for the Anderson-Schulz-Flory polymerization mechanism [38-41]. This reaction model enables the calculation of intrinsic rate constants for initiation, termination, and propagation, as well as values for the polymerization probability. This reaction model also has a provision which accounts for the formation of olefins and oxygenates in the case of the iron catalysts. In addition, the kinetics of the water-gas-shift reaction [42] will be added. The effects of pore diffusion resistance will not be considered at this point. The coupled differential equations will be solved by finite difference [43]. Model predictions will be closely compared with experimental results obtained at high conversions in the CSTR Berty reactor. The model will be used initially to predict catalytic activity, selectivity, reactant concentration, and temperature as functions of time and position in the fixed-bed reactor.

II. SUMMARY OF PROGRESS

Progress can be most efficiently summarized by task:

A. Task 1: Kinetic/Deactivation Studies

During the fifteenth quarter design of software for a computer-automated reactor system to be used in the kinetic and deactivation studies was continued. Further progress was made towards the completion of the control language, control routines, and software for operating this system. Progress was also made on testing of the system hardware and software.

Two new Fe/K/Al₂O₃ catalysts were prepared and H₂ adsorption data were obtained for these and unpromoted catalysts by two different methods. Kinetic and deactivation data were obtained for CO hydrogenation on K-promoted Fe as a function of time, temperature, and H₂/CO ratio.

B. Task 2: Study of Carbon Reactivities and Types

No experiments are scheduled for this Task until Spring 1991, although literature study is being conducted.

C. Task 3: Mathematical Modeling of Catalyst Deactivation by Carbon

This task is scheduled to begin in Summer 1991.

D. Task 4: Technical Communication and Miscellaneous Accomplishments

The PI attended the 1990 Spring National Meeting of the AIChE in Orlando, Florida, March 17-21 where he presented two invited papers at the Symposium on Fischer-Tropsch Synthesis and the 7th BES Catalysis and Surface Chemistry Research Conference held March 25-28 in Gaithersburg, Maryland where he presented a poster paper. He also hosted the annual ASME Corrosion Meeting April 5-6 at BYU which focused on coal mineral transformations at which he presented a paper on CaO catalysis of char oxidation. On April 30 Professor Bartholomew presented a short course on Catalyst Deactivation at Catalytica Associates; he also presented a 3-day course on the same subject at Shell R&D in Houston on May 21-23 and visited with Shell personnel on May 24th. On May 7th the Catalysis Laboratory hosted Dr. Lynn Slaugh, distinguished scientist at Shell.

III. DETAILED DESCRIPTION OF TECHNICAL PROGRESS

A. Task 1: Kinetic/Deactivation Studies

1. Construction and Testing of the Automated Bertly Reaction System.

During the fifteenth quarter design of software for a computer-automated reactor system to be used in the kinetic and deactivation studies was continued. Further progress was made towards the completion of the control language, control routines, and software for operating this system. Progress was also made on the testing of the system hardware and software. Some bugs in the control software were found and corrected.

2. Catalyst Preparation

A new potassium-promoted catalyst (Fe/K-A-30X) was prepared by dissolving KNO_3 in water and mixing a portion of the Fe-A-200 catalyst that was previously reduced and passivated. KNO_3 was added to achieve a total K/Fe molar ratio of 0.06. Arakawa and Bell [48] have shown that CO consumption and olefin production pass through a maximum at this ratio. The first (Fe/K-A-301) of two samples of this new catalyst was used to probe the conditions required for obtaining activity similar to the unpromoted catalysts. The second sample (Fe/K-A-302) was used to measure hydrogen chemisorption uptakes.

A batch of (Fe/K-A-40X) was prepared by dissolving 0.1118 g KNO_3 in 10 ml water and adding to 5.0009 g reduced and passivated Fe-A-200 catalyst to achieve a total K/Fe ratio of 0.013. The catalyst was then dried at 110°C .

3. Adsorption Measurements

a. **Hydrogen Adsorption Measurements.** Hydrogen chemisorption measurements were performed on a spent, reduced Fe-A-205 catalyst after evacuation at 400°C for 1 hr and cooling in hydrogen to room temperature. The average of seven measurements with the corresponding 95% confidence interval was 55.3 ± 2.8 $\mu\text{moles/g}$ catalyst.

Chemisorption measurements were also obtained on Fe-A-206, a catalyst from the same batch as Fe-A-205, resulting in an uptake of 54.3 ± 4.7 $\mu\text{moles/g}$. Based on these results, the quantity of zero-valent surface iron can be considered the same on both the fresh and spent catalysts.

It has been shown, however, that there may be significant spillover of hydrogen on iron catalysts at temperatures where these chemisorptions have been performed and that admitting hydrogen into the cell at 100°C and then measuring the uptake at that temperature gives results consistent with surface areas measured by CO chemisorption [48]. Indeed, when this new

method was performed on Fe-A-206, the average uptake was 32.9 ± 2.7 $\mu\text{moles/g}$, a decrease of 40% from the previous method.

Hydrogen uptakes were also measured for (Fe/K-A-302) using both methods previously discussed. Again, there were substantial differences in the results of the two methods. Cooling in hydrogen from 400°C to room temperature resulted in an uptake of 30.2 ± 6.7 $\mu\text{moles/g}$ while the adsorption at 100°C gave 9.66 ± 3.2 , a decrease of 68%.

Hydrogen uptake data are summarized for the catalysts studied thus far in Table 1. Chemisorption uptake data were obtained for the two methods for both K-promoted and unpromoted catalyst before and after reaction. There is a general trend of decreasing uptake from Method 1 to Method 2. The substantially larger uptakes obtained by the first method suggest that spill-over is important at high adsorption temperatures in both catalysts systems but more pronounced on the promoted catalyst.

The surface area of K-promoted iron (Fe/K-A-402) decreases 40% from the unpromoted catalyst, showing that even a very small amount of potassium has a large effect on the adsorption characteristics of the iron. Increasing the potassium content by 5 times (Fe/K-A-302)

TABLE 1

Hydrogen chemisorption uptakes ($\mu\text{moles/g}$) for various unpromoted and potassium-promoted catalysts. Numbers in parentheses are the 95% confidence intervals.

Catalyst	Hydrogen uptake, $\mu\text{moles/g}$		
	Fresh/Reduced	Spent/Unreduced	Spent/Reduced
Fe-A-205 ^a			55.3 (2.8)
Fe-A-206 ^a	54.3 (4.7)		
Fe-A-206 ^b	32.9 (2.7)		
Fe/K-A-302 ^{a,c}	30.2 (6.7)		
Fe/K-A-302 ^{b,c}	9.66 (3.2)		
Fe/K-A-401 ^{b,d}		4.77 (1.6)	11.0 (12.)
Fe/K-A-402 ^{b,d}	19.3 (3.5)	8.75 (1.1)	12.6 (2.7)
Fe/K-A-403 ^{b,d}		4.37 (3.6)	6.61 (3.5)

^a Method 1: Cool from 400°C to RT in hydrogen; isotherm measured at RT.

^b Method 2: Isotherm measured at 100°C.

^c K/Fe molar ratio = 0.061.

^d K/Fe molar ratio = 0.013.

reduces the uptake again by a factor of two. Measurement of the active surface area (zero-valent iron) by hydrogen chemisorption after synthesis indicates that deactivation of K-promoted iron occurs readily at mild reaction conditions. For example, after a series of reaction experiments, the uptake of Fe/K-A-402 decreases from 19.3 to 8.75 $\mu\text{moles/g}$. Upon regenerating the catalyst in hydrogen at 400°C for 24 hours, some of the active surface area is regained, but significant permanent deactivation has occurred as indicated by a final uptake of 12.6 $\mu\text{moles/g}$. On the other hand, the active surface area of the unpromoted catalyst is the same within experimental error before and after reaction, i.e. uptakes of two different unpromoted samples, one fresh and the other spent, were nearly identical.

Hydrogen chemisorptions made on the 400 series catalysts at various points along their schedules are shown in Figure 1. There is an obvious trend of active surface area decrease due to reaction but which may be partially recovered by re-reducing in hydrogen.

b. BET Surface Areas. Surface areas were measured for Fe-A-206 following ASTM standard test method D3663-84. Three separate tests on this catalyst resulted in a surface area of $11.6 \pm 0.2 \text{ m}^2/\text{g}$ catalyst. Several BET measurements were also made on the 400 series catalysts at various reaction times. The values for the spent/reduced Fe/K-A-402 and -403 were 9.75 and 7.66 m^2/g , respectively. A value of 8.36 was obtained for the fresh/reduced Fe/K-A-404.

4. Activity/Selectivity/Deactivation Measurements

Activity data were obtained as a function of temperature, time, and reactant concentrations for several Fe/K catalysts. The results are summarized by catalyst.

a. Fe/K-A-301. Reaction conditions were initially 200°C and $\text{H}_2/\text{CO} = 3$. Temperatures were increased in 10 degree increments after reacting at each temperature for 10 to 24 hours. The catalyst was not active enough for the thermal conductivity detector to register a methane peak until the reaction temperature reached 250°C. The CO conversion did not exceed 3% until a reaction temperature of 350°C. Based on the low activity of the potassium promoted catalyst it is concluded that the potassium content on the surface of the catalyst was significantly higher than the calculated total molar ratio. A rough estimate of the surface ratio based on hydrogen uptakes of the unpromoted and promoted catalysts gives a maximum K/Fe surface ratio of 20, nearly three orders of magnitude greater than the desired amount. When compared to activity data of catalysts with varying potassium contents [48], the activity of Fe/K-A-301 more closely resembles a catalyst having a K/Fe ratio of 0.2 to 0.3. Because of the low activity of Fe/K-A-301 it was decided that the amount of potassium added to make a new K-promoted catalyst would be decreased to one-fifth of the previous amount. No further reactions were performed with this catalyst.

Figure 1. Hydrogen adsorption data for fresh, spent and regenerated Fe/K catalysts.

b. Fe/K-A-400 Series. From the results for Fe/K-A-301, it is clear that potassium promoted catalysts require higher temperatures to achieve comparable CO conversions to those of the unpromoted catalysts. For this reason, the initial reaction conditions chosen for catalyst Fe/K-A-401 were 230°C at a H₂/CO ratio of 3/1. The activity was a maximum after one hour on stream and decreased by 75% over the next 19 hours.

The purpose of the unsupported kinetic study is to obtain kinetic data at conditions where the effect of deactivation is minimal or non-existent. The apparent deactivation at 230°C indicated that lower temperature tests were necessary if deactivation was to be minimized.

The sample was re-reduced in hydrogen at 400°C for about 24 hours prior to reacting further. This extended reduction time was necessary to obtain a state of catalyst in which no more (or very little) methane was being produced. Subsequent re-reductions on the potassium-promoted catalysts were done for a standard length of 20 hours. This compares to reduction times for the unpromoted catalysts of only two hours to obtain similar states.

Reaction temperatures for continued runs on Fe/K-A-401 ranged from 200 to 230°C. However, at 200°C the activity was too low to measure. Figure 2 shows the activity versus time curves at various temperatures. The two sets of data with the highest initial activities

were obtained (following reduction in hydrogen) at 210 and 230°C. The time zero point is the time at which the reactor reached the given temperature. Although sample data for each temperature do not cover the full range, they do indicate that after several (about 9) hours on stream the activity at each temperature reaches a value that is within about 20% of the other temperatures. For reaction sets at 210 and 230°C where data were obtained on the freshly reduced catalyst, the higher initial activity of the higher temperature leads to a lower "steady-state" value (about 20 hours). Thus, the effect of deactivation becomes more pronounced at higher temperatures.

Figure 2. Activity versus time for Fe/K-A-401 at 210-230°C.

Figure 3 shows the data from three different samples all reacted at 230°C at H₂/CO ratio of 3/1. The catalyst histories for the other two samples (Fe/K-A-402 and Fe/K-A-403) are given here. Hydrogen chemisorptions had been performed on the fresh Fe/K-A-402 catalyst. Reaction runs were then commenced at 210°C for 36 hours followed directly by reaction at 230°C. Fe/K-A-403 had been reacted at 210°C for 12 hours, reduced for 12 hours at 400°C and then reacted at 230°C. As seen in Fig. 3, the two freshly reduced samples (401 and 403) have similar initial activities but 401 drops to a significantly lower value than 403. After 20 hours at 230°C, 401 activity is about half of the measured activity for 403. The fact that catalyst 403 had previously been reacted at 210°C may be the reason for the difference,

even though the catalyst was reduced between the two runs. The conditions which the catalyst is subjected to initially appear to have a large impact on the "long-term" (ie, 20 hour) state of the catalyst.

After reaction for 36 hours at 210°C, the temperature for catalyst Fe/K-A-402 was increased to 230°C. While the initial activity was only about half that for the other two catalysts, the activity after 3 hours was similar to catalyst 401 and for the rest of the time shown was intermediate between the other two catalysts.

Another potassium-promoted sample (Fe/K-A-404) was used to measure activities as a function of H₂/CO ratio so that an estimate of the reaction orders for hydrogen and CO could be obtained, similar to what was done previously for the unpromoted catalysts. The catalyst was first reacted at 3/1 H₂/CO at temperatures ranging from 220-240°C so that the data for determining reaction orders would not be affected by errors introduced by using different samples. Subsequent treatment at 2/1 H₂/CO (with 1 part He diluent) showed a stronger effect of deactivation on the activity of the catalyst. No further reaction experiments were performed with the potassium-promoted catalyst since kinetic data could not be obtained due to deactivation.

Figure 3. Specific activity versus time for Fe/K-A-401, 402, and 403.

B. Task 2: Study of Carbon Reactivities and Types

No experiments are scheduled for this task until Spring 1991. The research assistants working on this project are presently familiarizing themselves with the literature dealing with deactivation by carbon.

C. Task 3: Mathematical Modeling of Catalyst Deactivation by Carbon

This task is scheduled to begin in the Summer 1991.

D. Task 4: Technical Communication and Miscellaneous Accomplishments

The PI attended the 1990 Spring National Meeting of the AIChE in Orlando, Florida, March 17-21 where he presented two invited papers at the Symposium on Applications of Fischer-Tropsch Synthesis dealing with "Hydrogen Adsorption on Supported Cobalt, Iron and Nickel" and "Recent Technological Developments in Fischer-Tropsch Catalysis" and the 7th BES Catalysis and Surface Chemistry Research Conference held March 25-28 in Gaithersburg, Maryland where he presented a poster paper on "Effects of Dispersion and Support on Adsorption, Catalytic and Electronic Properties of Cobalt/Alumina CO Hydrogenation Catalysts." He also hosted the annual ASME Corrosion Meeting April 5-6 at BYU which focused on coal mineral transformations at which he presented a paper on CaO catalysis of char oxidation. On April 30 Professor Bartholomew presented a short course on Catalyst Deactivation at Catalytica Associates; he also presented a 3-day course on the same subject at Shell R&D in Houston on May 21-23 and visited with Shell personnel on May 24th. On May 7th the Catalysis Laboratory hosted Dr. Lynn Slaugh, distinguished scientist at Shell.

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