

Figure 6.6. A Schematic Cross-Sectional Diagram of a Solenoid Used to Actuate the Sliding Plug.

The solenoid consists of a 187.3-mm long piece of 1/2-inch O.D. 316- stainless-steel (non-magnetizable) tubing with a 0.049-inch wall thickness. The winding is 111 mm in length and it starts 44 mm from the bottom end of the tube. It contains 2,880 turns of 23 AWG cooper-solenoid-winding wire, producing a force of 1.33 N at the start of the plunger stroke. The solenoid is connected at the base to a 1/2-inch to 1/4-inch Swagelok reducing union. This union serves as the resting point of the plunger when the solenoid is de-energized. When the plunger is in this position, approximately the top 22 mm is in the winding area.

At the top of the solenoid, an adjustable plunger stop extends down into the solenoid winding. The stop consists of a 10.0-mm diameter piece of 416- stainless steel (non-magnetizable) threaded into a 6.35-mm O.D. piece of 316- stainless steel. The stop serves to redirect the flux lines of the magnetic field so that the magnetic force at the end of the plunger stroke is greatly increased. This serves, in turn, to pull the sliding plug in the microreactor firmly against its seat. The plunger stop is fixed to the solenoid by a 1/2-inch stainless-steel Swagelok union. In this way, the solenoid can be used at high pressure with no gas leakage and the stop can still be adjusted.

The plunger itself is a piece of 416- stainless-steel rod, 76.2-mm long and 10.0 mm in diameter. Two grooves, 3.18-mm wide and 1.27-mm deep, run the length of the plunger. These grooves keep gas from building up in front of the plunger as it moves. The lower end of the plunger has a nipple to allow for attachment of the wire from the

sliding plug. The wire connecting the plungers to the sliding plug runs down from the plunger, around a 90-degree bend and through the flexible stainless-steel hose. After passing through the flexible hose, the wire goes through two more 90-degree bends and finally attaches to the plug. The feed gas enters the tubing just below the solenoid at a tee union. Therefore, the wire does not go around any sharp corners, but only 90-degree tubing bends. "Flexing" of the flexible hose during vibration causes no ill effects and the plug remains seated.

As in the cold-flow model, the solenoids are powered by a 24-VDC supply and are connected to a relay. The latter acts to alternately energize the solenoids. Therefore, one solenoid is energized while the other is de-energized. The relay is controlled via the computer interface and the H-89 microcomputer.

6.1.1.4 Associated Systems

The product-gas sampling system and the gas-chromatographic system, used in conjunction with the sliding-plug vibrofluidized-bed microreactor system are identical to the systems described in Sections 4.1.1.3 and 4.1.1.4.

6.1.2 Materials

The sliding-plug vibrofluidized-bed microreactor system for unsteady-state F-T synthesis was designed with the use of -150 ± 300 μ fused-iron ammonia-synthesis catalyst as described in Section 4.1.2.1. However, this system does not preclude the use of other size fractions or new types of catalysts.

Gases being used with this microreactor system are similarly described in Section 4.1.2.2.

6.1.3 Experimental Procedures

6.1.3.1 Microreactor Cleaning and Catalyst Loading

The procedure to be followed when cleaning and loading the sliding-plug vibrofluidized-bed microreactor is very similar to the procedure used for the steady-state vibrofluidized-bed microreactor.

First, however, the sliding plug had to be removed from the plenum zone. This was accomplished by removing the two Swagelok male connectors that screw into the base section of the microreactor and serve as plug seats. The mating surface of the three microreactor sections were then polished with number 500 emory cloth on a surfacing table. The entire interior surface of the microreactor was flushed with acetone and wiped with Kimwipes.

After the microreactor was thoroughly cleaned, the base section was placed in the wooden support apparatus and clamped in the vise. Approximately 1 meter of the 0.356-mm diameter stainless-steel wire was then attached to each end of the sliding plug. The plug was slid into the plenum zone; and the wire was threaded through the washers and the Swagelok male connectors. A small amount of "Silver Goop" thread lubricant was applied to the threads of the connectors to prevent seizing and to facilitate later removal. The male connectors were then tightened, compressing the copper washer.

The wire was threaded through the 1/4-inch O.D. stainless-steel tubing that is used to connect the microreactor to the flexible stainless-steel hose. Each piece of tubing has two 90-degree bends and is attached to the Swagelok fitting-end of the male connector in the base of the microreactor. Thread lubricant is also applied to the fitting threads which are exposed to the high temperature in the constant temperature bath.

Following the installation of the sliding plug, a new 2-micron sintered stainless-steel plate was made and positioned into the distributor plate recess in the base section. A thin, oval-shaped, Grafoil gasket was then placed on top of the distributor plate. This gasket prevents any gas from bypassing the distributor plate by sealing between the edges of the plate and the microreactor base-section.

A silver-plated stainless-steel O-ring was then inserted into the O-ring groove and the reaction section of the microreactor was installed. One gram of -150+300 micron fused-iron catalyst was weighted and carefully poured into the reaction zone. The thermocouples were typically left in place in the reaction section between experiments.

A 20-micron, sintered stainless-steel catalyst retention plate was fitted to the gas-exit section as was a silver plated O-ring. The gas-exit section was placed on top of the reaction section. Thread lubricant was used on the bolts that clamp the three sections (i.e., base section, reaction section, and gas-exit section) together and these bolts were torqued in sequence to 27 N-m.

6.1.3.2 Mounting the Microreactor

Once the microreactor was cleaned and loaded with fresh catalyst, it was ready for attachment to the rest of the system. Four threaded rods were screwed into the tapped holes in the base section.

The microreactor was lowered into the cool fluidized-bed constant-temperature bath. These rods were, in turn, bolted to the leaf-spring supports. The two stainless-steel plug wires, emanating from the microreactor feed tubes, were then carefully threaded up through the flexible metal hose and tubing to the solenoid mounting position. In order to do this, guide wires had to be used. The compression fittings between the flexible metal hose and the microreactor feed and gas-exit lines were then tightened. The thermocouples from the microreactor were then connected to the panel meter.

At this point, the vibrator itself was mounted to the underside of the I-beam support and connected to the microreactor support system. The frequency generator was then adjusted to the point where the microreactor was vibrating at the maximum amplitude. This usually corresponded to a resonance frequency of 18-24 Hz with a peak-to-peak amplitude of 4 mm. The solenoid plungers were next attached to the plug wires. The plug was first drawn up tight against the left-hand plug stop by pulling on the plug wire.

The plunger was next attached to the plug wire 57.2 mm up from the point where the reducing union expands from 1/4- to 1/2-inch. Note that the reducing union serves as the resting point of the plunger when the solenoid is de-energized. In addition, the stroke of the plug in the

plenum is 50.8 mm. Consequently, when the solenoid is de-energized, there should be approximately 6.4 mm of slack in the plug wire. This provides enough slack so that the plunger in the de-energized solenoid does not keep the plug from resting on the opposite plug-seat.

After attaching the left plunger, the left solenoid was slipped down over that plunger and attached to the reducing union. The right-hand plunger and solenoid were then installed in a similar fashion and the solenoid cooling fans were turned on.

The final step in the installation involved optimizing the pulling force at the ends of the plug stroke. This was done by adjusting the length of the plunger stops in the solenoids. These stops were constructed so that they could be adjusted to make up for any difference in plug-wire length between experiments.

6.1.3.3 System Startup and Catalyst Reduction

Before an experiment, the mass-flow meters as well as the pressure transducers were calibrated. The system was then pressure-tested at 3,446 kPa for possible leaks. The portion of the system located downstream of needle valves 1-4 (Figure 6.2) was thoroughly flushed with helium. This was done by directing three-way valves V6, V9 and V10, so that helium could flow through them. Shut-off valve V11 was opened so as to keep the pressure on either side of the sliding plugs equilized. Valves V3 and V12, and solenoid valve 5 were opened, allowing helium to flow. The solenoids were then alternately switched moving the plug

back and forth. Valve V12, parallel to the back-pressure regulator, was closed and the system pressure downstream of solenoid valves 1-4 was brought up to 2,220 kPa using helium.

The F-gas feed line located upstream of solenoid valves 1 and 2 was pressurized to 4,807 kPa, as was the S-gas feed-line located upstream of solenoid valves 3 and 4. During an experiment, three-way valves V7 and V8 were always turned so that the downstream pressure was monitored. If these valves are turned from their upstream position to the downstream position during an experiment, a burst of gas will be transmitted through the microreactor.

At this point, the nitrogen ballast-gas flow was started by opening valve V1 and adjusting the associated needle valve. The back-pressure regulator was adjusted so that a downstream system-pressure of 2,220 kPa was maintained. The helium flow was stopped by shutting valve V3 and solenoid valve 5.

The next major step involved setting the F-gas, S-gas, percarburizing and reducing gas flow rates through the microreactor. The S-gas flow rate was set first. Three-way valves V9 and V10 were directed toward the F-gas and S-gas feed-lines and shut-off valve V11 remained open. The right solenoid, R, was activated, causing the plug to rest against the right-hand stop. Solenoid valves 3, 4, and 5 were then simultaneously opened, purging the reactor with S-gas at 6.67×10^4 standard mm^3/s for one minute. Solenoid valve 3 was closed and the system pressure was allowed to stabilize for several minutes with a low

flow of S-gas. Valve V11 was then shut, isolating the F-gas and S-gas feed lines.

The needle valve associated with solenoid valve 4 was adjusted so that the mass-flow meter was reading the desired value for the S-gas flow rate. Solenoid valve 4 was closed and three-way valves V6 and V10 were turned so that the H₂:CO:Ar precarburizing-gas mixture was flowing through the microreactor. Valve V11 was temporarily opened to assure pressure equilization across the sliding plug and then closed.

The flow rate of precarburizing gas was then set using the appropriate needle valve and the mass-flow meter. The pressure upstream of the precarburization needle valve was kept at 4,807 kPa in order to maintain a critical pressure drop. The precarburization flow was stopped by directing three-way valve V10 toward the S-gas feed line.

The reducing-gas flow rate was set in a similar fashion to the S-gas flow rate. Hydrogen was used as both F-gas and the reducing gas. Different flow rates of hydrogen were used during reduction and unsteady-state synthesis. Consequently, the needle valve associated with solenoid valve 2 had to be adjusted accordingly after the catalyst reduction period.

After the downstream system was purged with hydrogen and the reduction flow was set to 3,670 standard mm³/s, the fluidized constant-temperature bath was heated to 450°C and the heating tapes were turned on. The bath-heating period took approximately two and one-half hours. The actual reduction period consisted of six hours of isothermal reduction of the catalyst at 450°C. At the end of the reduction period,

the hydrogen flow rate had to be adjusted. Hydrogen was used as F-gas in the later stages of the unsteady-state experiment. Its flow rate, however, must be set during a period when it is flowing steadily. As the final step in the reduction period, the temperature of the fluidized constant-temperature bath was lowered to that desired for the precarburization and unsteady-state synthesis experiments.

6.1.3.4 Precarburization and Unsteady-State Synthesis

Precarburization of the reduced fused-iron catalyst was used as a means of creating a bulk carbide structure before unsteady-state synthesis began. In this way, different unsteady-state experiments could be performed from a common starting composition of catalyst, and the rate of carbon deposition could be more easily determined. After the fused-iron catalyst had been reduced, precarburization was initiated simply by closing solenoid valve 2 and then simultaneously activating the right solenoid and turning three-way valve V10 toward the precarburization stream.

The precarburization gas typically used was a synthesis gas of a 4:1 H_2/CO ratio with a small percentage of argon. Argon was used as an internal standard for gas-chromatographic analysis.

At the start of precarburization, the microcomputer program, which contains the sampling-valve timing loops, was started. After the first twenty minutes of precarburization, a light gas sample was automatically flushed into the gas chromatograph. Seventeen minutes later, all light gas compounds of interest had eluted and the microcomputer switched the sampling valve, backflushing the packed column. This process was

repeated every 37 minutes throughout the precarburization and unsteady-state synthesis portions of the experiment.

After two hours of catalyst precarburization with the 4:1 H₂/CO synthesis gas, the unsteady-state synthesis was started. The flow rates of F-gas and S-gas had been previously set to their desired values for unsteady-state synthesis. Hence, the only steps required to start unsteady-state synthesis were to switch three-way valve V10 toward the S-gas feed-line and to run the solenoid-switching microcomputer program. The program, used to slide the plug and switch between solenoid valves 2 and 4, is presented in Appendix C.

When solenoid valve 2 was opened, the plug was simultaneously pulled to the left. When solenoid valve 4 was opened, the sliding plug was pulled to the right. The program allowed control of the sliding plug and solenoid valves to within hundredths of a second. The response times of the solenoid valves, however, were only on the order of one-tenth of a second. As stated earlier, light gas samples were taken every 37 minutes during the unsteady-state gas pulsing. The volume of the tubing between the reaction zone and the sampling point is approximately 30 times the volume of the reaction zone itself. Therefore, the exit-gases should be well mixed by the time they reach the sampling valves. As in the steady-state experiments, gas samples to be separated using the capillary column were taken only at the end of an experiment. The gas chromatograph oven was cooled to -20°C and a sample was then flushed onto the capillary column. The column was held at -20°C for 2 minutes and then temperature programmed to 150°C at 4°C/min.

6.1.3.5 System Shut-Down

At the completion of the unsteady-state reaction period, it was desirable to rapidly stop the reaction by flushing the sliding-plug microreactor and feed-gas lines with helium. This was done by first stopping the computer program and making certain that solenoid valves 2 and 4 were closed and 5 was open. Valve V11 was then rapidly opened and three-way valves V6, V9 and V10 were switched so that helium was flowing through the microreactor.

As helium flowed through the microreactor, the nitrogen ballast-gas was shut off. Valve V12, parallel to the back-pressure regulator, was slowly opened over the course of several minutes. During this period, the plug was slid back and forth several times to insure purging of both feed lines by helium.

Once the system had reached atmospheric pressure, the constant-temperature bath was shut off and the microreactor was allowed to cool. The catalyst was still vibrofluidized as the microreactor cooled. Cooling took place over five to six hours under a maximum helium flow rate of 2,200 standard mm^3/s . The heating tapes were maintained at 200°C during the cool-down period to keep any residual F-T products from condensing in the heated portion of the equipment, including the sampling valves.

6.1.3.6 Catalyst Collection and Analysis

Once the sliding-plug microreactor had been cooled to ambient temperatures, it could be removed from the constant-temperature bath. In order to do this, the solenoids were disconnected from the reducing

unions, and the plug wires were cut, releasing the solenoid plungers. The compression fittings between the flexible hose and the microreactor were disconnected, and the plug wires were removed from these hoses.

The vibrational support apparatus for the microreactor was then unbolted and the microreactor was clamped in the vise. All eight bolts holding the three sections of the microreactor together were removed. The gas-exit section was lifted off with care and the spent catalyst and any bugdust present were removed using the suction-filter apparatus. This procedure was previously described in Section 4.1.3.6.

After the spent catalyst had been meticulously removed and weighed, the sliding plug was removed from the plenum zone. Spent catalyst was stored in vials under nitrogen until being sent for total carbon and iron analyses along with Mössbauer spectroscopic determination of iron-containing phases.

CHAPTER 7

CONCLUSIONS, SIGNIFICANCE AND RECOMMENDATIONS

7.1 Conclusions

Following a review of relevant literature on F-T synthesis, vibrofluidized-beds, and unsteady-state methods for kinetic studies, an experimental investigation into the development of a microreactor system for unsteady-state F-T synthesis was carried out. Steady-state F-T synthesis experiments using a commercial fused-iron catalyst produced information on catalyst defluidization, hydrocarbon product distribution and baseline carbon deposition. Investigations in a cold-flow vibrofluidized-bed microreactor model revealed information on gas mixing in the unsteady-state system. In addition, the cold-flow model allowed observation of characteristics of the vibrofluidized catalyst in the microreactor. In the final stages of the studies, a vibrofluidized-bed microreactor system for unsteady-state F-T synthesis at commercially important reaction conditions was designed and constructed.

The following conclusions can be drawn based on the experimental studies.

1. In a vibrofluidized microreactor system for F-T synthesis under steady-state conditions using a commercial promoted fused-iron catalyst:
 - a. Catalyst defluidization occurs within several hours at temperatures below 395°C when using a feed-gas H₂/CO ratio of 2:1 or less.
 - b. Catalyst defluidization can be detected through observation of thermocouple temperature fluctuations in the reaction zone.

- c. A shift in the probability of chain growth of hydrocarbon products to lower values occurs, as the reaction temperature is increased and as the feed-gas H_2/CO ratio is increased.
- d. Bugdust is a fine, black powder produced due to excessive carbon formation which in turn causes physical degradation of the catalyst. Its structure is highly porous and bugdust contains 18-30 weight percent carbon and 50-64 weight percent iron.
- e. Discrete fractions of free-flowing catalyst and bugdust (powdery, low-density carbon-rich particles) can be easily collected under conditions where liquid products and waxes do not condense in the reaction zone.
- f. The rate of free carbon formation (mainly in the form of bugdust) is much greater when a feed-gas H_2/CO ratio of 1:1 was used than when a higher ratio of 2:1 is used.

2. In a cold-flow vibrofluidized-bed microreactor model for unsteady-state gas feeding:

- a. Experiments with a manual 3-way ball valve substituting for the sliding-plug microreactor show quantitative gas replacement after 2.4 seconds at all flow rates investigated.
- b. A 20-micron distributor plate induces feed-gas mixing by allowing gas to backflow from the reaction zone to the plenum zone during the sliding-plug movement.
- c. The use of a 2-micron distributor plate eliminates the backflow of gas from the reaction zone to the plenum zone during the sliding-plug movement.
- d. The geometry of the microreactor induces some mixing of the feed gases, particularly when the gases pass from the reaction zone to the gas-exit zone.
- e. More gas-mixing occurs during the transition from argon to helium feeding than during the transition from helium to argon feeding. This is thought to be due to the density differences between the two gases.
- f. Vibrofluidization of the catalyst in the reaction zone induces only a small amount of gas backmixing at low feed-gas velocities.
- g. The use of high gas flow rates and feed-gas staggering significantly reduces undesirable gas mixing in the microreactor.

3. Experimental characterizations of a vibrofluidized-bed of fused-iron catalyst in a cold-flow microreactor model show that:

- a. The solid mixing is intense, even at very low gas velocities.
- b. At feed-gas velocities somewhat below those for normal gas-fluidization (below the minimum gas-fluidization velocity, U_{mf}) the surface of the vibrofluidized catalyst-bed levels out and begins to oscillate.

4. A vibrofluidized-bed microreactor system for unsteady-state F-T synthesis:

- a. Has been designed and constructed, and it can be operated at commercially important reaction conditions.
- b. Allows for rapid switching of feed gases on the order of several seconds.

5. In order to simulate the catalyst behavior in the freeboard region and the shallow-bed region of a "heat-tray" reactor (Figure 1.1) using the unsteady-state vibrofluidized-bed microreactor system:

- a. A flow rate of approximately 1,650 actual mm^3/s should be used. This will permit rapid switching of feed gases over the catalyst in the reaction zone of the microreactor.
- b. A reaction temperature of 395°C is necessary to prevent defluidization of the fused-iron catalyst. This temperature is higher than that desired for operation of a "heat-tray" reactor. Therefore, a means should be developed for reducing the operating temperature in the microreactor, while maintaining a fluidized catalyst.

7.2 Significance of the Results

The development of a vibrofluidized-bed microreactor for both steady-state and unsteady-state catalytic gas-solid reactions has far-reaching significance. Before this development, there was no easy way of accurately determining integral fluid-bed kinetics in a laboratory reactor.

Fixed-bed reactors rely on changes in gas composition over static catalyst particles. Laboratory gas-fluidized-bed reactors require large flow rates of feed gas and therefore deep catalyst beds (requiring large quantities of catalyst) in order to obtain integral conversions.

The unique ability of the new microreactor system to rapidly switch feed-gas flows over an intensely-mixed solid makes this development an even more significant contribution to the areas of chemical kinetics and reaction engineering.

7.3 Recommendations for Further Studies

Based on the results of this work, the following recommendations are forwarded for future studies:

1. Repeat the steady-state carbon-deposition experiments utilizing a bifunctional catalyst, such as synthetic zeolite Fe-HZSM-5, in order to eliminate catalyst defluidization caused by accumulation of high molecular-weight products. This will allow for use of lower operating temperatures.
2. Determine the vibrofluidization characteristics of new catalysts in the cold-flow microreactor model.
3. Further explore effective means of improving feed-gas transitions in the unsteady-state cold-flow vibrofluidized-bed microreactor model.
4. Undertake model-reaction studies in the vibrofluidized-bed microreactor system. By examining some simple reactions with well-characterized kinetics, quantitative mixing tests can be performed. Some candidates for such model-reaction studies include hydrogenation of

ethylene (Wynkoop and Wilhelm, 1950) and ethanol dehydration (Bock et al., 1984). These reaction studies could be used to determine heat- and mass-transfer effects in the reaction zone of the microreactor.

5. Experimentally determine the mass-transfer coefficient in the vibrofluidized-bed microreactor. This could be done by studying the sublimation of naphthalene in nitrogen as a function of flow rate and particle size.

6. Perform feed-gas-cycling F-T synthesis experiments in the unsteady-state vibrofluidized-bed microreactor system in order to determine carbon deposition rates on: (a) a fused-iron catalyst; and (b) different formulations of Fe-HZSM-5.

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APPENDIX A

Calculations for (1) Minimum Fluidization Velocity of the Fused-Iron Catalyst in the Microreactor, (2) Pressure Drop Across the Distributor Plates and (3) Changes in Feed-Line Volume Upon Switching the Sliding Plenum Across the Plenum Zone

A.1. Minimum Fluidization Velocity of the Fused-Iron Catalyst in the Microreactor

For the calculation, the smoothed correlation of particulate fluidization as given by Zenz and Othmer (1960) was used. The minimum fluidization velocity v_e , under actual conditions was read from Figure A.1 after first calculating Ω and Δ . A void fraction of 0.5 was assumed.

$$\Omega = \frac{4}{3} \frac{\mu_f(\rho_p - \rho_f)g}{\rho_f^2}^{1/3}$$

$$\Delta = \frac{3}{4} \frac{\mu_f^2}{\rho_f(\rho_p - \rho_f)g}^{1/3}$$

where:

v_e = superficial velocity ($\frac{ft}{s}$)

D_p = particle diameter (ft)

μ_f = fluid viscosity (lb/ft-s)

ρ_p = apparent particle density (lb/ft³)

ρ_f = fluid density (lb/ft³)

$g = 32.2 \text{ ft/s}$

An average particle diameter of 225 μ was assumed as well.

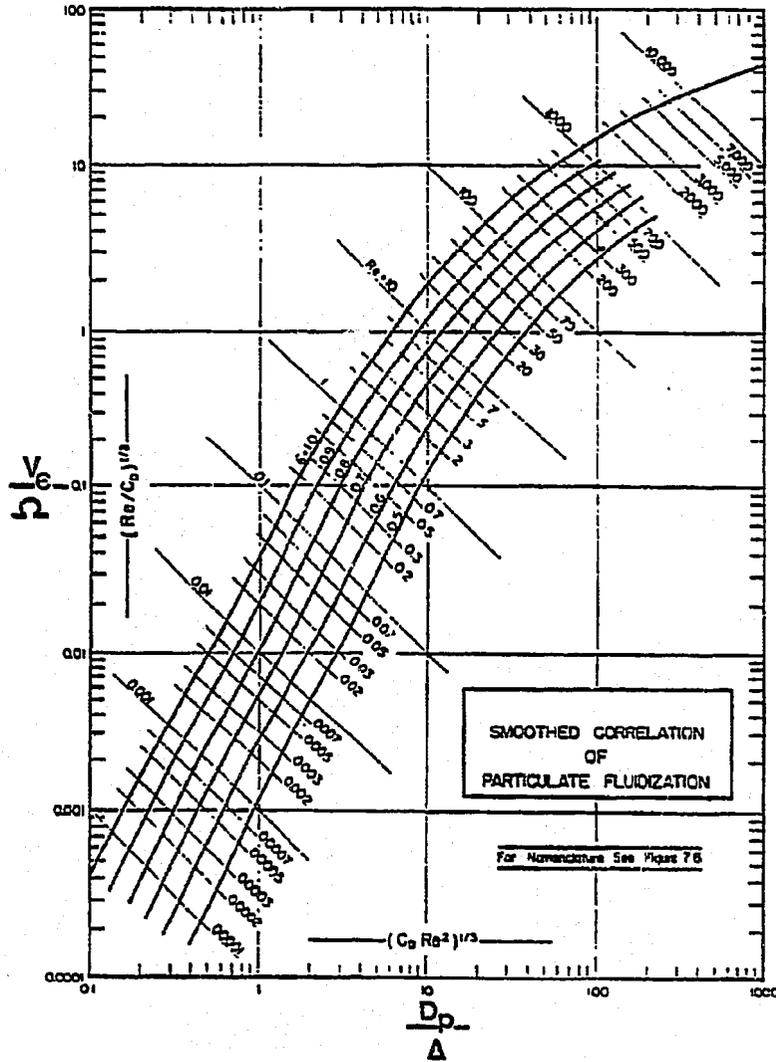


Figure A.1. The Smoothed Correlation of Particulate Fluidization Used to Calculate the Minimum Gas-Fluidization Velocity (V_c) of a Fused-Iron Catalyst (Taken from Zenz and Othmer, 1960). D_p is the Particle Diameter, Ω and Δ are Defined in Section A.1.

A.2 Pressure Drop Across Different Micron-Grade Sintered Stainless-Steel Distributor Plates

The following equation relating the fluid flow to pressure drop across porous plates has been provided by Mott Metallurgical Corporation for their products:

$$\Delta P^2 = p_{\text{upstream}}^2 - p_{\text{downstream}}^2 = \delta \mu R T \frac{\rho_s}{30} t \left[1 + \frac{8 \rho_s}{60 \alpha \mu} Q \right] Q$$

P = pressure (psi)

α = viscous resistance coefficient (in⁻²)

β = inertial resistance coefficient (in⁻¹)

ρ_s = density of gas at S.T.P. (slugs/ft³)

R = gas constant = 1.71×10^3 (ft.lb/slug °R)

T = temperature (°R)

t = porous wall thickness (in)

Q = flow (SCFM/in²)

μ = viscosity of flow (slugs/in.sec.)

For 1/16-inch thick porous stainless steel the following coefficients are specified:

Micron Grade	α (in ⁻²)	β (in ⁻¹)
2	8.41×10^8	1.25×10^5
20	3.55×10^7	6.02×10^3

An approximation to the volume of gas backflowing across the distributor plate can be made. This is done by measuring the magnitude and duration

of the pressure inversion with a rapid-response differential-pressure transducer. The pressure drop across the distributor plate for the same gas at a typical flow rate is then calculated. By ratioing the measured pressure inversion and the calculated pressure drop, the volume of gas backflowing can be approximated. For example:

Given a 20- μ distributor plate and argon flowing at 400 actual mm^3/s and conditions of 25°C and 101 kPa, what is the pressure drop

$$\Delta P = 1.42 \times 10^{-2} \text{ kPa}$$

If a pressure inversion of 0.346 kPa is observed for a duration of 0.013 seconds after the feed gas is switched from argon to helium, what is the volume of gas backflowing across the distributor plate

$$\frac{0.346 \text{ kPa}}{0.0142 \text{ kPa}} \cdot 400 \frac{\text{mm}^3}{\text{s}} \cdot 0.013 \text{ s} = 127 \text{ mm}^3$$

A.3 Changes in Feed-Line Volume Upon Switching the Sliding Plug Across the Plenum Zone.

When the sliding plug is drawn across the plenum zone, gas is compressed into the feed line ahead of the plug. By measuring the increase in pressure in the appropriate feed line, the amount of gas entering that feed line by compression can be calculated. The remainder of the gas originally in the plenum is either compressed through the distributor plate or flows anularly around the plug.

$$\text{Volume of Feed Line} = 26,383 \text{ mm}^3$$

$$\Delta P_{\text{Ar} \rightarrow \text{He}} = \Delta P \text{ upon switching from Ar to He} = 3.175 \text{ kPa}$$

$$\Delta P_{\text{He} \rightarrow \text{Ar}} = \Delta P \text{ upon switching from He to Ar} = 2.864 \text{ kPa}$$

$$P_{\text{final Ar} \rightarrow \text{He}} = \text{final feed-line pressure upon switching from Ar to He} = 141.000 \text{ kPa}$$

$$P_{\text{final He} \rightarrow \text{Ar}} = \text{final feed-line pressure upon switching from He to Ar} = 140.685 \text{ kPa}$$

$$\text{Absolute System Pressure} = 137.825 \text{ kPa}$$

$$\Delta V_{\text{Feed Line}} = \text{change in volume of the feed line upon plug switching}$$

$$\Delta V_{\text{Feed Line}} = \frac{\Delta P \cdot V_{\text{Feed Line}}}{P_{\text{final}}}$$

For the transition from argon-to-helium flow how much argon is compressed into the feed line? (Experiment 1-4)

$$\Delta V_{\text{feed line, Ar} \rightarrow \text{He}} = 594 \text{ mm}^3 \text{ or } 37\% \text{ of the gas in the plenum}$$

For the transition from helium-to-argon flow how much helium is compressed into the feed liner

$$\Delta V_{\text{feed line, He} \rightarrow \text{Ar}} = 537 \text{ mm}^3 \text{ or } 33\% \text{ of the gas in the plenum.}$$

APPENDIX B

Steady-State Analysis Results Including Definitions of Input Parameters and Output Labels on Gas-Chromatographic Data Tables for (1) Light Gas Analyses and Mass Balances and (2) Hydrocarbon Product Distribution and Rate of Production from Capillary Analyses. In Addition (3) Temperature-Fluctuation Plots are Presented for Steady-State Experiments.

B.1 Light Gas Analysis--Output from the Microcomputer Data Compilation Program "MASSBAL. BAS."

1. Input

- A. Number of moles of CO fed per mole of Ar fed
 - i. obtained by GC analysis of S-gas.
- B. H₂/CO ratio of feed gas
 - i. As specified by AIRCO.
- C. Temperature
- D. Number of data points.
- E. Peak areas from light gas chromatogram for Co, Ar, CH₄ and CO₂.

2. Output

- A. CO CONV: Fractional molar conversion of CO fed to the microreactor.
- B. CO₂/CO CONV: The number of moles of CO₂ produced per mole of CO converted (fraction of C from CO converted that goes to CO₂).
- C. CH₄/CO CONV: The number of moles of CH₄ produced per mole of CO converted (fraction of CO converted that goes to CH₄).
- D. CO/Ar FED; The number of moles of CO fed per mole of Ar fed. An input parameter.
- E. H₂/CO RATIO: Molar ratio of feed gases. An input parameter.
- F. H₂O IMPLIED: An approximation of water production. Calculation of this value assumes the following:
 - i. All oxygen produced from the reacted amount of CO and not as as CO₂ is present as H₂O.
 - ii. No oxygenates are produced. Huff (1982) states that with the same catalyst in a slurry reactor, less than 1.1% of oxygen is present as oxygenates.
- G. -CH₂-IMPLIED: Carbon which is not produced as CO, CO₂, or CH₄ is assumed to be in the form of -CH₂-. This is the mole fraction of C fed converted to -CH₂-.

- H. H₂ CONV IMPLIED: An approximation based on actual CH₄ production and the above approximations for H₂O and -CH₂- production.
- I. H₂ USED IMPLIED: Estimate of the number of moles of H₂ used. The maximum number of moles of H₂ that can be used is the H₂/CO ratio of the feed gas.
- J. H₂/CO USAGE: An estimate of the number of moles of H₂ used divided by the number of moles of CO used, the H₂/CO usage ratio.
- K. -CH₂-/CO CONV: The mole fraction of converted carbon that went into making -CH₂-.
- L. CALC KEQ: The calculated equilibrium constant for the water-gas shift reaction at the temperature of the reaction.

$$K_{eq} = 0.0102e^{4730/T}$$

- M. EXPT KEQ: The estimated experimental value of the equilibrium constant for the water-gas shift reaction.

$$K_{eq} = \frac{x_{CO_2} x_{H_2}}{x_{CO} x_{H_2O}}$$

- N. SUM = 1π: The sum of the moles of CO₂, CH₄ and -CH₂- produced per mole of CO converted should add up to 1. This is an internal check on the calculation.
- O. SAMPLE NUMBER: The light-gas sample identification listed chronologically. The first sample is taken 17 minutes after the start of the reaction. Subsequent samples are taken every 37 minutes.

Table B-2

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment B-2.

DATE OF EXPERIMENT 9/6/84 STEADY STATE EXPERIMENT B-2
THIS EXPERIMENT USES 2.08:1 S-GAS FOR A 2 HOUR AND 3 MIN RUN.

TEMPERATURE	633	# DATA PTS.=	3		
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO ₂ /AR FED	H ₂ /CO RATIO
1	.963068	.13424	.142716	4.636	2.08
2	.892212	.329646	.0831131	4.636	2.08
3	.754651	.363142	.0994475	4.636	2.08
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
1	.805642	.656341	.704804	1.67573	1.74
2	.473608	.915004	.303248	.385105	1.10412
3	.366449	.405557	.20656	.762214	1.01002
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.73044	17.9392	9.00872	1	
2	.577221	17.9392	9.00872	1	
3	.537411	17.9392	7.12582	1	

Table B-3

The Light Gas Analysis and Implied Mass Balance from Steady-State Experiment B-3.

DATE OF EXPERIMENT 3/10/34 STEADY STATE EXPERIMENT B-3
 THIS EXPERIMENT USES 4.0:1 S-GAS FOR A 10 HOURS AND 0 MIN RUN.

TEMPERATURE= 633		# DATA PTS. = 15			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
0073547	0.073547	0.0622746	0.20199	4.00000	4
0073548	0.073548	0.1772201	0.1506909	4.00000	4
0073549	0.073549	0.0334587	0.1447233	4.00000	4
0073550	0.073550	0.1757733	0.1690884	4.00000	4
0073551	0.073551	0.1322433	0.1740733	4.00000	4
0073552	0.073552	0.1781166	0.1317233	4.00000	4
0073553	0.073553	0.1797166	0.1911233	4.00000	4
0073554	0.073554	0.1001166	0.1945033	4.00000	4
0073555	0.073555	0.1001166	0.2001166	4.00000	4
0073556	0.073556	0.1001166	0.1960033	4.00000	4
0073557	0.073557	0.1001166	0.1919933	4.00000	4
0073558	0.073558	0.1001166	0.1919933	4.00000	4
0073559	0.073559	0.1001166	0.1919933	4.00000	4
0073560	0.073560	0.1001166	0.1919933	4.00000	4
0073561	0.073561	0.1001166	0.1919933	4.00000	4
0073562	0.073562	0.1001166	0.1919933	4.00000	4
0073563	0.073563	0.1001166	0.1919933	4.00000	4
0073564	0.073564	0.1001166	0.1919933	4.00000	4
0073565	0.073565	0.1001166	0.1919933	4.00000	4
0073566	0.073566	0.1001166	0.1919933	4.00000	4
0073567	0.073567	0.1001166	0.1919933	4.00000	4
0073568	0.073568	0.1001166	0.1919933	4.00000	4
0073569	0.073569	0.1001166	0.1919933	4.00000	4
0073570	0.073570	0.1001166	0.1919933	4.00000	4
0073571	0.073571	0.1001166	0.1919933	4.00000	4
0073572	0.073572	0.1001166	0.1919933	4.00000	4
0073573	0.073573	0.1001166	0.1919933	4.00000	4
0073574	0.073574	0.1001166	0.1919933	4.00000	4
0073575	0.073575	0.1001166	0.1919933	4.00000	4
0073576	0.073576	0.1001166	0.1919933	4.00000	4
0073577	0.073577	0.1001166	0.1919933	4.00000	4
0073578	0.073578	0.1001166	0.1919933	4.00000	4
0073579	0.073579	0.1001166	0.1919933	4.00000	4
0073580	0.073580	0.1001166	0.1919933	4.00000	4
0073581	0.073581	0.1001166	0.1919933	4.00000	4
0073582	0.073582	0.1001166	0.1919933	4.00000	4
0073583	0.073583	0.1001166	0.1919933	4.00000	4
0073584	0.073584	0.1001166	0.1919933	4.00000	4
0073585	0.073585	0.1001166	0.1919933	4.00000	4
0073586	0.073586	0.1001166	0.1919933	4.00000	4
0073587	0.073587	0.1001166	0.1919933	4.00000	4
0073588	0.073588	0.1001166	0.1919933	4.00000	4
0073589	0.073589	0.1001166	0.1919933	4.00000	4
0073590	0.073590	0.1001166	0.1919933	4.00000	4
0073591	0.073591	0.1001166	0.1919933	4.00000	4
0073592	0.073592	0.1001166	0.1919933	4.00000	4
0073593	0.073593	0.1001166	0.1919933	4.00000	4
0073594	0.073594	0.1001166	0.1919933	4.00000	4
0073595	0.073595	0.1001166	0.1919933	4.00000	4
0073596	0.073596	0.1001166	0.1919933	4.00000	4
0073597	0.073597	0.1001166	0.1919933	4.00000	4
0073598	0.073598	0.1001166	0.1919933	4.00000	4
0073599	0.073599	0.1001166	0.1919933	4.00000	4
0073600	0.073600	0.1001166	0.1919933	4.00000	4

SAMPLE NUMBER	H2 CONV IMPLIED	CH4 IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
0073547	0.411601	0.063173	0.786108	0.00000	1.191317
0073548	0.411601	0.063173	0.614108	0.00000	1.180000
0073549	0.411601	0.063173	0.614108	0.00000	1.180000
0073550	0.411601	0.063173	0.614108	0.00000	1.180000
0073551	0.411601	0.063173	0.614108	0.00000	1.180000
0073552	0.411601	0.063173	0.614108	0.00000	1.180000
0073553	0.411601	0.063173	0.614108	0.00000	1.180000
0073554	0.411601	0.063173	0.614108	0.00000	1.180000
0073555	0.411601	0.063173	0.614108	0.00000	1.180000
0073556	0.411601	0.063173	0.614108	0.00000	1.180000
0073557	0.411601	0.063173	0.614108	0.00000	1.180000
0073558	0.411601	0.063173	0.614108	0.00000	1.180000
0073559	0.411601	0.063173	0.614108	0.00000	1.180000
0073560	0.411601	0.063173	0.614108	0.00000	1.180000
0073561	0.411601	0.063173	0.614108	0.00000	1.180000
0073562	0.411601	0.063173	0.614108	0.00000	1.180000
0073563	0.411601	0.063173	0.614108	0.00000	1.180000
0073564	0.411601	0.063173	0.614108	0.00000	1.180000
0073565	0.411601	0.063173	0.614108	0.00000	1.180000
0073566	0.411601	0.063173	0.614108	0.00000	1.180000
0073567	0.411601	0.063173	0.614108	0.00000	1.180000
0073568	0.411601	0.063173	0.614108	0.00000	1.180000
0073569	0.411601	0.063173	0.614108	0.00000	1.180000
0073570	0.411601	0.063173	0.614108	0.00000	1.180000
0073571	0.411601	0.063173	0.614108	0.00000	1.180000
0073572	0.411601	0.063173	0.614108	0.00000	1.180000
0073573	0.411601	0.063173	0.614108	0.00000	1.180000
0073574	0.411601	0.063173	0.614108	0.00000	1.180000
0073575	0.411601	0.063173	0.614108	0.00000	1.180000
0073576	0.411601	0.063173	0.614108	0.00000	1.180000
0073577	0.411601	0.063173	0.614108	0.00000	1.180000
0073578	0.411601	0.063173	0.614108	0.00000	1.180000
0073579	0.411601	0.063173	0.614108	0.00000	1.180000
0073580	0.411601	0.063173	0.614108	0.00000	1.180000
0073581	0.411601	0.063173	0.614108	0.00000	1.180000
0073582	0.411601	0.063173	0.614108	0.00000	1.180000
0073583	0.411601	0.063173	0.614108	0.00000	1.180000
0073584	0.411601	0.063173	0.614108	0.00000	1.180000
0073585	0.411601	0.063173	0.614108	0.00000	1.180000
0073586	0.411601	0.063173	0.614108	0.00000	1.180000
0073587	0.411601	0.063173	0.614108	0.00000	1.180000
0073588	0.411601	0.063173	0.614108	0.00000	1.180000
0073589	0.411601	0.063173	0.614108	0.00000	1.180000
0073590	0.411601	0.063173	0.614108	0.00000	1.180000
0073591	0.411601	0.063173	0.614108	0.00000	1.180000
0073592	0.411601	0.063173	0.614108	0.00000	1.180000
0073593	0.411601	0.063173	0.614108	0.00000	1.180000
0073594	0.411601	0.063173	0.614108	0.00000	1.180000
0073595	0.411601	0.063173	0.614108	0.00000	1.180000
0073596	0.411601	0.063173	0.614108	0.00000	1.180000
0073597	0.411601	0.063173	0.614108	0.00000	1.180000
0073598	0.411601	0.063173	0.614108	0.00000	1.180000
0073599	0.411601	0.063173	0.614108	0.00000	1.180000
0073600	0.411601	0.063173	0.614108	0.00000	1.180000

SAMPLE NUMBER	CH4/CO CONV	CALC KEY	EXPT KEY	SUM=10
0073547	0.20199	N	0.41160	1
0073548	0.15069	N	0.41160	1
0073549	0.14472	N	0.41160	1
0073550	0.16908	N	0.41160	1
0073551	0.17407	N	0.41160	1
0073552	0.13172	N	0.41160	1
0073553	0.19112	N	0.41160	1
0073554	0.19450	N	0.41160	1
0073555	0.20011	N	0.41160	1
0073556	0.19600	N	0.41160	1
0073557	0.19199	N	0.41160	1
0073558	0.19199	N	0.41160	1
0073559	0.19199	N	0.41160	1
0073560	0.19199	N	0.41160	1
0073561	0.19199	N	0.41160	1
0073562	0.19199	N	0.41160	1
0073563	0.19199	N	0.41160	1
0073564	0.19199	N	0.41160	1
0073565	0.19199	N	0.41160	1
0073566	0.19199	N	0.41160	1
0073567	0.19199	N	0.41160	1
0073568	0.19199	N	0.41160	1
0073569	0.19199	N	0.41160	1
0073570	0.19199	N	0.41160	1
0073571	0.19199	N	0.41160	1
0073572	0.19199	N	0.41160	1
0073573	0.19199	N	0.41160	1
0073574	0.19199	N	0.41160	1
0073575	0.19199	N	0.41160	1
0073576	0.19199	N	0.41160	1
0073577	0.19199	N	0.41160	1
0073578	0.19199	N	0.41160	1
0073579	0.19199	N	0.41160	1
0073580	0.19199	N	0.41160	1
0073581	0.19199	N	0.41160	1
0073582	0.19199	N	0.41160	1
0073583	0.19199	N	0.41160	1
0073584	0.19199	N	0.41160	1
0073585	0.19199	N	0.41160	1
0073586	0.19199	N	0.41160	1
0073587	0.19199	N	0.41160	1
0073588	0.19199	N	0.41160	1
0073589	0.19199	N	0.41160	1
0073590	0.19199	N	0.41160	1
0073591	0.19199	N	0.41160	1
0073592	0.19199	N	0.41160	1
0073593	0.19199	N	0.41160	1
0073594	0.19199	N	0.41160	1
0073595	0.19199	N	0.41160	1
0073596	0.19199	N	0.41160	1
0073597	0.19199	N	0.41160	1
0073598	0.19199	N	0.41160	1
0073599	0.19199	N	0.41160	1
0073600	0.19199	N	0.41160	1

Table B-4

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment B-4.

DATE OF EXPERIMENT 8/14/84 STEADY STATE EXPERIMENT B-4
THIS EXPERIMENT USES 1.03:1 S-GAS FOR A 1 HOURS AND 2 MIN RUN.

TEMPERATURE=	633	# DATA PTS.=	2		
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO/AR FED	H ₂ /CO RATIO
1	.962333	.152279	.0953146	10.832	1.03
2	.368091	.423382	.0931238	10.832	1.03
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
1	1.53092	.724106	.663084	1.57385	1.63348
2	.304436	.1857	.0555333	.313663	.207973
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.752406	17.9392	-3.18361	1	
2	.478494	17.9392	3.50159	1	

Table B-5

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment B-5.

DATE OF EXPERIMENT 8/16/94 STEADY STATE EXPERIMENT B-5
THIS EXPERIMENT USES 1.0311 S-OAS FOR A 2 HOURS AND 13 MIN RUN.

TEMPERATURE= 633		# DATA PTS.= 4			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
1	.76013	.152638	.0943774	10.883	1.03
402497	.402497	.465347	.0911527	10.883	1.03
344551	.344551	.43463	.0937697	10.883	1.03
329153	.329153	.449026	.10219	10.883	1.03
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	1.52638	.722963	.667026	1.57122	1.63646
402497	.402497	.178308	.0279259	.479731	.625113
344551	.344551	.162459	.0450085	.427073	.723731
329153	.329153	.147276	.0334546	.447736	.755033
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.722963	17.9332	-2.98244	1	
402497	.443501	17.9332	0.45039	1	
471551	.471551	17.9332	.6473	1	
443504	.443504	17.9332	.12759	1	

Table B-6

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment B-6.

DATE OF EXPERIMENT 8/19/84 STEADY STATE EXPERIMENT B-6
THIS EXPERIMENT USES 2.08:1 S-GAS FOR A 2 HOURS AND 57 MIN RUN.

TEMPERATURE= 633		# DATA PTS.= 3			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
1	.968713	.103859	.125136	4.636	2.08
2	.711443	.383734	.0769916	4.636	2.08
3	.738021	.383734	.0769916	4.636	2.08
4	.603073	.370037	.0814453	4.636	2.08
5	.418807	.35195	.0998239	4.636	2.08
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	.837639	.74204	.757808	1.74228	1.79856
2	.486536	.54758	.624065	1.01168	1.11022
3	.387118	.430664	.523484	.805206	1.03377
4	.234518	.324766	.356755	.591819	.81334
5	.210204	.229601	.124009	.437224	1.04397
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.766006	17.9392	1.50202	1	
2	.600783	17.9392	10.9227	1	
3	.600783	17.9392	6.3488	1	
4	.383717	17.9392	6.3276	1	
5	.469116	17.9392	3.3597	1	

Table B-7

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment B-7.

DATE OF EXPERIMENT 8/21/84 STEADY STATE EXPERIMENT B-7					
THIS EXPERIMENT USES 2.08:1 S-GAS FOR A 2 HOURS AND 45 MIN RUN.					
TEMPERATURE= 633		# DATA PTS.= 4			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	HC/CC RATIO
1	.972577	.103765	.137887	4.636	1.0000
2	.915845	.321632	.072172	4.636	1.0000
3	.74340	.267079	.026437	4.636	1.0000
4	.562199	.375146	.090487	4.636	1.0000
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	.349411	.747277	.770737	1.75577	1.3165
2	.49062	.548766	.226705	1.02049	1.1124
3	.349034	.32136	.19393	.74503	.95203
4	.263625	.303627	.141884	.59334	.66048
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.768348	17.9339	1.49555	1	
2	.59919	17.9339	11.3516	1	
3	.532424	17.9339	6.2115	1	
4	.554366	17.9339	3.32904	1	

Table B-8

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment C-1.

DATE OF EXPERIMENT		3/24/84		STEADY STATE EXPERIMENT C-1	
THIS EXPERIMENT USES 2.03:1 S-GAS FOR A 2 HOURS AND 4 MIN RUN.					
TEMPERATURE=		673		# DATA PTS.= 3	
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO/AR FED	H ₂ /CO RATIO
W1-1	.967754	.102517	.175733	4.436	2.08
W1-2	.879722	.323356	.162606	4.436	2.08
W1-3	.934139	.300694	.129202	4.436	2.08
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
W1-1	.369202	.698477	.769332	1.80794	1.86916
W1-2	.504376	.432211	.310798	1.0491	1.19346
W1-3	.551155	.532599	.372401	1.1464	1.21976
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEQ	EXPT KEQ	SUM=10	
W1-1	.721791	11.5059	1.088	1	
W1-2	.514033	11.5059	7.84473	1	
W1-3	.570114	11.5059	10.702	1	

Table B-9

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment C-2.

DATE OF EXPERIMENT 3/27/84 STEADY STATE EXPERIMENT C-2
THIS EXPERIMENT USES 1.03:1 S-GAS FOR A 1 HOUR AND 0 MIN RUN.

TEMPERATURE=	673	# DATA PTS.=	2		
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO/AR FED	H ₂ /CO RATIO
1	.95979	.19042	.132979	10.882	1.03
2	.947319	.396654	.0796436	10.882	1.03
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
1	1.36699	.687883	.671048	1.614	1.63162
2	.817712	.495923	.195424	.342243	.339081
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.716702	11.5089	-3.12471	:	
2	.523502	11.5089	6.85627	1	

Table B-10.

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment D-1.

DATE OF EXPERIMENT 3/29/84 STEADY STATE EXPERIMENT D-1
THIS EXPERIMENT USES 1.03:1 S-GAS FOR A 1 HOUR AND 15 MIN RUN.

TEMPERATURE= 653 # DATA PTS.= 2

SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO ₂ /AR FED	H ₂ /CO RATIO
1	.769372	.117161	.12634	10.882	1.03
2	.489233	.436336	.112811	10.882	1.03

SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
1	1.66866	.732573	.741461	1.71870	1.77486
2	.379339	.21959	.0603374	.390307	.767811

SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?
1	.756499	14.2695	-3.33199	1
2	.448853	14.2695	4.45107	1

Table B-11

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment D-2.

TEMPERATURE=		653	# DATA PTS.=	5		
DATE OF EXPERIMENT 9/4/84 STEADY STATE EXPERIMENT D-2						
THIS EXPERIMENT USES 2.00:1 S-GAS FOR A 2 HOUR AND 40 MIN RUN.						
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO	
012-001	.39133	.0654104	.183736	4.636	1.000	
012-002	.413697	.315628	.115818	4.636	1.000	
012-003	.403707	.315628	.11064	4.636	1.000	
012-004	.397258	.315628	.101275	4.636	1.000	
012-005	.46992	.315628	.10012	4.636	1.000	
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE	
012-001	.27691	.736835	.852951	1.3504	1.88751	
012-002	.513486	.519486	.33692	1.06805	1.18623	
012-003	.455026	.512067	.316509	1.02965	1.1331	
012-004	.500981	.5009781	.315954	1.04204	1.12272	
012-005	.46992	.803121	.396649	.977434	1.10164	
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?		
012-001	.750895	14.32683	9.1391	1		
012-002	.513486	14.32683	10.0368	1		
012-003	.455026	14.32683	10.7626	1		
012-004	.500981	14.32683	11.8048	1		
012-005	.46992	14.32683	9.7352	1		

Table B-12

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment E-1.

DATE OF EXPERIMENT 7/9/84 STEADY STATE EXPERIMENT E-1
THIS EXPERIMENT USES 3.08:1 S-GAS FOR A 2 HOUR AND 50 MIN RUN.

TEMPERATURE= 663		# DATA PTS.= 5			
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO ₂ /R FED	H ₂ /CO RATIO
015010	.959778	.153064	.146365	4.636	1.08
015011	.951051	.339254	.144345	4.636	1.08
015012	.931853	.314166	.116154	4.636	1.08
015013	.932193	.313923	.110444	4.636	1.08
015014	.94235	.300319	.110492	4.636	1.08
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
015010	.778475	.672358	.665929	1.661052	1.66717
015011	.460951	.439483	.373406	.953773	1.10658
015012	.523804	.530857	.346329	1.09367	1.17345
015013	.523768	.536604	.346971	1.08944	1.16848
015014	.547979	.555231	.376333	1.1098	1.1098
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KEY	EXPT KEY	SUM=1?	
015010	.700371	13.7926	3.52393		
015011	.516401	13.7926	3.96345		
015012	.56768	13.7926	13.7926		
015013	.575634	13.7926	13.7926		
015014	.589198	13.7926	13.7926		

Table B-13

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment F-1.

DATE OF EXPERIMENT 9/11/84 STEADY STATE EXPERIMENT F-1
THIS EXPERIMENT USES 4.0:1 S-GAS FOR A 3 HOUR AND 30 MIN RUN.

TEMPERATURE= 668		# DATA PTS.= 6			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
0-081013	.991424	.0230512	.33336	4.636	4
0-081014	.951072	.148536	.245336	4.636	4
0-081015	.953104	.143242	.265973	4.636	4
0-081016	.948116	.151278	.319167	4.636	4
0-081017	.937733	.163631	.323821	4.636	4
0-081018	.933078	.166705	.322957	4.636	4
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
0-081013	.455637	.057733	.245717	.73547	1.7354
0-081014	.428344	.087633	.069144	1.21333	1.6833
0-081015	.445014	.050633	.479544	1.76833	1.6833
0-081016	.433136	.050079	.661133	1.74833	1.6833
0-081017	.429333	.475933	.630733	1.72333	1.6833
0-081018	.4214	.476133	.62193	1.70033	1.6833
SAMPLE NUMBER	-CH2- /CO CONV	CALC REQ	EXPT REQ	SUM=17	
0-081013	.652333	12.1274	4.9722	1	
0-081014	.605033	12.1274	10.0843	1	
0-081015	.570333	12.1274	9.56203	1	
0-081016	.529333	12.1274	9.33646	1	
0-081017	.507333	12.1274	8.33713	1	
0-081018	.510333	12.1274	8.59133	1	

Table B-14

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment F-2.

DATE OF EXPERIMENT 9/13/84 STEADY STATE EXPERIMENT F-2
THIS EXPERIMENT USES 4.0:1 S-GAS FOR A 2 HOUR AND 0 MIN RUN.

TEMPERATURE*	668	# DATA PTS.*	3		
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
1	.971771	*****	.296196	4.636	4
2	.964579	.10431	.267961	4.636	4
3	.965401	.0996195	.33198	4.636	4
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	.587842	.683934	.971754	2.23127	1.23619
2	.476273	.986184	.763348	1.90509	1.97505
3	.49067	.548331	.773055	1.96268	2.03302
SAMPLE NUMBER	CO CONV	CALC REQ	EXPT REQ	SUM=1?	
1	.703301	11.1274	*****	1	
2	.607709	11.1274	7.79565	1	
3	.568501	12.1274	7.3294	1	

***** INDICATES THAT THE CO2 PEAK WAS NOT INTEGRATED IN THIS SAMPLE

Table B-15

The Light Gas Analysis and Implied Mass Balance from Steady-State Experiment F-3.

DATE OF EXPERIMENT 9/18/84 STEADY STATE EXPERIMENT F-3

THIS EXPERIMENT USES 2.03:1 S-GAS FOR A 1 HOUR AND 0 MIN RUN AFTER FIRST EXPOSING IT TO 4:1 PRECARB. GAS FOR 2 HOURS.

TEMPERATURE= 663		# DATA PTS.= 5			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
1	.925622	.0361131	.312424	4.636	4
2	.925101	.133341	.249323	4.636	4
3	.920854	.145242	.262584	4.636	4
4	.942613	.147303	.319799	4.636	13.03
5	.912643	.312974	.160159	4.636	11.02
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	.543093	.642096	.913434	2.17239	11.0403
2	.426473	.534365	.679974	1.74666	11.0403
3	.439023	.344034	.674642	1.75600	11.0403
4	.854661	.505575	.669906	1.78186	11.0403
5	.535643	.480841	.341376	1.11435	11.0403
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1?	
1	.651463	12.1274	4.94773	1	
2	.611836	12.1274	9.74309	1	
3	.672175	12.1274	9.34629	1	
4	.592399	12.1274	1.24172	1	
5	.526866	12.1274	9.2472	1	

Table B-16

The Light Gas Analysis and Implied Mass Balance from Steady-State Experiment F-4.

DATE OF EXPERIMENT 9/20/84 STEADY STATE EXPERIMENT F-4
 THIS EXPERIMENT USES 3.03:1 S-GAS FOR A 2 HOUR RUN
 AFTER FIRST EXPOSING IT TO 4:1 PRECARB. GAS FOR 2 HOURS.

TEMPERATURE= 643		# DATA PTS.= 6			
SAMPLE NUMBER	CO CONV	CO2/CO CONV	CH4/CO CONV	CO/AR FED	H2/CO RATIO
1	.384279	.0403736	.32122	4.636	4.4
0-040311	.951694	.145327	.145327	4.636	4.4
	.949076	.149319	.163944	4.636	4.4
	.942934	.153835	.314231	4.636	4.4
0	.920779	.309185	.152234	4.636	4.4
0	.93619	.296109	.134311	4.636	4.4
SAMPLE NUMBER	H2 CONV IMPLIED	-CH2- IMPLIED	H2O IMPLIED	H2 USED IMPLIED	H2/CO USAGE
1	.534163	.69121	.97501	7.12667	7.1
0-040311	.430539	.99121	.675271	1.74214	1.7
	.436596	.932087	.644697	1.74214	1.7
	.940561	.901155	.654694	1.74214	1.7
0	.422454	.493369	.381397	1.74214	1.7
0	.560307	.533236	.381762	1.13646	1.1
SAMPLE NUMBER	-CH2- /CO CONV	CALC KEQ	EXPT KEQ	SUM=1.0	
1	.667707	12.1374	9.20561	1	
0-040311	.60944	12.1374	9.65094	1	
	.550637	12.1374	9.45677	1	
	.531464	12.1374	9.78216	1	
0	.53763	12.1374	9.78216	1	
0	.569581	12.1374	10.6957	1	

Table B-17

The Light Gas Analysis and Implied Mass Balance
from Steady-State Experiment F-5.

DATE OF EXPERIMENT 9/25/64 STEADY STATE EXPERIMENT F-5
THIS EXPERIMENT USES 1.03:1 S-GAS FOR A 22 MINUTE RUN
AFTER FIRST EXPOSING IT TO 4:1 PRECARB. GAS FOR 2 HOURS.

TEMPERATURE=	668	# DATA PTS.=	3		
SAMPLE NUMBER	CO CONV	CO ₂ /CO CONV	CH ₄ /CO CONV	CO/AR FED	H ₂ /CO RATIO
1	.937643	.242925	.171306	10.839	4
2	.93993	.234843	.194517	10.839	4
3	.930952	.26168	.178697	10.839	4
SAMPLE NUMBER	H ₂ CONV IMPLIED	-CH ₂ - IMPLIED	H ₂ O IMPLIED	H ₂ USED IMPLIED	H ₂ /CO USAGE
1	.338145	.343243	.48209	1.33453	1.44456
2	.278536	.461536	.382915	1.19422	1.34136
3	.323703	.523589	.443729	1.29482	1.39086
SAMPLE NUMBER	-CH ₂ - /CO CONV	CALC KER	EXPT KER	SUM=1?	
1	.353769	12.1274	20.0596	1	
2	.308621	12.1274	16.8761	1	
3	.342423	12.1274	21.5092	1	

B.2 Major Hydrocarbon Product Analysis--Output from the Microcomputer Data Compilation Program "HEAVY. BAS."

1. Input

- A. Moles of CH₄ produced per mole of CO converted.
 - i. Obtained from light-gas analysis.
- B. Flow Rate of the synthesis gas.
- C. Fraction of CO in the S-gas feed.
- D. Moles of CO converted per mole of CO fed.
 - i. Obtained from the light-gas analysis.
- E. Moles of CO₂ produced per mole of CO converted.
 - i. Obtained from the light-gas analysis.
- F. Peak areas for 24 hydrocarbons.

2. Output

- A. NORM AREA: Normalized peak areas of the 24 hydrocarbon. Normalized to CH₄.
- B. WT FRACT: The weight fraction of each hydrocarbon peak. Assumes FID response factors for all hydrocarbons are 1.
- C. HC/CO CONV: The moles of hydrocarbon produced per mole of CO consumed.
- D. RATE PROD: The rate of production of each hydrocarbon product i. mmoles per hour.
- E. M.W.: The molecular weight of each hydrocarbon. For fused peaks (C₂ and C₃) the average molecular weight is used.
- F. MOLE CA: The number of moles of each carbon number hydrocarbon product produced per mole of CO converted.
- G. MOLFRAC CA: The mole fraction of each carbon number hydrocarbon product produced.
- H. WT CA: The weight fraction of each carbon number of hydrocarbon product.

- I. WTFRAC C_n: The weight fraction of each carbon number hydrocarbon product.
- J. RATE C_n: The rate of production of each carbon number hydrocarbon product in mmoles per hour.

Table B-18

The Hydrocarbon Product Distribution and Rate of Production as Analyzed by Gas Chromatography for Steady-State Experiment B-1.

DATE OF EXPERIMENT 3/4/84 STEADY STATE W/D PRECARB.

EXPERIMENT B-1: THIS EXPERIMENT CONSISTS OF 10 HOURS OF 2.08:1 S-GAS FLOW AT 632K.

PEAK #	NORM AREA	WT FRACT.	HC/CO CONV	RATE PROD	M.W.
1	.573734	.262092	.06645	10.784	16.040
2	.696402	.151698	.0317747	3.44574	29.064
3	.429139	.132256	.005786	1.78431	28.064
4	.066338	.112276	.0112026	1.32256	56.108
5	.0162383	.0175181	1.33467E-03	.133467	56.108
6	.019747	4.25601E-03	4.61748E-04	.0500734	56.108
7	.271543	5.17545E-03	5.61571E-04	.0608933	56.108
8	.0493735	.0711739	6.17728E-03	.669926	70.136
9	.0123193	.0130717	1.10239E-03	.113597	70.136
10	.0105137	1.33599E-03	1.31621E-04	.0216242	70.136
11	.089597	1.73679E-03	1.33327E-04	.0239447	70.136
12	.0377479	1.33243E-03	1.33243E-03	.423401	86.176
13	.0127713	1.33423E-03	1.33423E-03	.0757358	86.176
14	.12513	1.33231E-03	1.41161E-04	.0261873	86.176
15	.0261281	6.34811E-03	1.02423E-03	.0451139	100.164
16	3.37005E-03	6.34811E-03	4.16015E-04	.0451139	100.164
17	6.60057E-03	6.33233E-04	5.47401E-05	5.93335E-03	98.130
18	.0220441	2.25419E-03	1.39731E-04	.015155	98.130
19	.0255406	6.02437E-03	1.33231E-03	.147433	114.166
20	.0633107	6.69813E-03	1.45774E-04	.0336893	114.166
21	.0174623	4.0167246	8.06444E-04	.0274537	128.192
22	.0302017	4.57683E-03	3.17227E-04	.0235547	128.192
23	.012958	3.0993E-03	3.51487E-04	.0231147	142.218
24		3.394E-03	1.453E-04	.0157833	142.218

CARBON #	MOLES C#	MOLFRAC C#	WT C#	WTFRAC C#	RATE C#
1	.09948	.521249	.262092	.262092	10.7847
2	.021747	.166733	.151698	.151698	3.44574
3	.015786	.132208	.132208	.132208	1.78431
4	7.81145E-03	.0790796	.139426	.139426	1.32256
5	4.84433E-03	.0409893	.0902643	.0902643	.0470358
6	2.44474E-03	.0254201	.0672093	.0672093	.0417973
7	1.6799E-03	.0138779	.0427973	.0427973	.0417973
8	1.02367E-03	8.81503E-03	.031084	.031084	.021774
9	4.96786E-04	1.37155E-03	.0213014	.0213014	.11101
10		1.60331E-03	.0114956	.0114956	.0593712

TOTAL PEAK AREA= 467574
 TOTAL MOLE CARBON PRODUCED AS OLEPAR/MOLE CO CONV= .414357
 MOLE RATIO C1/(C2-C5)= 1.16619
 WEIGHT FRACTION C1/(C2-C5)= .415219
 RATES ARE IN UNITS OF MMOL PER HOUR
 DWS MOL WTS ARE USED FOR C2 AND C3 HYDROCBNS DUE TO FUNED PEAKS
 TOT MOLE C PRODUCED AS CO2 AND OLEPAR/MOLE CO CONV= .768346

Table B-19

The Hydrocarbon Product Distribution and Rate of Production as Analyzed by Gas Chromatography for Steady-State Experiment B-2.

DATE OF EXPERIMENT 8/9/64 STEADY STATE W/O PRECURB.
 EXPERIMENT B-2: THIS EXPERIMENT CONSISTS OF 2 HOURS AND 3 MIN
 OF 2.08:1 S-GAS FLOW AT 633K.

PEAK #	NORM AREA	WT FRACT.	HC/CO CONV	RATE PROD	N.W.
1	.601216	.268172	.019245	13.4465	16.0443
2	.681714	.161225	.023006	4.46273	5.5742
3	.415909	.182317	.043347	3.41557	4.2843
4	.0607859	.111535	.011377	1.59907	1.9958
5	.0161563	.0143011	1.68554E-03	.229682	.28764
6	.0176762	4.33266E-03	1.82417E-03	.0521173	.65142
7	.262424	4.74026E-03	1.02437E-03	.0521173	.65142
8	.0126878	.0703748	1.62973E-03	.027163	.33953
9	.012990	.0114476	1.49948E-04	.12763	.15953
10	.012990	.0114476	1.49948E-04	.12763	.15953
11	.012990	.0114476	1.49948E-04	.12763	.15953
12	.012990	.0114476	1.49948E-04	.12763	.15953
13	.012990	.0114476	1.49948E-04	.12763	.15953
14	.012990	.0114476	1.49948E-04	.12763	.15953
15	.012990	.0114476	1.49948E-04	.12763	.15953
16	.012990	.0114476	1.49948E-04	.12763	.15953
17	.012990	.0114476	1.49948E-04	.12763	.15953
18	.012990	.0114476	1.49948E-04	.12763	.15953
19	.012990	.0114476	1.49948E-04	.12763	.15953
20	.012990	.0114476	1.49948E-04	.12763	.15953
21	.012990	.0114476	1.49948E-04	.12763	.15953
22	.012990	.0114476	1.49948E-04	.12763	.15953
23	.012990	.0114476	1.49948E-04	.12763	.15953
24	.012990	.0114476	1.49948E-04	.12763	.15953
25	.012990	.0114476	1.49948E-04	.12763	.15953
26	.012990	.0114476	1.49948E-04	.12763	.15953
27	.012990	.0114476	1.49948E-04	.12763	.15953
28	.012990	.0114476	1.49948E-04	.12763	.15953
29	.012990	.0114476	1.49948E-04	.12763	.15953
30	.012990	.0114476	1.49948E-04	.12763	.15953
31	.012990	.0114476	1.49948E-04	.12763	.15953
32	.012990	.0114476	1.49948E-04	.12763	.15953
33	.012990	.0114476	1.49948E-04	.12763	.15953
34	.012990	.0114476	1.49948E-04	.12763	.15953
35	.012990	.0114476	1.49948E-04	.12763	.15953
36	.012990	.0114476	1.49948E-04	.12763	.15953
37	.012990	.0114476	1.49948E-04	.12763	.15953
38	.012990	.0114476	1.49948E-04	.12763	.15953
39	.012990	.0114476	1.49948E-04	.12763	.15953
40	.012990	.0114476	1.49948E-04	.12763	.15953
41	.012990	.0114476	1.49948E-04	.12763	.15953
42	.012990	.0114476	1.49948E-04	.12763	.15953
43	.012990	.0114476	1.49948E-04	.12763	.15953
44	.012990	.0114476	1.49948E-04	.12763	.15953
45	.012990	.0114476	1.49948E-04	.12763	.15953
46	.012990	.0114476	1.49948E-04	.12763	.15953
47	.012990	.0114476	1.49948E-04	.12763	.15953
48	.012990	.0114476	1.49948E-04	.12763	.15953
49	.012990	.0114476	1.49948E-04	.12763	.15953
50	.012990	.0114476	1.49948E-04	.12763	.15953
51	.012990	.0114476	1.49948E-04	.12763	.15953
52	.012990	.0114476	1.49948E-04	.12763	.15953
53	.012990	.0114476	1.49948E-04	.12763	.15953
54	.012990	.0114476	1.49948E-04	.12763	.15953
55	.012990	.0114476	1.49948E-04	.12763	.15953
56	.012990	.0114476	1.49948E-04	.12763	.15953
57	.012990	.0114476	1.49948E-04	.12763	.15953
58	.012990	.0114476	1.49948E-04	.12763	.15953
59	.012990	.0114476	1.49948E-04	.12763	.15953
60	.012990	.0114476	1.49948E-04	.12763	.15953
61	.012990	.0114476	1.49948E-04	.12763	.15953
62	.012990	.0114476	1.49948E-04	.12763	.15953
63	.012990	.0114476	1.49948E-04	.12763	.15953
64	.012990	.0114476	1.49948E-04	.12763	.15953
65	.012990	.0114476	1.49948E-04	.12763	.15953
66	.012990	.0114476	1.49948E-04	.12763	.15953
67	.012990	.0114476	1.49948E-04	.12763	.15953
68	.012990	.0114476	1.49948E-04	.12763	.15953
69	.012990	.0114476	1.49948E-04	.12763	.15953
70	.012990	.0114476	1.49948E-04	.12763	.15953
71	.012990	.0114476	1.49948E-04	.12763	.15953
72	.012990	.0114476	1.49948E-04	.12763	.15953
73	.012990	.0114476	1.49948E-04	.12763	.15953
74	.012990	.0114476	1.49948E-04	.12763	.15953
75	.012990	.0114476	1.49948E-04	.12763	.15953
76	.012990	.0114476	1.49948E-04	.12763	.15953
77	.012990	.0114476	1.49948E-04	.12763	.15953
78	.012990	.0114476	1.49948E-04	.12763	.15953
79	.012990	.0114476	1.49948E-04	.12763	.15953
80	.012990	.0114476	1.49948E-04	.12763	.15953
81	.012990	.0114476	1.49948E-04	.12763	.15953
82	.012990	.0114476	1.49948E-04	.12763	.15953
83	.012990	.0114476	1.49948E-04	.12763	.15953
84	.012990	.0114476	1.49948E-04	.12763	.15953
85	.012990	.0114476	1.49948E-04	.12763	.15953
86	.012990	.0114476	1.49948E-04	.12763	.15953
87	.012990	.0114476	1.49948E-04	.12763	.15953
88	.012990	.0114476	1.49948E-04	.12763	.15953
89	.012990	.0114476	1.49948E-04	.12763	.15953
90	.012990	.0114476	1.49948E-04	.12763	.15953
91	.012990	.0114476	1.49948E-04	.12763	.15953
92	.012990	.0114476	1.49948E-04	.12763	.15953
93	.012990	.0114476	1.49948E-04	.12763	.15953
94	.012990	.0114476	1.49948E-04	.12763	.15953
95	.012990	.0114476	1.49948E-04	.12763	.15953
96	.012990	.0114476	1.49948E-04	.12763	.15953
97	.012990	.0114476	1.49948E-04	.12763	.15953
98	.012990	.0114476	1.49948E-04	.12763	.15953
99	.012990	.0114476	1.49948E-04	.12763	.15953
100	.012990	.0114476	1.49948E-04	.12763	.15953

TOTAL PEAK AREA= 662411
 TOTAL MOLE CARBON PRODUCED AS OLEFINS/MOLE CO CONV= .40506
 MOLE RATIO C1/(C2-C6)= 1.16866
 WEIGHT FRACTION C1/(C2-C5) .419514
 RATES ARE IN UNITS OF MMOL PER HOUR
 100 MOL WTS ARE USED FOR C2 AND C3 HYDROCBNS DUE TO FUSED PEAKS
 TOT MOLE C PRODUCED AS CO2 AND OLEFINS/MOLE CO CONV= .748057

Table B-20

The Hydrocarbon Product Distribution and Rate of Production as Analyzed by Gas Chromatography for Steady-State Experiment B-3.

DATE OF EXPERIMENT 8/10/64 STEADY STATE W/O PRECARR.
 EXPERIMENT B-3: THIS EXPERIMENT CONSISTS OF 10 HOURS
 OF 3.0:1 S-GAS FLOW AT 633K.

PEAK #	NORM AREA	WT FRACT.	HC/CO CONV	RATE PROD	M.W.
1	.47654	.327338	.1791	18.8321	14.0
2	.57979	.153889	.0471145	4.95811	40.0
3	.347677	.113808	.038643	4.04237	42.0
4	.0570124	.0186623	.0173046	1.87212	58.0
5	.0136335	4.44038E-03	.813355E-03	.0762374	70.0
6	.0147805	4.93333E-03	5.97799E-04	.0798371	70.0
7	.038017	.0280939E-03	2.95209E-03	.0396063	70.0
8	.038925	.0177413	1.95016E-03	.1639397	70.0
9	.0105235	3.44444E-03	3.10301E-04	.0439136	70.0
10	.112713	3.34753E-03	3.43033E-04	.0311364	70.0
11	.0241421	7.90263E-03	5.04335E-04	.0442135	70.0
12	.7.63145E-03	1.49806E-03	3.60539E-04	.0343073	70.0
13	.053626	.0175533	1.89318E-03	.0173935	70.0
14	.0112655	3.63761E-03	1.38027E-04	.125005	70.0
15	1.62034E-03	3.30563E-04	4.74006E-04	.033265	100.0
16	4.00413E-03	1.96539E-03	1.74906E-04	4.53725E-03	100.0
17	.0360765	.011809	1.377E-04	.0184745	100.0
18	9.4967E-03	3.10845E-03	3.33733E-04	.0713301	110.0
19	.0196077	3.41835E-03	1.33733E-04	.0251171	110.0
20	5.26559E-03	1.95376E-03	1.32473E-04	.0489047	120.0
21	5.44585E-03	3.05315E-03	1.33643E-04	.0140074	120.0
22	5.54999E-03	1.15008E-03	7.14366E-04	.0311091	120.0
23			7.15666E-04	7.52519E-03	140.0

CARBON #	MOLES C#	MOLFRAC C#	WT C#	WTFRAC C#	RATE C#
1	.1791	.593317	.327338	.327338	18.8321
2	.0471145	.153889	.153889	.153889	4.95811
3	.038643	.113808	.113808	.113808	4.04237
4	.0173046	.0173046	.0173046	.0173046	1.87212
5	.813355E-03	.0352033	.0352033	.0352033	3.52143
6	.597799E-04	.0266438	.0266438	.0266438	1.12547
7	.310301E-03	.0223737	.0223737	.0223737	5.12547
8	.1639397E-03	3.78931E-03	.0149173	.0149173	1.12547
9	.0439136E-03	1.89031E-03	3.37103E-03	3.37103E-03	.0609771
10	.0343073E-03	3.57313E-04	4.21922E-03	4.21922E-03	.0276542

TOTAL PEAK AREA= 949937
 TOTAL MOLE CARBON PRODUCED AS OLE&PAR/MOLE CO CONV= .593021
 MOLE RATIO C1/(C2-C5) 1.44958
 WEIGHT FRACTION C1/(C2-C5) .52676
 RATES ARE IN UNITS OF MMOL PER HOUR
 AVG MOL WTS ARE USED FOR C2 AND C3 HYDROCBNS DUE TO FUSED PEAKS
 TOT MOLE C PRODUCED AS CO2 AND OLE&PAR/MOLE CO CONV= .800321

Table B-21

The Hydrocarbon Product Distribution and Rate of Production as Analyzed by Gas Chromatography for Steady-State Experiment C-1.

DATE OF EXPERIMENT 8/24/84 STEADY STATE W/O PRECARB.

EXPERIMENT C-1: THIS EXPERIMENT CONSISTS OF 2 HOURS AND 4 MIN OF 2.08:1 S-GAS FLOW AT 673K.

PEAK #	NORM AREA	WT FRACT.	HC/CO CONV	RATE PROD	M.W.
1	342877	.1292	1.1292E-03	1.1292E-03	16.043
2	107139	.0382	3.82E-04	3.82E-04	28.053
3	125039	.0443	4.43E-04	4.43E-04	44.099
4	145113	.0515	5.15E-04	5.15E-04	58.120
5	179031	.0641	6.41E-04	6.41E-04	72.150
6	446748	.1591	1.591E-03	1.591E-03	86.171
7	671193	.2411	2.411E-03	2.411E-03	100.200
8	107139	.0382	3.82E-04	3.82E-04	114.229
9	125039	.0443	4.43E-04	4.43E-04	128.258
10	145113	.0515	5.15E-04	5.15E-04	142.287
11	179031	.0641	6.41E-04	6.41E-04	156.316
12	446748	.1591	1.591E-03	1.591E-03	170.345
13	671193	.2411	2.411E-03	2.411E-03	184.374
14	107139	.0382	3.82E-04	3.82E-04	198.403
15	125039	.0443	4.43E-04	4.43E-04	212.432
16	145113	.0515	5.15E-04	5.15E-04	226.461
17	179031	.0641	6.41E-04	6.41E-04	240.490
18	446748	.1591	1.591E-03	1.591E-03	254.519
19	671193	.2411	2.411E-03	2.411E-03	268.548
20	107139	.0382	3.82E-04	3.82E-04	282.577
21	125039	.0443	4.43E-04	4.43E-04	296.606
22	145113	.0515	5.15E-04	5.15E-04	310.635
23	179031	.0641	6.41E-04	6.41E-04	324.664
24	446748	.1591	1.591E-03	1.591E-03	338.693
25	671193	.2411	2.411E-03	2.411E-03	352.722
26	107139	.0382	3.82E-04	3.82E-04	366.751
27	125039	.0443	4.43E-04	4.43E-04	380.780
28	145113	.0515	5.15E-04	5.15E-04	394.809
29	179031	.0641	6.41E-04	6.41E-04	408.838
30	446748	.1591	1.591E-03	1.591E-03	422.867
31	671193	.2411	2.411E-03	2.411E-03	436.896
32	107139	.0382	3.82E-04	3.82E-04	450.925
33	125039	.0443	4.43E-04	4.43E-04	464.954
34	145113	.0515	5.15E-04	5.15E-04	478.983
35	179031	.0641	6.41E-04	6.41E-04	493.012
36	446748	.1591	1.591E-03	1.591E-03	507.041
37	671193	.2411	2.411E-03	2.411E-03	521.070
38	107139	.0382	3.82E-04	3.82E-04	535.099
39	125039	.0443	4.43E-04	4.43E-04	549.128
40	145113	.0515	5.15E-04	5.15E-04	563.157
41	179031	.0641	6.41E-04	6.41E-04	577.186
42	446748	.1591	1.591E-03	1.591E-03	591.215
43	671193	.2411	2.411E-03	2.411E-03	605.244
44	107139	.0382	3.82E-04	3.82E-04	619.273
45	125039	.0443	4.43E-04	4.43E-04	633.302
46	145113	.0515	5.15E-04	5.15E-04	647.331
47	179031	.0641	6.41E-04	6.41E-04	661.360
48	446748	.1591	1.591E-03	1.591E-03	675.389
49	671193	.2411	2.411E-03	2.411E-03	689.418
50	107139	.0382	3.82E-04	3.82E-04	703.447
51	125039	.0443	4.43E-04	4.43E-04	717.476
52	145113	.0515	5.15E-04	5.15E-04	731.505
53	179031	.0641	6.41E-04	6.41E-04	745.534
54	446748	.1591	1.591E-03	1.591E-03	759.563
55	671193	.2411	2.411E-03	2.411E-03	773.592
56	107139	.0382	3.82E-04	3.82E-04	787.621
57	125039	.0443	4.43E-04	4.43E-04	801.650
58	145113	.0515	5.15E-04	5.15E-04	815.679
59	179031	.0641	6.41E-04	6.41E-04	829.708
60	446748	.1591	1.591E-03	1.591E-03	843.737
61	671193	.2411	2.411E-03	2.411E-03	857.766
62	107139	.0382	3.82E-04	3.82E-04	871.795
63	125039	.0443	4.43E-04	4.43E-04	885.824
64	145113	.0515	5.15E-04	5.15E-04	899.853
65	179031	.0641	6.41E-04	6.41E-04	913.882
66	446748	.1591	1.591E-03	1.591E-03	927.911
67	671193	.2411	2.411E-03	2.411E-03	941.940
68	107139	.0382	3.82E-04	3.82E-04	955.969
69	125039	.0443	4.43E-04	4.43E-04	969.998
70	145113	.0515	5.15E-04	5.15E-04	984.027
71	179031	.0641	6.41E-04	6.41E-04	998.056
72	446748	.1591	1.591E-03	1.591E-03	1012.085
73	671193	.2411	2.411E-03	2.411E-03	1026.114
74	107139	.0382	3.82E-04	3.82E-04	1040.143
75	125039	.0443	4.43E-04	4.43E-04	1054.172
76	145113	.0515	5.15E-04	5.15E-04	1068.201
77	179031	.0641	6.41E-04	6.41E-04	1082.230
78	446748	.1591	1.591E-03	1.591E-03	1096.259
79	671193	.2411	2.411E-03	2.411E-03	1110.288
80	107139	.0382	3.82E-04	3.82E-04	1124.317
81	125039	.0443	4.43E-04	4.43E-04	1138.346
82	145113	.0515	5.15E-04	5.15E-04	1152.375
83	179031	.0641	6.41E-04	6.41E-04	1166.404
84	446748	.1591	1.591E-03	1.591E-03	1180.433
85	671193	.2411	2.411E-03	2.411E-03	1194.462
86	107139	.0382	3.82E-04	3.82E-04	1208.491
87	125039	.0443	4.43E-04	4.43E-04	1222.520
88	145113	.0515	5.15E-04	5.15E-04	1236.549
89	179031	.0641	6.41E-04	6.41E-04	1250.578
90	446748	.1591	1.591E-03	1.591E-03	1264.607
91	671193	.2411	2.411E-03	2.411E-03	1278.636
92	107139	.0382	3.82E-04	3.82E-04	1292.665
93	125039	.0443	4.43E-04	4.43E-04	1306.694
94	145113	.0515	5.15E-04	5.15E-04	1320.723
95	179031	.0641	6.41E-04	6.41E-04	1334.752
96	446748	.1591	1.591E-03	1.591E-03	1348.781
97	671193	.2411	2.411E-03	2.411E-03	1362.810
98	107139	.0382	3.82E-04	3.82E-04	1376.839
99	125039	.0443	4.43E-04	4.43E-04	1390.868
100	145113	.0515	5.15E-04	5.15E-04	1404.897
101	179031	.0641	6.41E-04	6.41E-04	1418.926
102	446748	.1591	1.591E-03	1.591E-03	1432.955
103	671193	.2411	2.411E-03	2.411E-03	1446.984
104	107139	.0382	3.82E-04	3.82E-04	1461.013
105	125039	.0443	4.43E-04	4.43E-04	1475.042
106	145113	.0515	5.15E-04	5.15E-04	1489.071
107	179031	.0641	6.41E-04	6.41E-04	1503.100
108	446748	.1591	1.591E-03	1.591E-03	1517.129
109	671193	.2411	2.411E-03	2.411E-03	1531.158
110	107139	.0382	3.82E-04	3.82E-04	1545.187
111	125039	.0443	4.43E-04	4.43E-04	1559.216
112	145113	.0515	5.15E-04	5.15E-04	1573.245
113	179031	.0641	6.41E-04	6.41E-04	1587.274
114	446748	.1591	1.591E-03	1.591E-03	1601.303
115	671193	.2411	2.411E-03	2.411E-03	1615.332
116	107139	.0382	3.82E-04	3.82E-04	1629.361
117	125039	.0443	4.43E-04	4.43E-04	1643.390
118	145113	.0515	5.15E-04	5.15E-04	1657.419
119	179031	.0641	6.41E-04	6.41E-04	1671.448
120	446748	.1591	1.591E-03	1.591E-03	1685.477
121	671193	.2411	2.411E-03	2.411E-03	1699.506
122	107139	.0382	3.82E-04	3.82E-04	1713.535
123	125039	.0443	4.43E-04	4.43E-04	1727.564
124	145113	.0515	5.15E-04	5.15E-04	1741.593
125	179031	.0641	6.41E-04	6.41E-04	1755.622
126	446748	.1591	1.591E-03	1.591E-03	1769.651
127	671193	.2411	2.411E-03	2.411E-03	1783.680
128	107139	.0382	3.82E-04	3.82E-04	1797.709
129	125039	.0443	4.43E-04	4.43E-04	1811.738
130	145113	.0515	5.15E-04	5.15E-04	1825.767
131	179031	.0641	6.41E-04	6.41E-04	1839.796
132	446748	.1591	1.591E-03	1.591E-03	1853.825
133	671193	.2411	2.411E-03	2.411E-03	1867.854
134	107139	.0382	3.82E-04	3.82E-04	1881.883
135	125039	.0443	4.43E-04	4.43E-04	1895.912
136	145113	.0515	5.15E-04	5.15E-04	1909.941
137	179031	.0641	6.41E-04	6.41E-04	1923.970
138	446748	.1591	1.591E-03	1.591E-03	1938.000
139	671193	.2411	2.411E-03	2.411E-03	1952.029
140	107139	.0382	3.82E-04	3.82E-04	1966.058
141	125039	.0443	4.43E-04	4.43E-04	1980.087
142	145113	.0515	5.15E-04	5.15E-04	1994.116
143	179031	.0641	6.41E-04	6.41E-04	2008.145
144	446748	.1591	1.591E-03	1.591E-03	2022.174
145	671193	.2411	2.411E-03	2.411E-03	2036.203
146	107139	.0382	3.82E-04	3.82E-04	2050.232
147	125039	.0443	4.43E-04	4.43E-04	2064.261
148	145113	.0515	5.15E-04	5.15E-04	2078.290
149	179031	.0641	6.41E-04	6.41E-04	2092.319
150	446748	.1591	1.591E-03	1.591E-03	2106.348
151	671193	.2411	2.411E-03	2.411E-03	2120.377

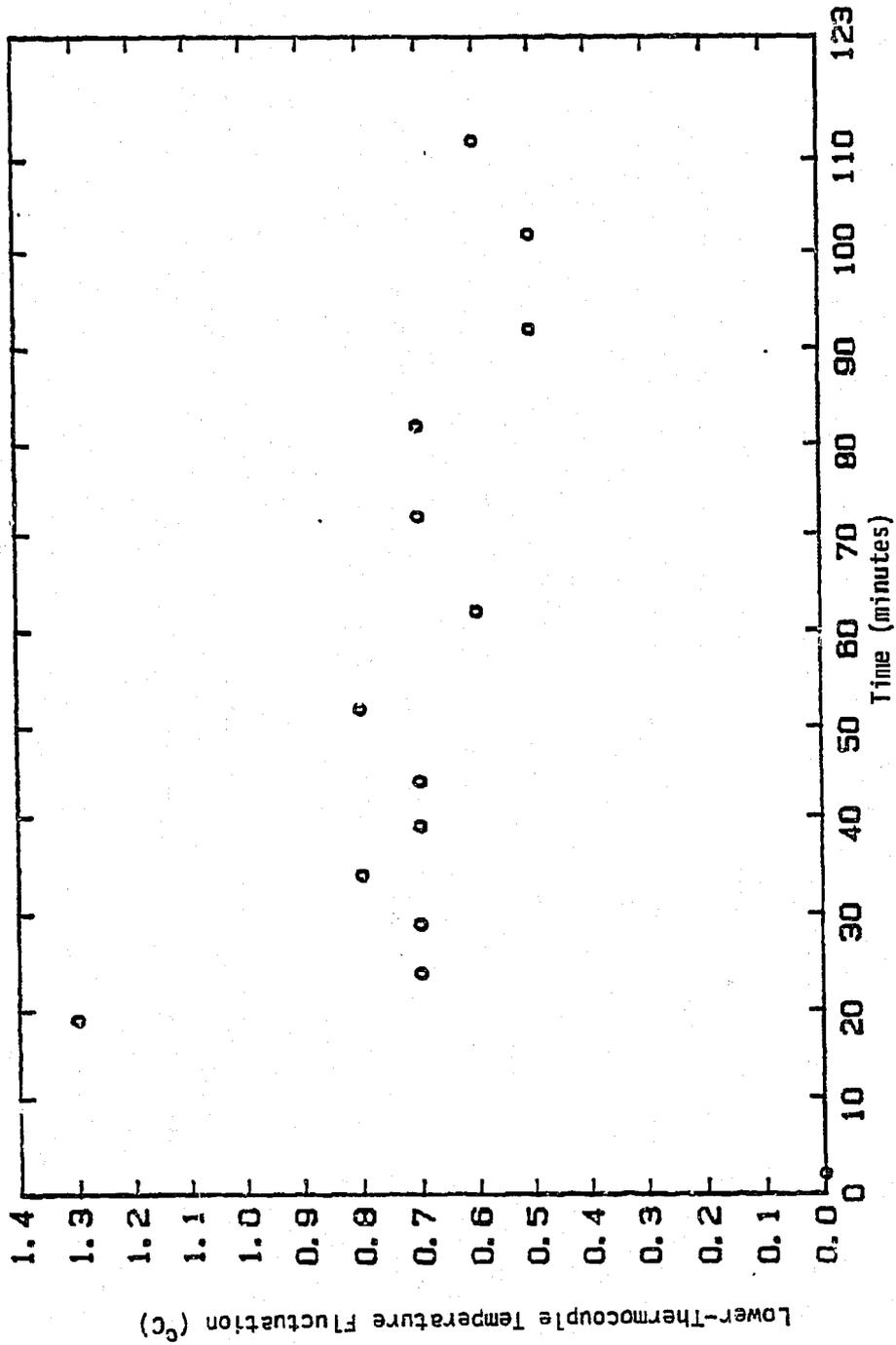


Figure B.1. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run B-2 Using a Feed Gas of 2.08:1 H₂/CO Ratio at 360°C and 2220 kPa.

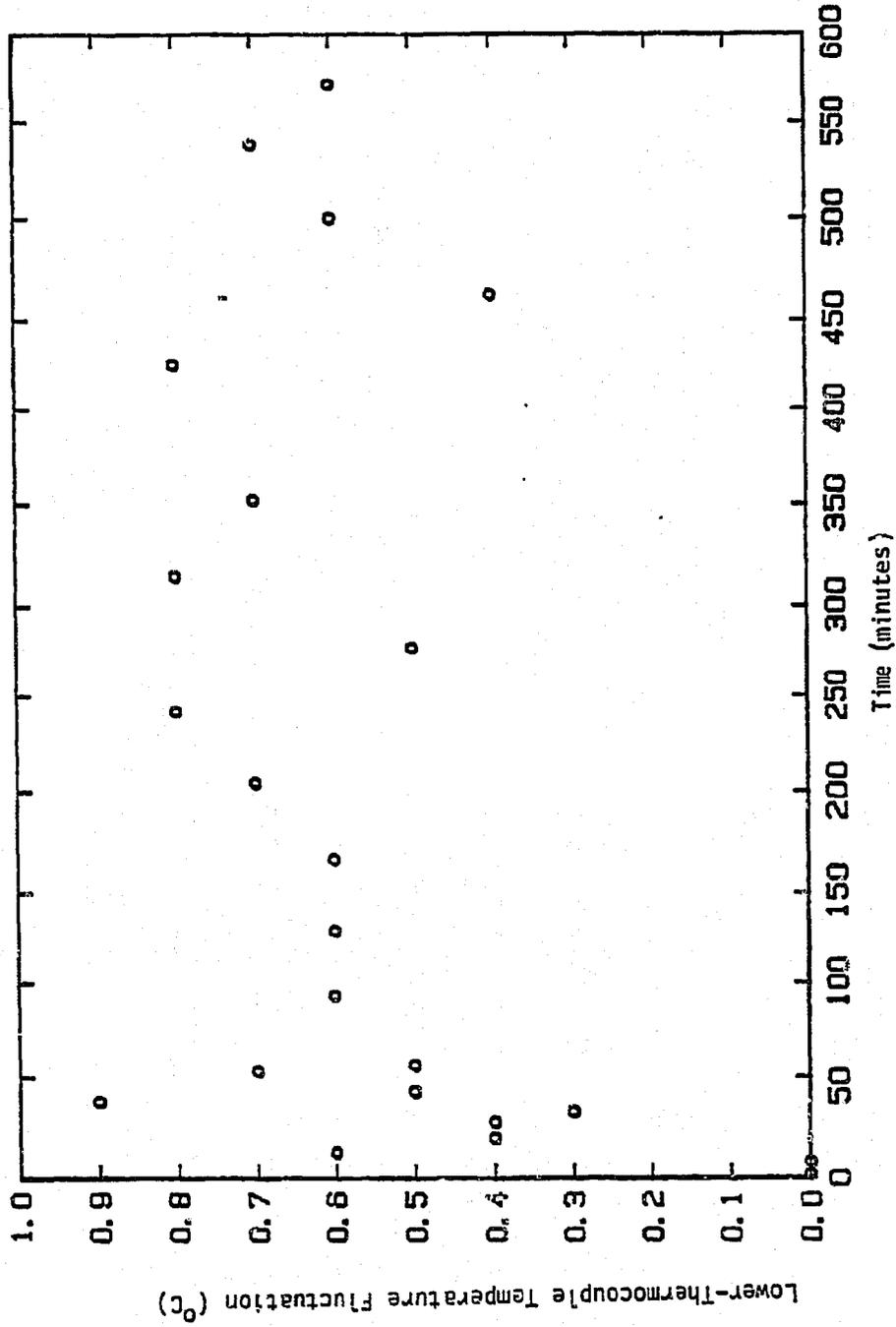


Figure B.2. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run B-3 Using a Feed Gas of 4:1 H₂/CO Ratio at 360°C and 2220 kPa.

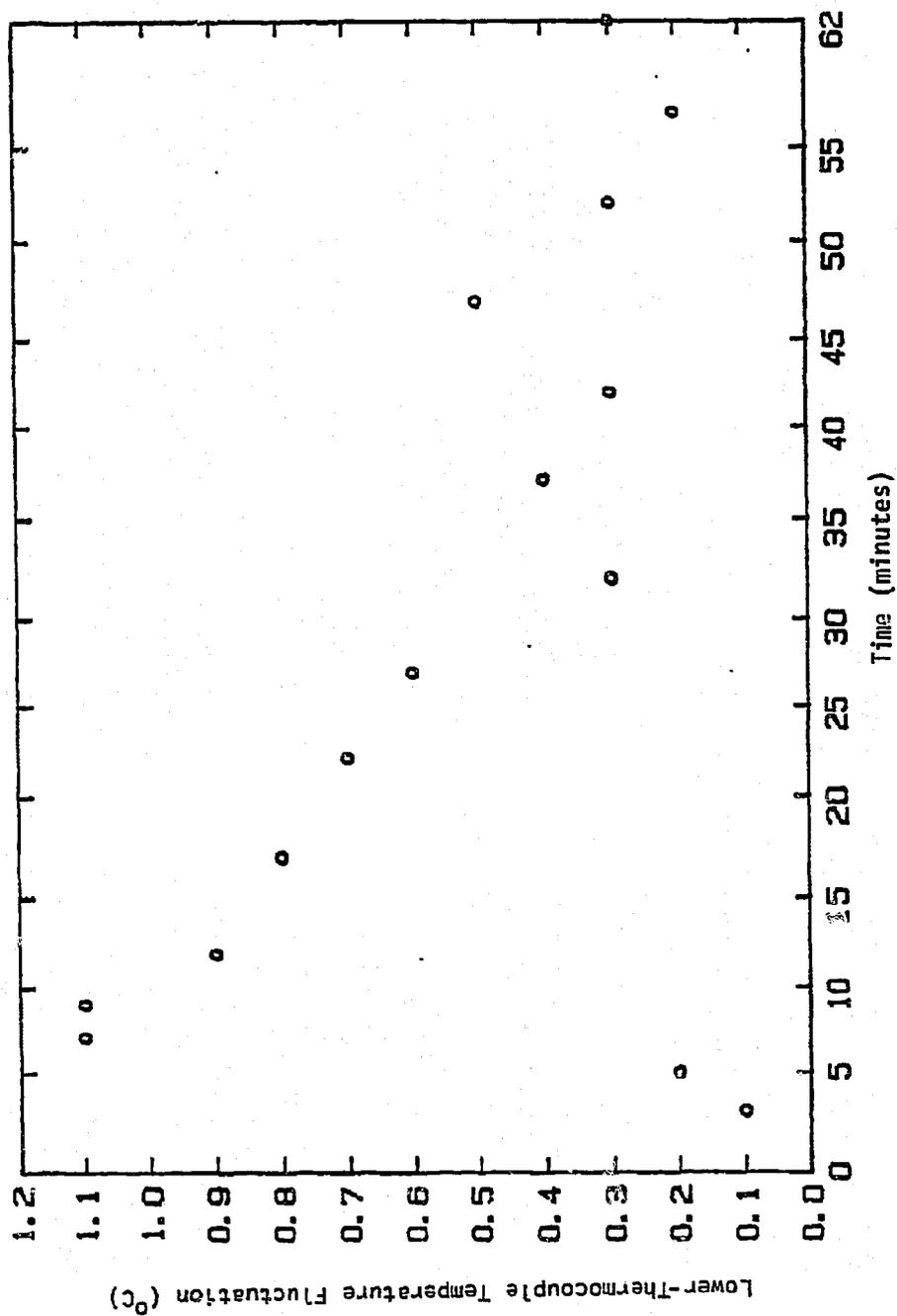


Figure B.3. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run B-4 Using a Feed Gas of 1.03:1 H₂/CO Ratio at 360°C and 2220 kPa.

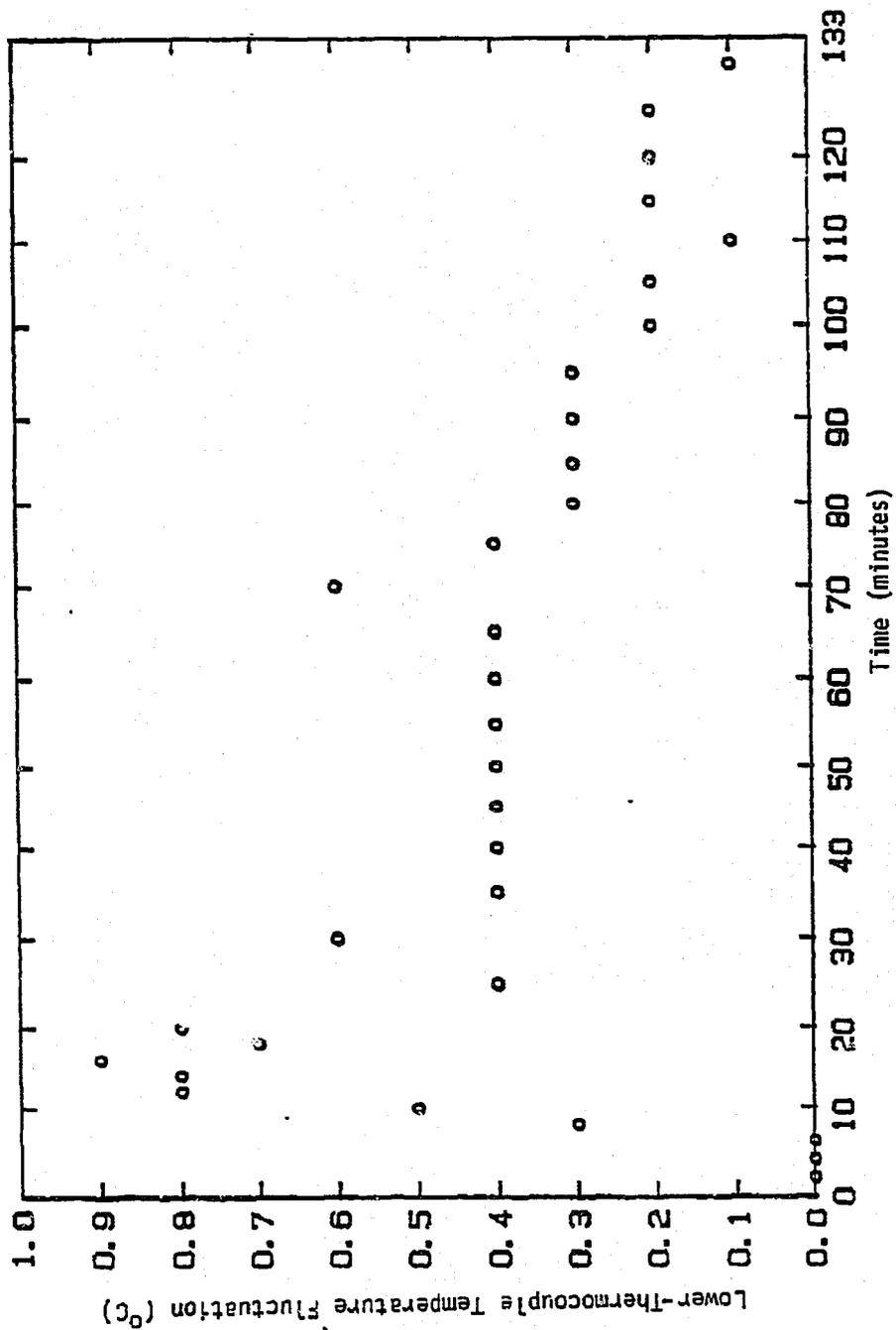


Figure B.4. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run B-5 Using a Feed Gas of 1.03:1 H₂/CO Ratio at 360°C and 2220 kPa.

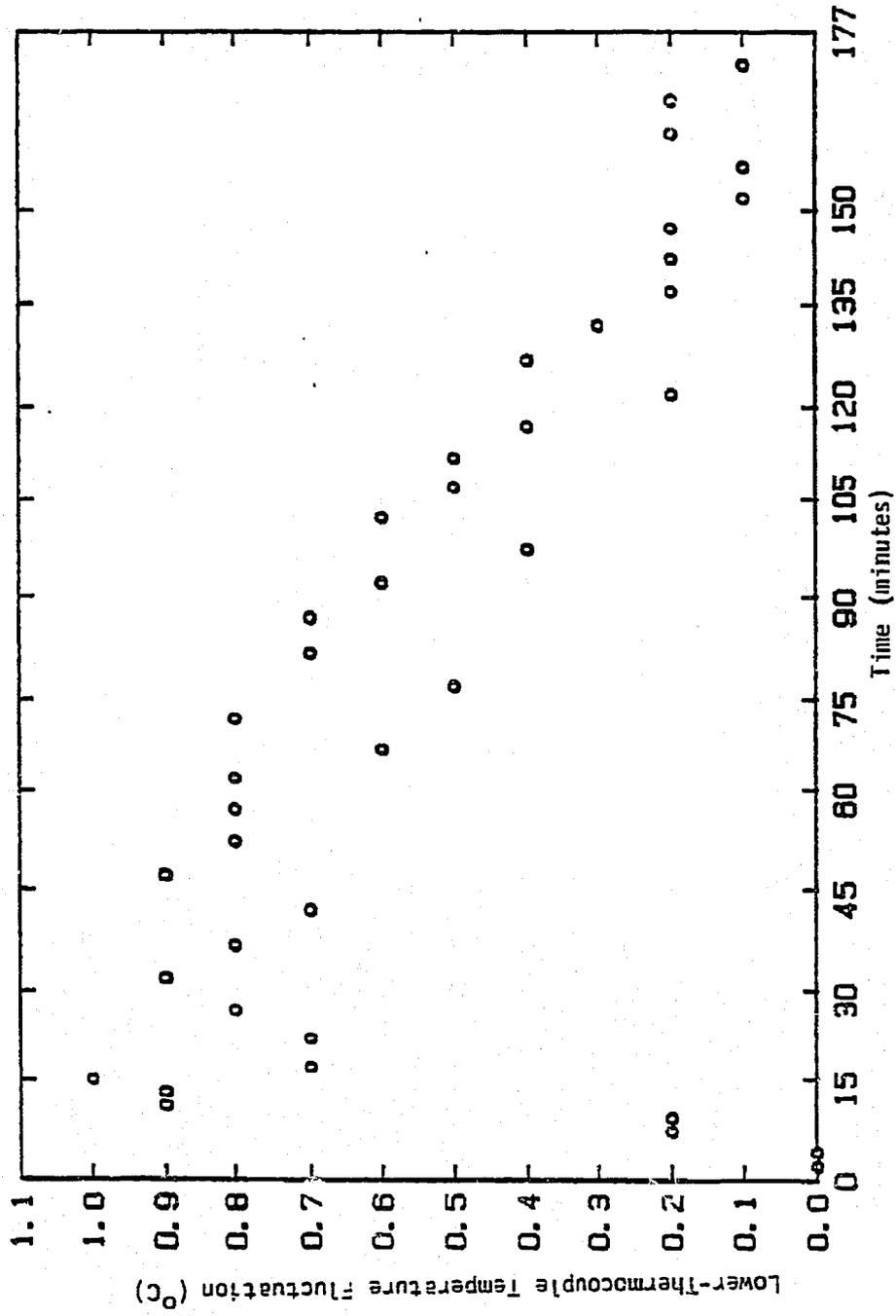


Figure B.5. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run B-6 Using a Feed Gas of 2.08:1 H_2/CO Ratio at 360°C and 2220 kPa.

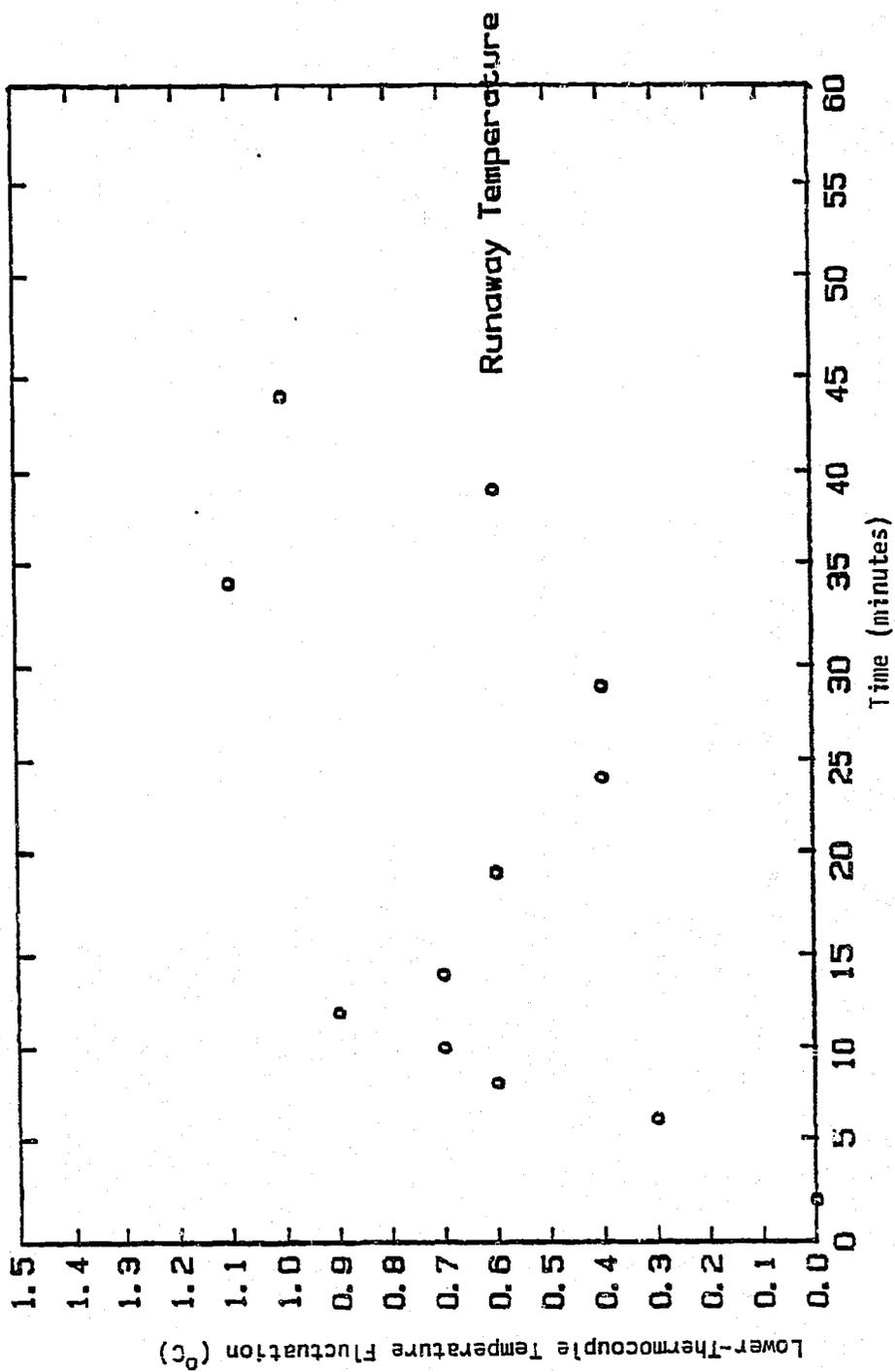


Figure B.6. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run C-2 Using a Feed Gas of 1.03:1 H_2/CO Ratio at 400°C and 2220 kPa.

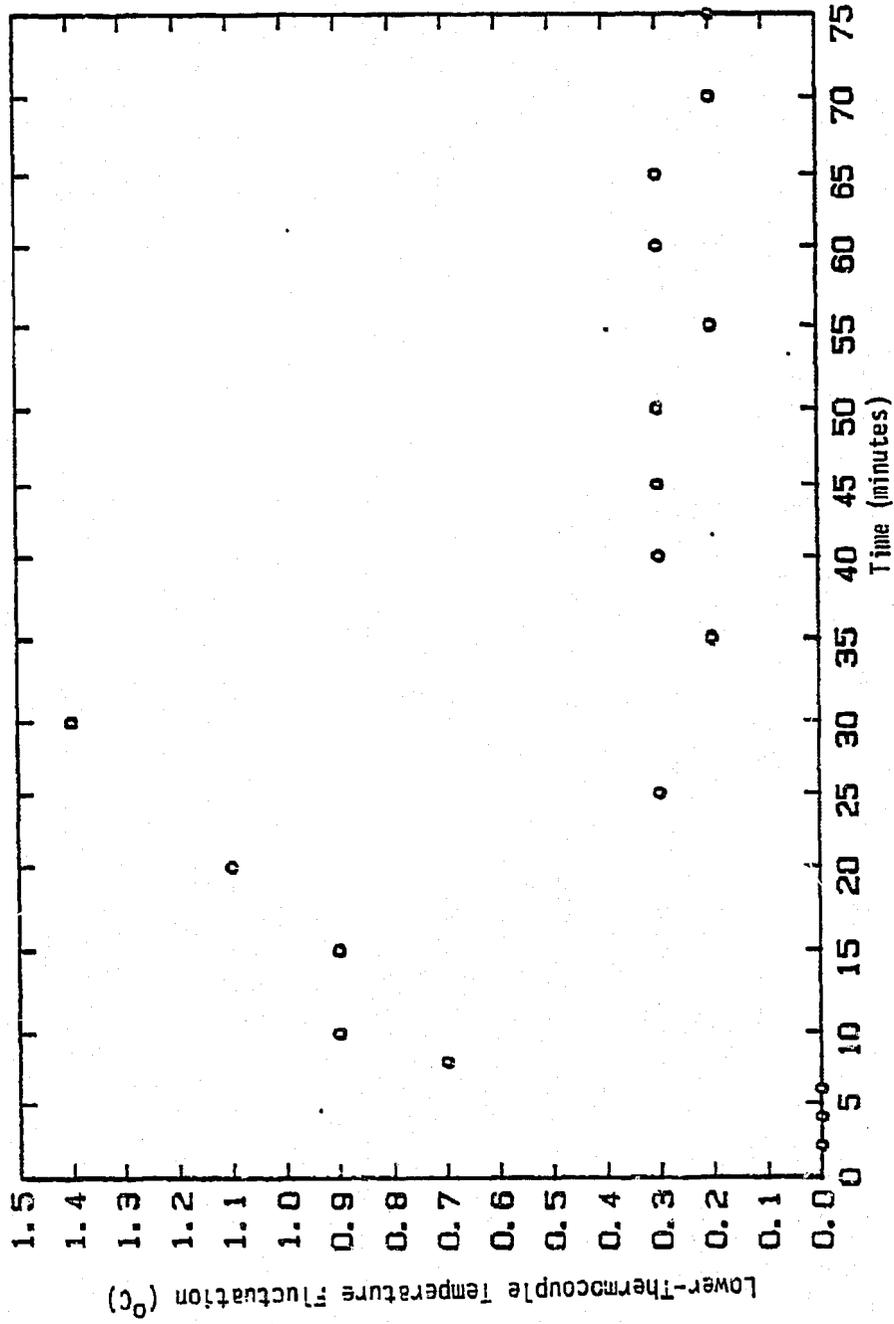


Figure B.7. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run D-1 Using a Feed Gas of 1.03:1 H₂/CO Ratio at 380°C and 2220 kPa.

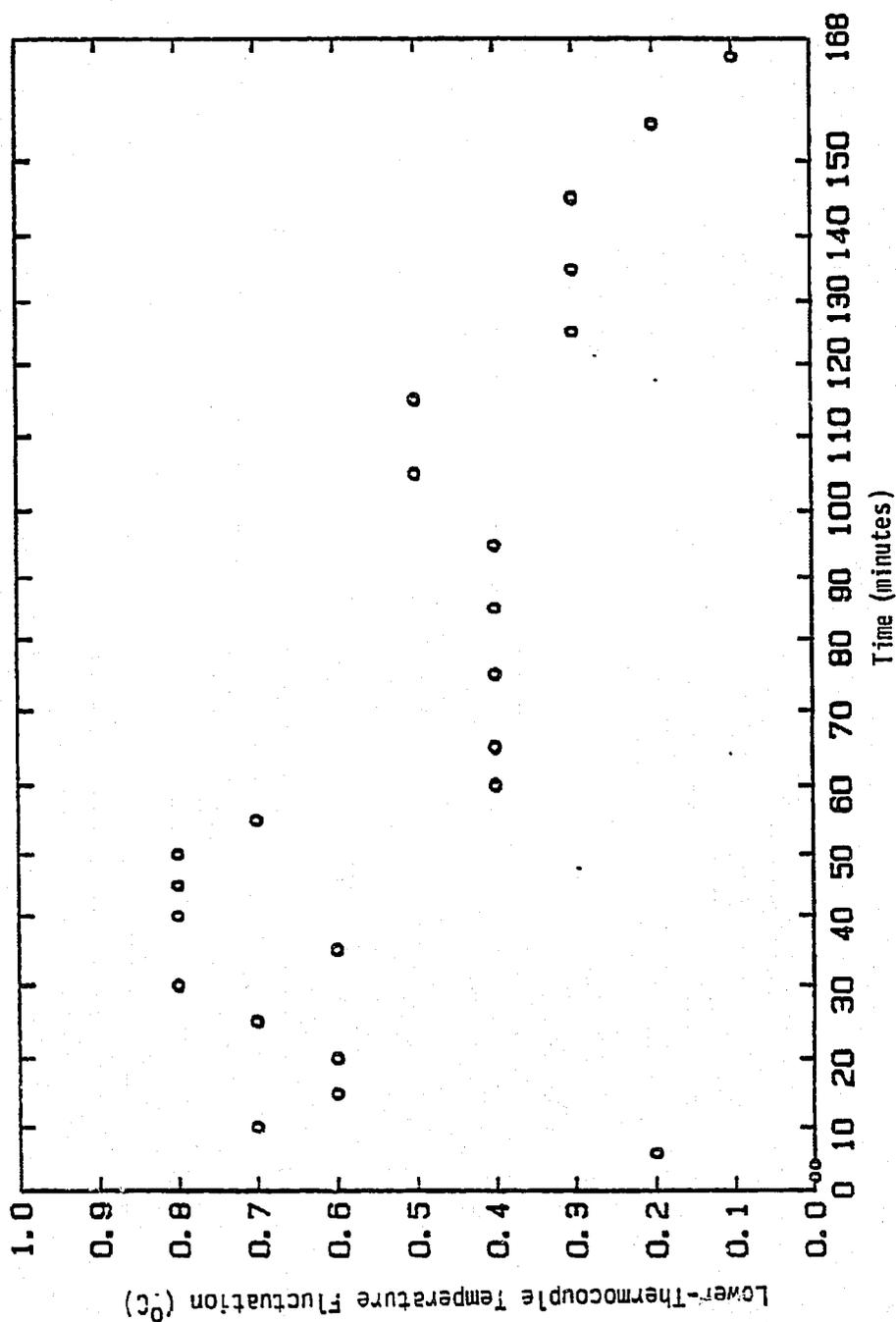


Figure B.8. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run D-2 Using a Feed Gas of 2.08:1 H₂/CO Ratio at 380°C and 2220 kPa.

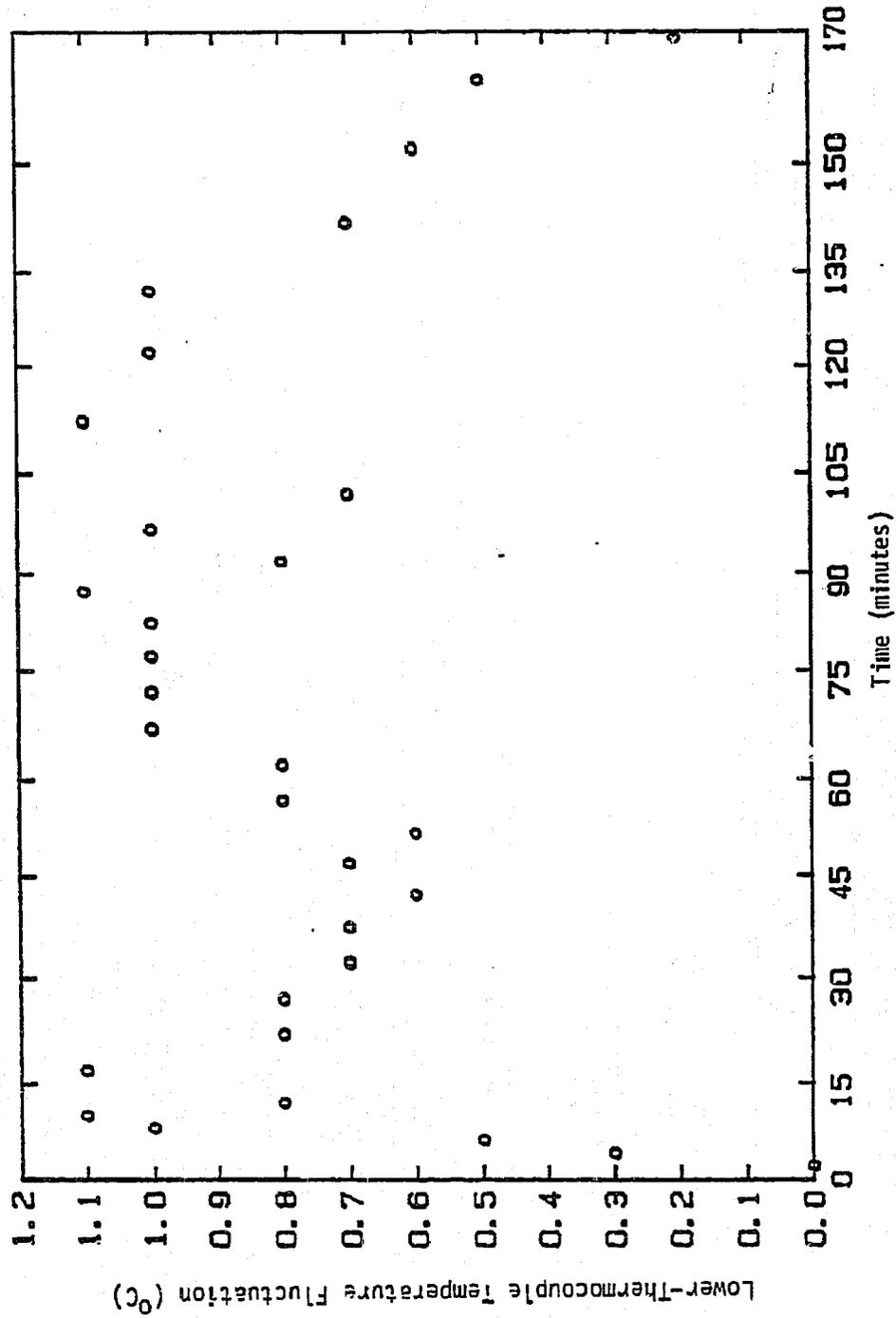


Figure B.9. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run E-1 Using a Feed Gas of 208:1 H_2/CO Ratio at 390°C and 2220 kPa.

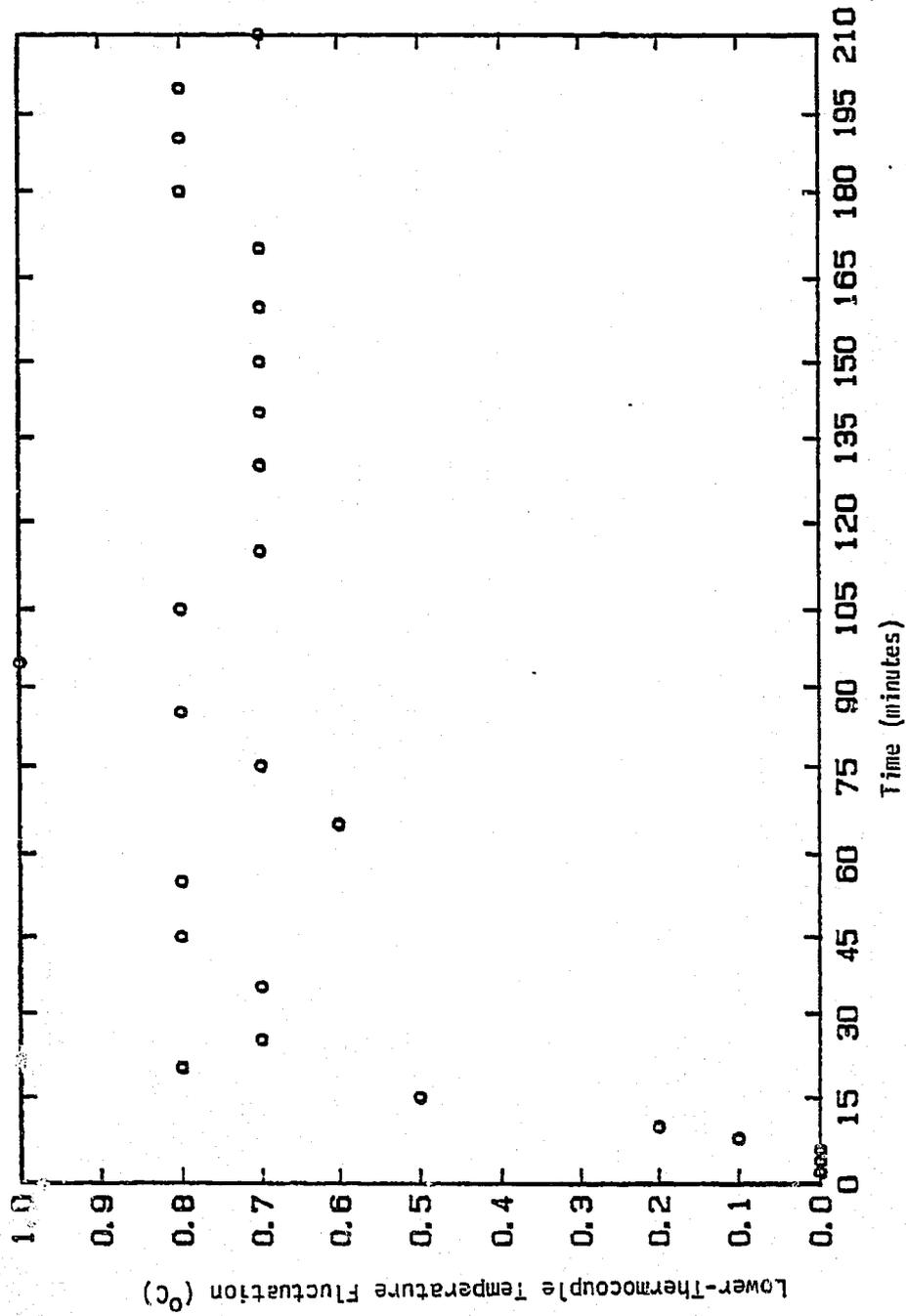


Figure B.10. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run F-1 Using a Feed Gas of 4:1 H₂/CO Ratio at 395°C and 2220 kPa.

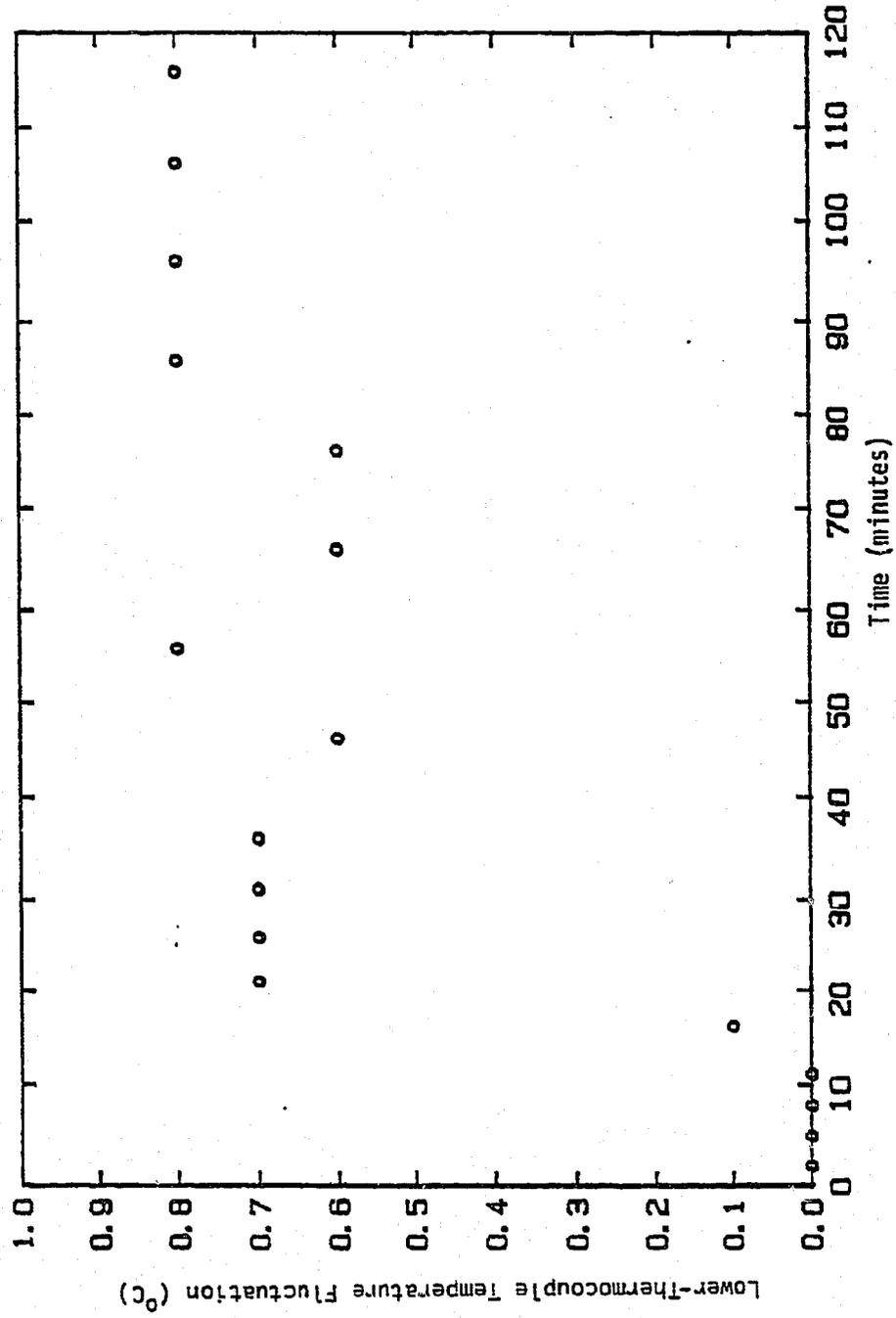


Figure B.11. Lower-Thermocouple Temperature Fluctuation as a Function of Time for Run F-2 Using a Feed Gas of 4:1 H₂/CO Ratio at 395°C and 2220 kPa.

APPENDIX C

Microcomputer Programs for: (1) Feed-Gas Cycling and Product Analysis During Unsteady-State Fischer-Tropsch Synthesis; (2) Data Compilation for Light-Gas Products (MASSBAL.BAS); and (3) Data Compilation for the Hydrocarbon Product Distribution from Capillary Analysis (HEAVY.BAS).


```

730 PRINT CHR$(96)
740 NEXT I
750 FOR J=1 TO 35
760 PRINT CHR$(32):
770 NEXT J
780 PRINT CHR$(102):
790 FOR J=1 TO 3
800 PRINT CHR$(97):
810 NEXT J
820 PRINT CHR$(96):
830 FOR J=1 TO 4
840 PRINT CHR$(97):
850 NEXT J
860 PRINT CHR$(32):
870 PRINT "SPLIT PRODUCT"
880 FOR I=1 TO 3
890 FOR J=1 TO 4
900 PRINT CHR$(32):
910 NEXT J
920 PRINT CHR$(32); CHR$(96); CHR$(32); CHR$(32); CHR$(32); CHR$(32); CHR$(32):
930 FOR J=1 TO 3
940 PRINT CHR$(32):
950 NEXT J
960 PRINT CHR$(96):
970 FOR J=1 TO 4
980 PRINT CHR$(32):
990 NEXT J
1000 PRINT CHR$(96):
1010 FOR J=1 TO 5
1020 PRINT CHR$(32):
1030 NEXT J
1040 PRINT CHR$(96):
1050 FOR I=1 TO 3
1060 FOR J=1 TO 3
1070 PRINT CHR$(32):
1080 NEXT J
1090 PRINT CHR$(96):
1100 FOR J=1 TO 5
1110 PRINT CHR$(32):
1120 NEXT J
1130 PRINT CHR$(96):
1140 FOR J=1 TO 3
1150 PRINT CHR$(32):
1160 NEXT J
1170 PRINT CHR$(96):
1180 FOR J=1 TO 5
1190 PRINT CHR$(105):
1200 NEXT J
1210 PRINT CHR$(96):
1220 FOR I=1 TO 3
1230 PRINT CHR$(32):
1240 NEXT I
1250 PRINT CHR$(96):
1260 FOR J=1 TO 3
1270 PRINT CHR$(32):
1280 NEXT J
1290 PRINT CHR$(96):
1300 NEXT I
1310 FOR J=1 TO 5
1320 PRINT CHR$(32):
1330 NEXT J
1340 PRINT CHR$(101):
1350 FOR J=1 TO 3
1360 PRINT CHR$(97):
1370 NEXT J
1380 PRINT CHR$(117):
1390 FOR J=1 TO 3
1400 PRINT CHR$(32):
1410 NEXT J
1420 PRINT CHR$(96):
1430 FOR J=1 TO 3
1440 PRINT CHR$(32):
1450 NEXT J

```

Figure C.1 (Continued)

