Section VIII: DESIGN AND FABRICATION OF THE CATALYST TESTING UNIT

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The screening and evaluation of candidate catalysts and the process variable studies to be conducted for both the aromatics formation step and the aromatics hydrogenation step required the design and fabrication of a bench scale catalyst testing unit. The unit was designed to be capable of conducting all the investigations outlined in the research proposal and for maximum flexibility with regard to process operating variables and process configurations.

Reactor Design

A schematic of the high pressure flow reactor system for aviation turbine fuel synthesis is presented in Figure 91. The reactor was designed on the assumption that it would operate as a fixed or packed bed reactor. Four critical process operating variables were selected to establish the design basis: temperature, pressure, gas and liquid space velocities, and feed ratios. It was required that all process variables must be capable of being monitored and adjusted in both the manual and automatic control operating modes. The ranges of the process operating conditions selected in the design process were as follows:

Catalyst Volume:	10-100 cm^3
Temperature:	373-773 K

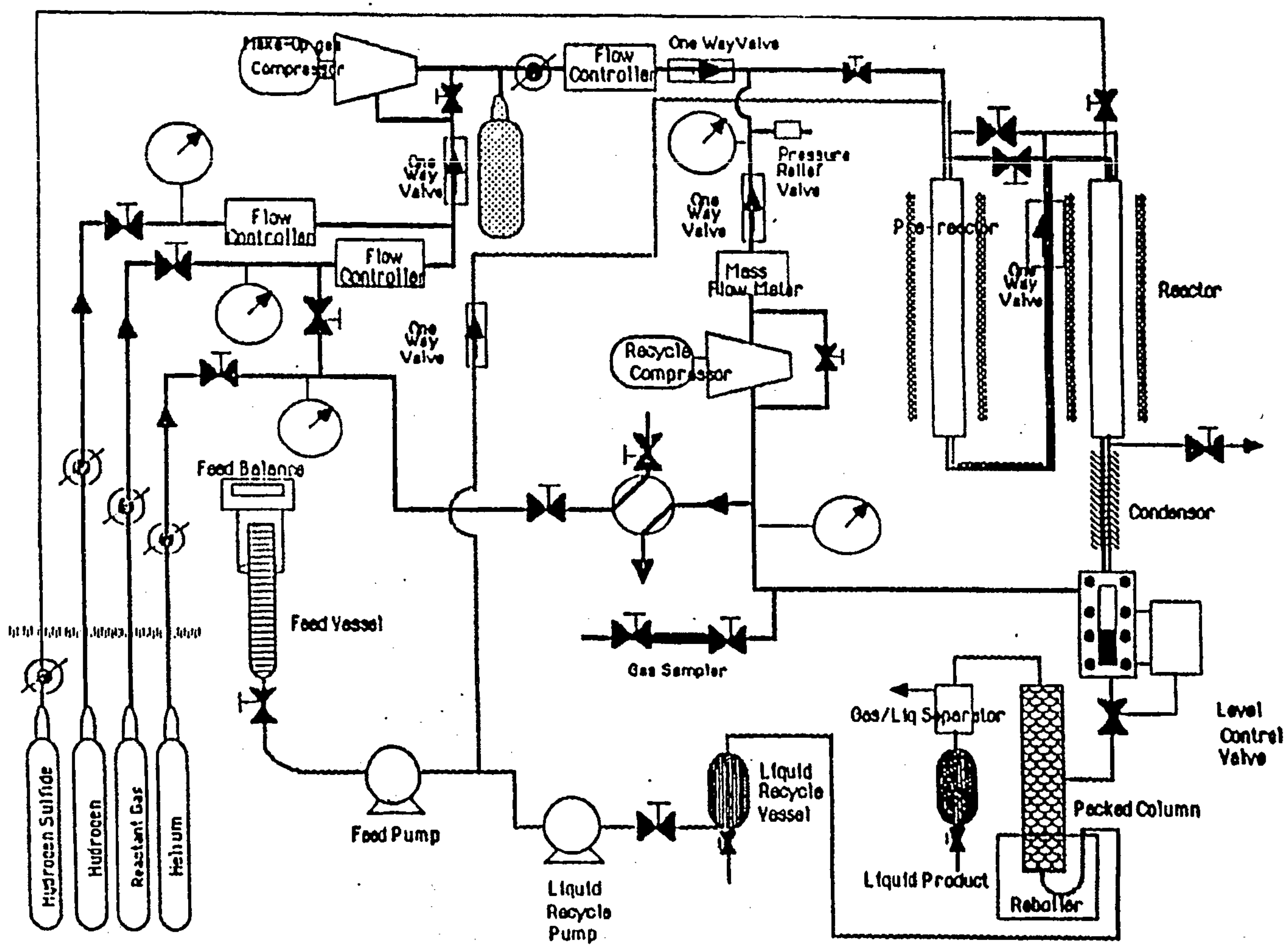


Figure 91. Schematic of Catalyst Evaluation Unit

Pressure: 0-3000 psig

Liquid Feed: 0-500 cm^3/h

LHSV: 0.1-50 h^{-1}

Gas Feed: 2-60 l/h

GHSV: 20-5000 h^{-1}

The reactor was fabricated with flanged entrance and exit regions to facilitate cleaning and catalyst loading procedures.

Temperature Controllers

The reactor furnace temperature controllers, capable of operating in both the manual and automatic control modes, can be provided by several controller manufacturers such as Love Control, Omega, and Barber-Coleman. Four Love temperature controllers were installed for the initial manual control operating phase and will be converted to automatic control mode at the appropriate time.

Pressure

High-pressure controllers (up to 3000 psig) for small-scale testing units were not commercially available. Therefore, one back-pressure regulator from Mity-Mite Inc., and two high-pressure gas solenoid valves from Atkomatic Valve Inc. coupled with capillary tubes were used to control the system pressure. A schematic of the circuit for the manual and automatic control modes for the reactor system pressure is presented in Figure 92. Helium was supplied to the control loop as the instrument gas. The pressure reading obtained from the pressure transducer is used to activate the solenoid valves depending on whether the system pressure needs to be

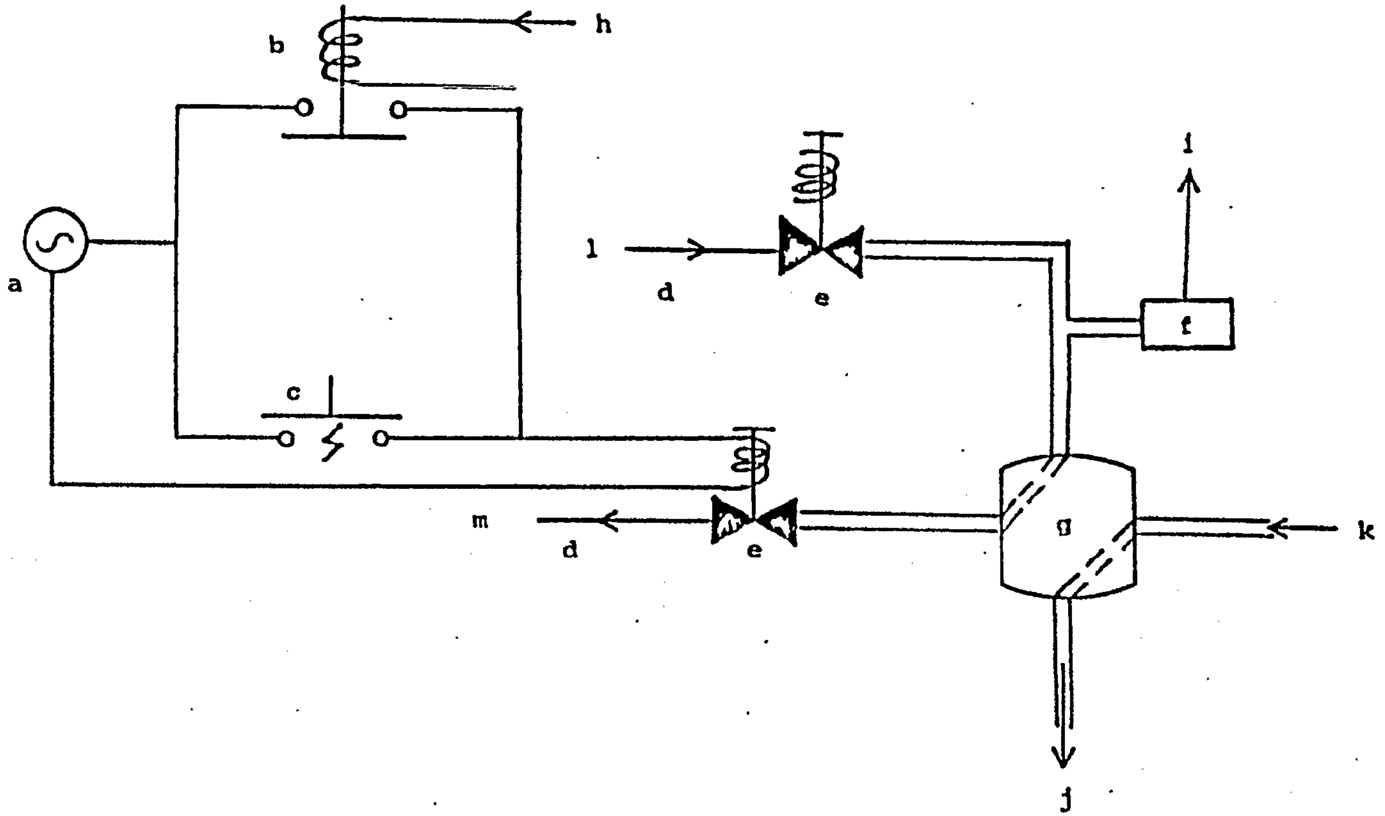


Figure 92. Design for Manual and Automatic Control Modes for the Reactor System Pressure

(a) Electrical Source; (b) Relay; (C) Push Button Switch; (d) Capillary Tube; (e) High Pressure Gas Solenoid Valve; (f) Pressure Transducer; (g) Back Pressure Regulator; (h) Signal from Microcomputer; (i) Signal into Microcomputer; (j) System Pressure; (k) System Outlet; (1) Instrument Gas Inlet; (m) Instrument Gas Outlet increased or decreased. For instance, if the pressure transducer reading is low compared to the set point pressure, the upstream solenoid valve is opened and the pressure in the control loop is increased, resulting in an increase in the system pressure. The capillary tubes were used in order to obtain a slow rate of change of pressure during pressure adjustment. The unit can be operated in both manual and automatic control modes.

Space Velocity and Mixing Ratio

Gas Feed and Mixing Ratio

The gases flowing into the reactor system (Figure 91) are controlled by Linde mass flow meters and controllers. Mixing of up to four different gases can be controlled and monitored at the same time with the manual and automatic control functions. The control range for gas flow rates is 0-3000 cm^3/min.

Liquid Feed

The liquid feed to the reactor system is supplied by the Milton Roy high pressure metering pump. The rated capacity of this pump is 1000 cm^3/hr at a pressure of 5000 psig. However, the automatic control mode is not commercially available for this pump, and a step motor from Thurst Inc. can be installed and used to control the liquid feed pump in the automatic control mode.

Gas-Liquid Separator

A gas-liquid separator, located downstream of the reactor, is used to separate the gas and liquid products into two streams. A Brooks high pressure (up to 3000 psig) site glass served as the gas-liquid separator, and it can be modified for both manual and automatic control operating modes. A high-pressure liquid solenoid valve from Atkomatic Inc. and two high-pressure liquid level sensors from FCI were utilized to achieve the liquid level control in the gas-liquid separator. The design of a high-pressure gas-liquid separator is presented in Figure 93.

Two-Stage Compressor

A two-stage compressor from PPI, Inc., was acquired to compress the low-pressure gas feed (70 psig) into the high pressure gas storage cylinder (maximum 5000 psig) (see Figure 91). The reactor system can be economically operated with this compressor whenever high gas space velocity or high pressure reaction conditions are required. The preliminary design for make-up compressor system is presented in Figure 94. The control circuit for this two-stage compressor system is presented in Figure 95.

Gas Recycle Pump

A Whitney laboratory compressor was purchased for use as a gas recycle pump whenever the recycle mode of operation is required. The rating of this pump is: a discharge pressure of 5000 psig and gas flow capacity of 10,000 cm^3/hr. The compressor can be operated in both the manual and automatic control modes.

Packed Distillation Column

The column was made from a two-foot long, two-inch I.D. stainless steel tube. The inside of both ends of the tube are threaded for pipe plugs. Two holes were drilled and threaded with 1/4 inch NPT 2 and 10 inches down from the top. Drilling through Swagelock fittings placed in

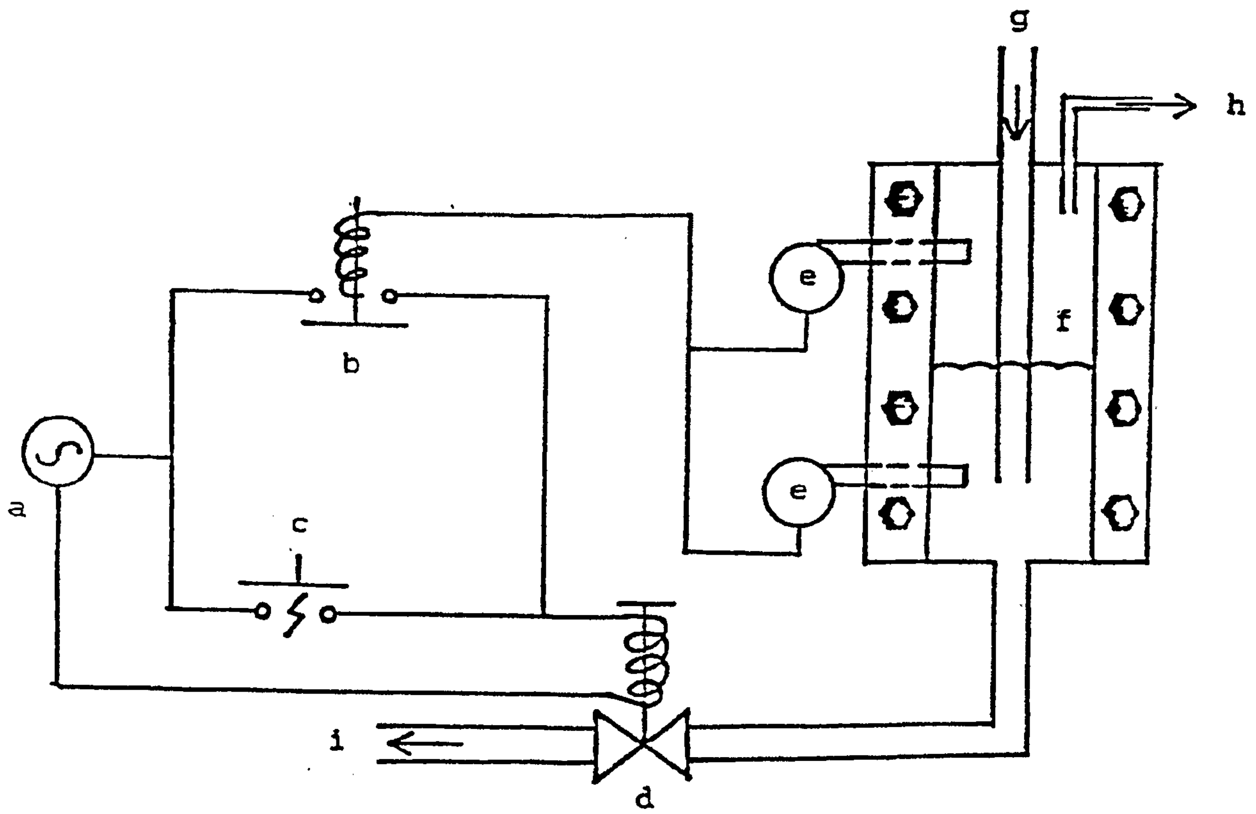


Figure 93. Design of the High Pressure Gas-Liquid Separator

(a) Electrical Source; (b) Relay; (c) Push Button Switch; (d) High Pressure Liquid Solenoid Valve; (e) High Pressure Liquid Level Sensor; (f) High Pressure Brooks Site Glass; (g) Reactor Effluent; (h) Gas Product Outlet; (i) Liquid Product Outlet

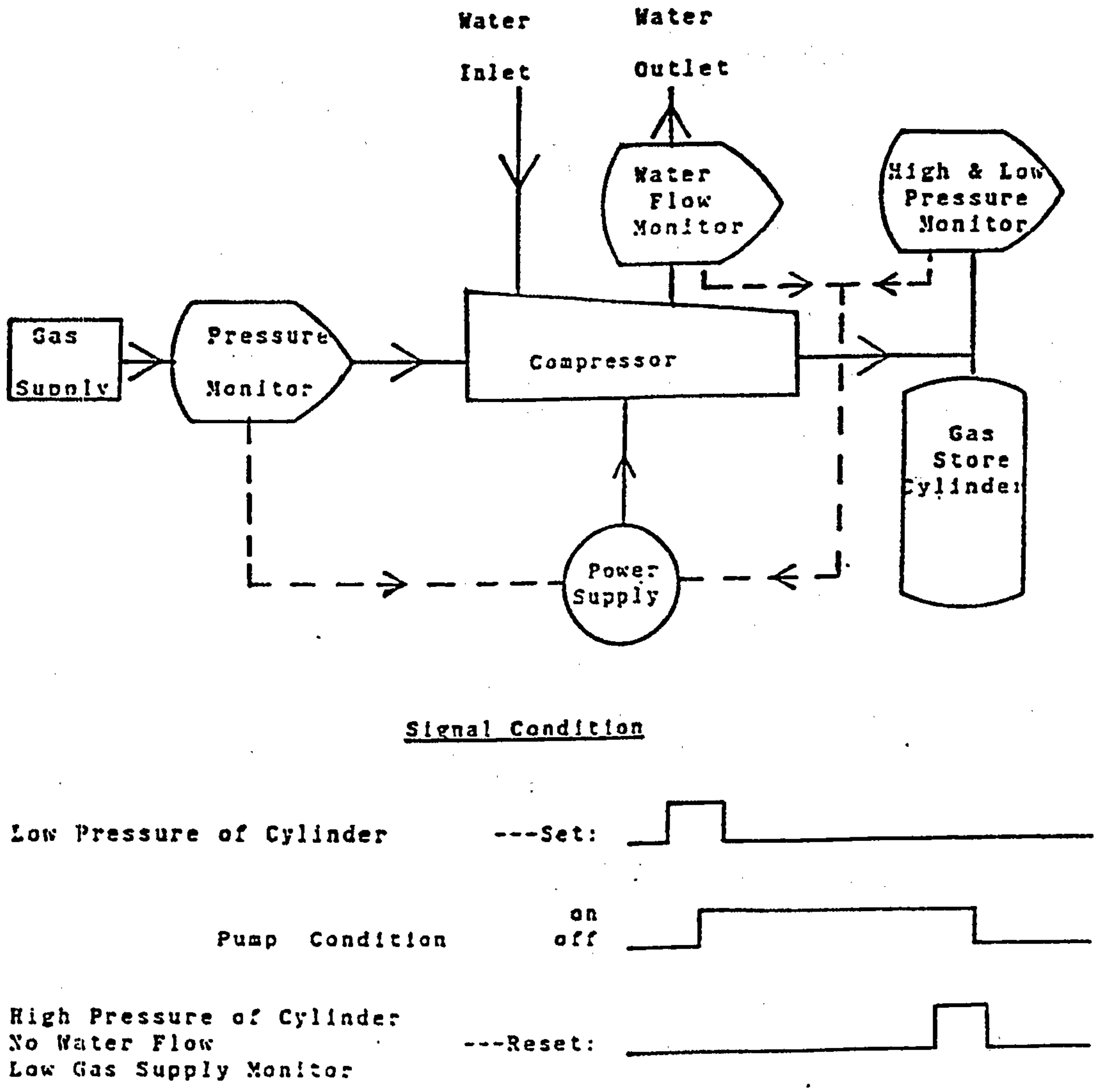
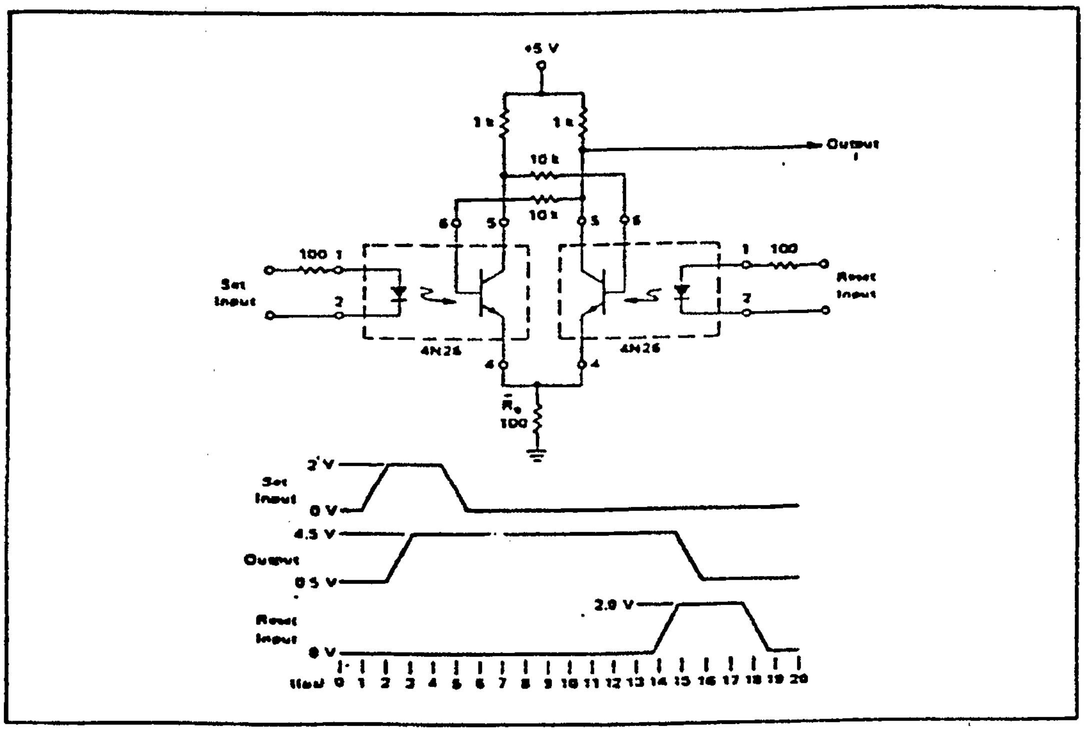


Figure 94. Two-State Feed Compressor Safety and Automatic Control Schematic



Optically Coupled R-S Flip-Flop

Figure 95. Control Circuit Design for the Two-State Feed Compressor

these taps secured the feed and recycle lines, and the pipe plugs on each end are machined to receive fittings for the vapor and liquid effluent streams. The recycle ratio is controlled by positioning a valve which allows flow back to the column. This can be adjusted, based on input from various sources throughout the system, by the computer. Temperature is controlled by two controllers, one for the reboiler and the other for the column itself. The column is heated with a single layer of heating tapes and insulation, giving a maximum operating temperature of approximately 350°C.

The packing material is stainless steel coils approximately 1/4 inch in diameter and 3/8 inch long. The reboiler section is created by a three-inch vertical rise of the exit stream. This is a 1/8 inch tube which passes under the heat tapes which surround the reboiler section of the column. A schematic of the distillation column is presented in Figure 96. The reactor system operated at the proposed specifications without significant problems.

Automation of the Reactor System

The following electronic circuit designs were completed for use in the automation of the apparatus and underwent preliminary testing:

Thermocouple Amplifier (Figure 97).

Pressure Transducer Interface (Figure 98).

Software Program (Appendix H) for Translation Technique for the Digital to Analog Converter and Analog to Digital Converter. Fourth-order polynomial equations are used to correlate the relationship between temperature and millivoltage for J-type thermocouples:

$$T(mV) = C_1 + C_2 *mV + C_3 *mV^2 + C_4 *mV^3 + C_5 *mV^4 \quad (8\text{-}1)$$

$$mV(T) = C_1 + C_2 *T + C_3 *T^2 + C_4 *T^3 + C_5 *T^4 \quad (8\text{-}2)$$

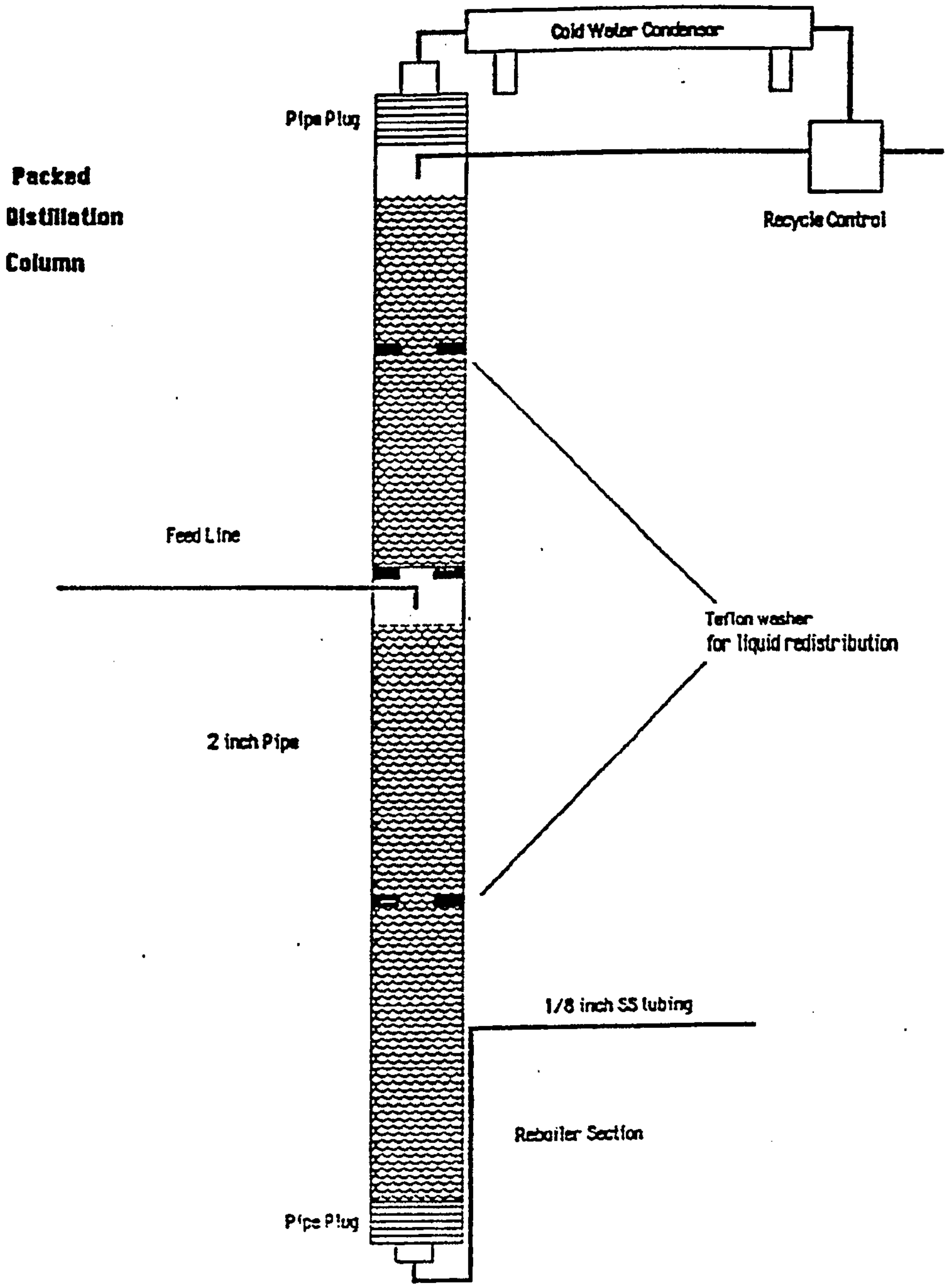


Figure 96. Packed Distillation Column

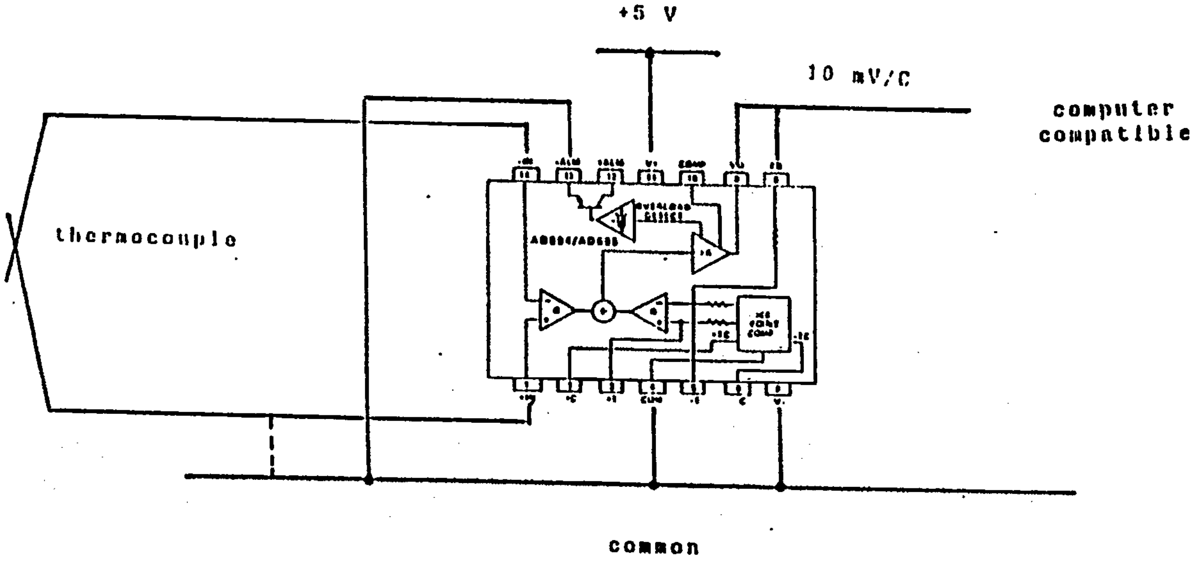


Figure 97. Thermocouple Amplifier

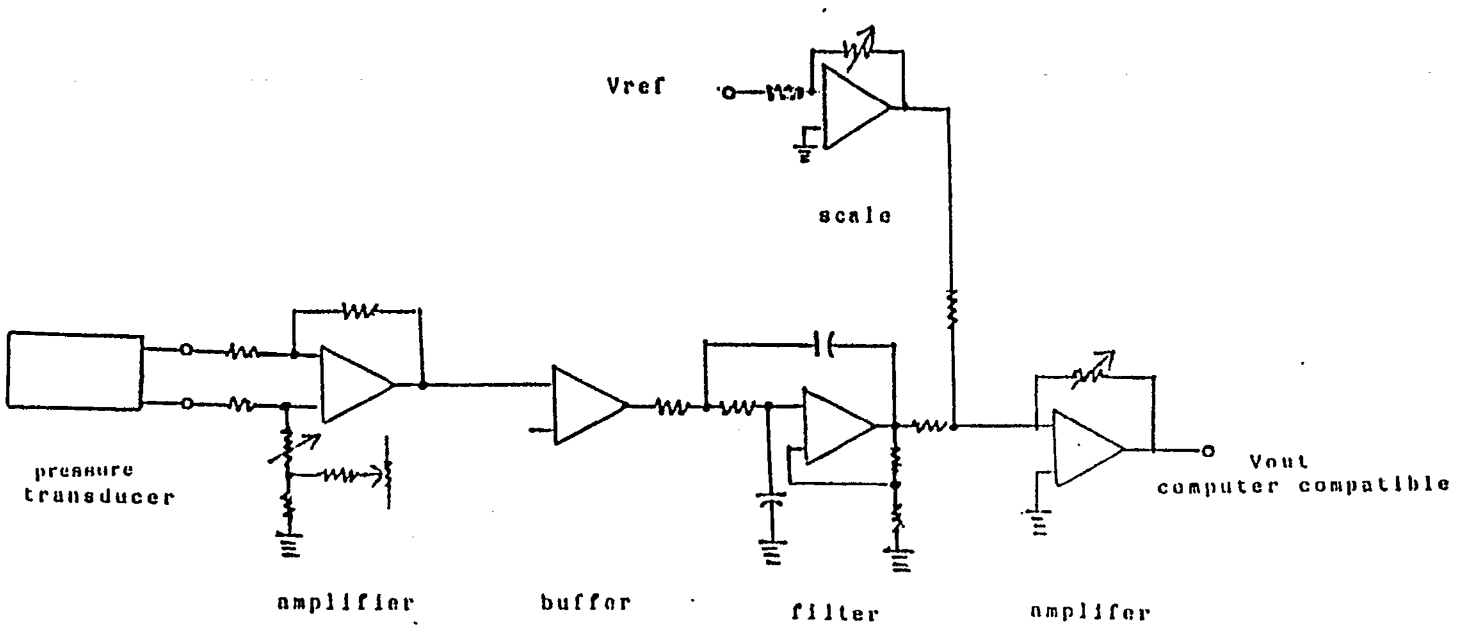


Figure 98. Pressure Transducer Interface

Equations (8-1) and (8-2) are applied to the A/D and the D/A translations, respectively. The program, named fit.c (Appendix H), for data fitting can treat the millivoltage as a function of temperature for J-type thermocouples and the temperature as a function of millivoltage for J-type thermocouples.

Section IX: LITERATURE SURVEY

Research Personnel:	
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	H. Paul Wang Graduate Student
	Kien-Ru Chen Postdoctoral Fellow
	Nabin K. Nag Assistant Research Professor
	Francis V. Hanson Associate Professor

INTRODUCTION

The literature survey to be conducted in conjunction with the high-density aviation turbine fuel research project was designed to be readily accessible to the University of Utah research team and to the personnel at the Wright Aeronautical Laboratories. A database management system based on the concept of "Information Automation" was set up on the IBM PC-AT and consisted of the following components:

1. Literature database files;
2. Data Transition: Addition, Edit, and Deletion; and
3. Data File Searching and Maintenance.

The relationship between these procedures is illustrated in Figure 99.

The database files are structured to record up to six authors, the journal reference, the volume, page numbers, year of publication, and title of the article. The field also contains eight (8) indices which permit classification and retrieval of information/key words related to each entry

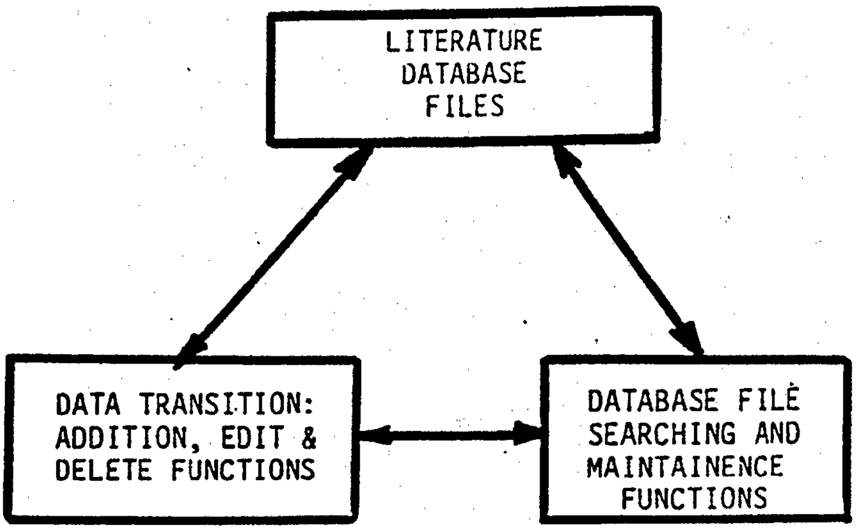

Figure 99. Relationships Between Functions for the Literature Survey Database Management System

in the database file. The search routine is capable of both single entry and multiple entry searches of the database file.

The technical subjects which were intended to be covered included the following:

1. shape selective catalysis;
2. zeolite catalyst preparation, characterization, and evaluation;
3. reactions of oxygenates over solid oxide materials;
4. supported metals catalysis;
5. preparation, characterization, and evaluation of supported metal catalysts;
6. hydrogenation of aromatic hydrocarbons and feedstocks; and
7. design concepts in catalytic reactor systems.

A printout of the database file as it had evolved at the termination of funding by the Air Force Wright Aeronautical Laboratories of the United States Air Force is included for record purposes.

Database File

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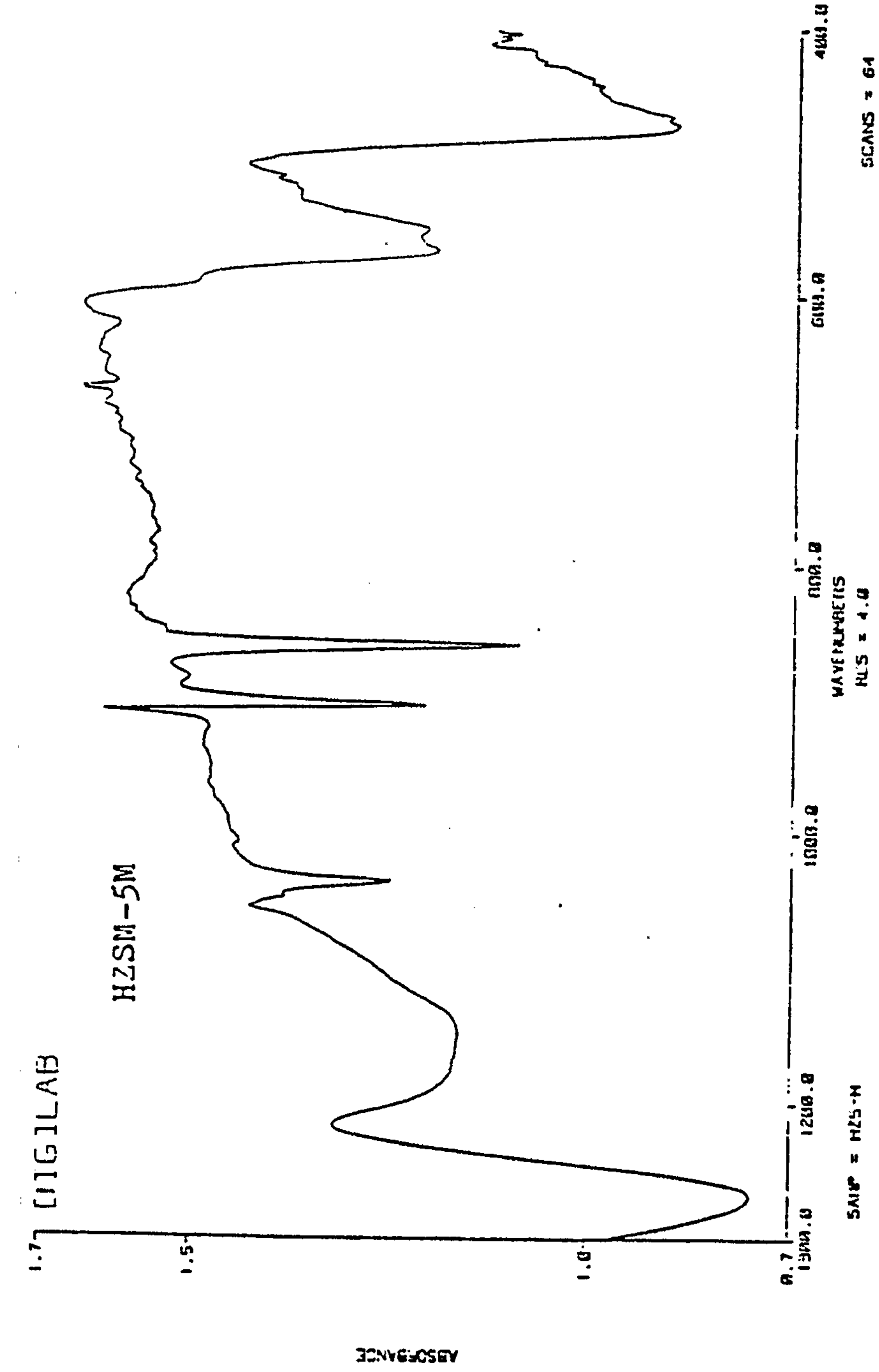
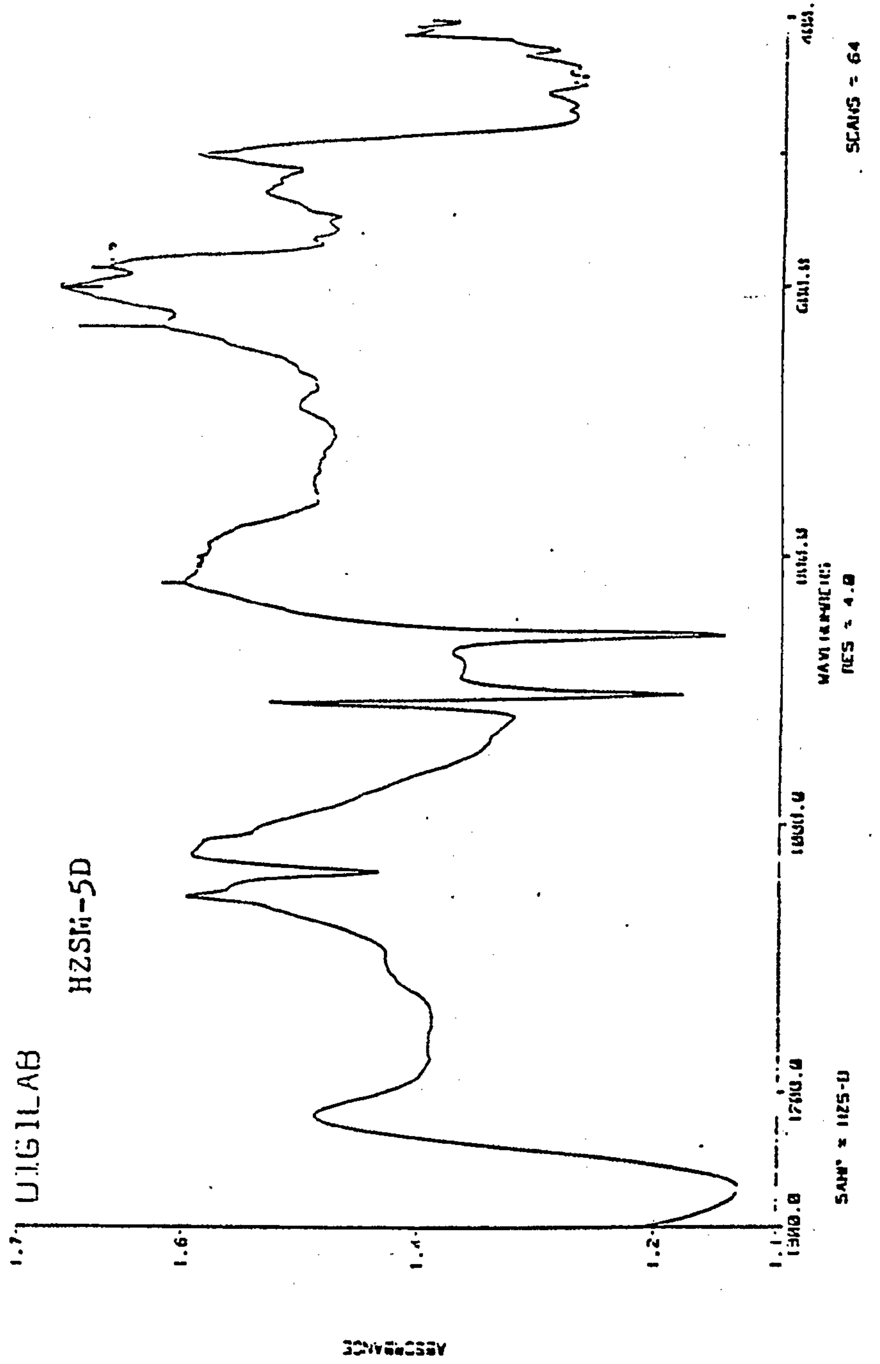
APPENDIX A

STRUCTURAL FTIR SPECTRA OF SYNTHESIZED ZEOLITES

IR spectra of synthetic zeolites were measured by the use of diffuse reflectance FTIR spectroscopy. The IR spectra in the lattice vibrational mode region are presented in this Appendix. Furthermore, a criterion (optical density ratio) for determining the structural characteristics of the zeolite frameworks was established using the data derived from these spectra.


DIGILAB
HZSM-5M
ABSORBANCE
1.7
1.5
1.0
0.7
1400.0
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
RES = 4.0
SAMP = HZS-M
SCANS = 64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HZSM-5D
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1.6
1.4
1.2
1.1
1300.0
1200.0
1000.0
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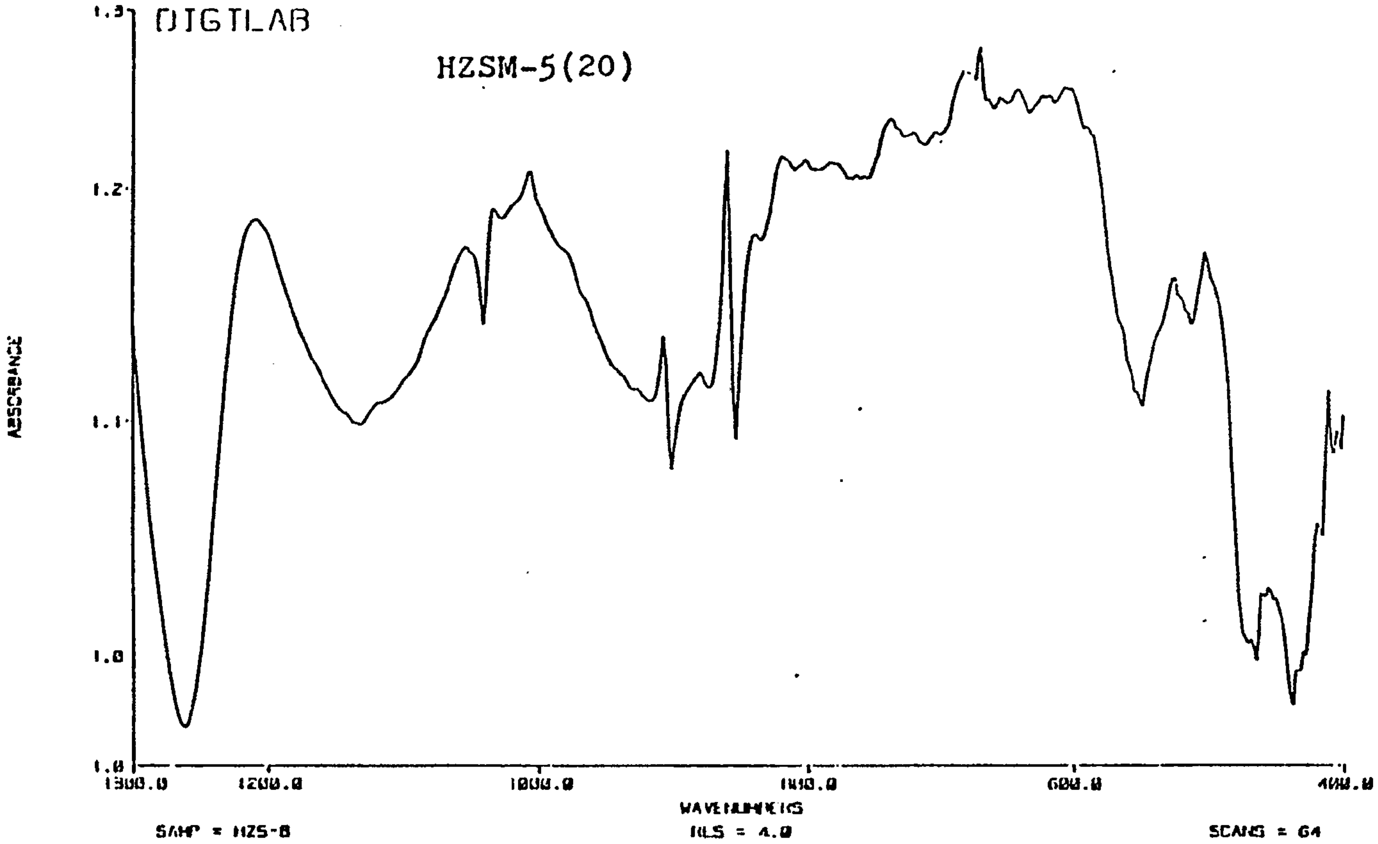
600.0
400.0
WAVENUMBERS
RES = 4.0
SCANS = 64
SAMP = HZS-D
ABSORBANCE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HZSM-5(20)
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1.2
1.1
1.0
1.0
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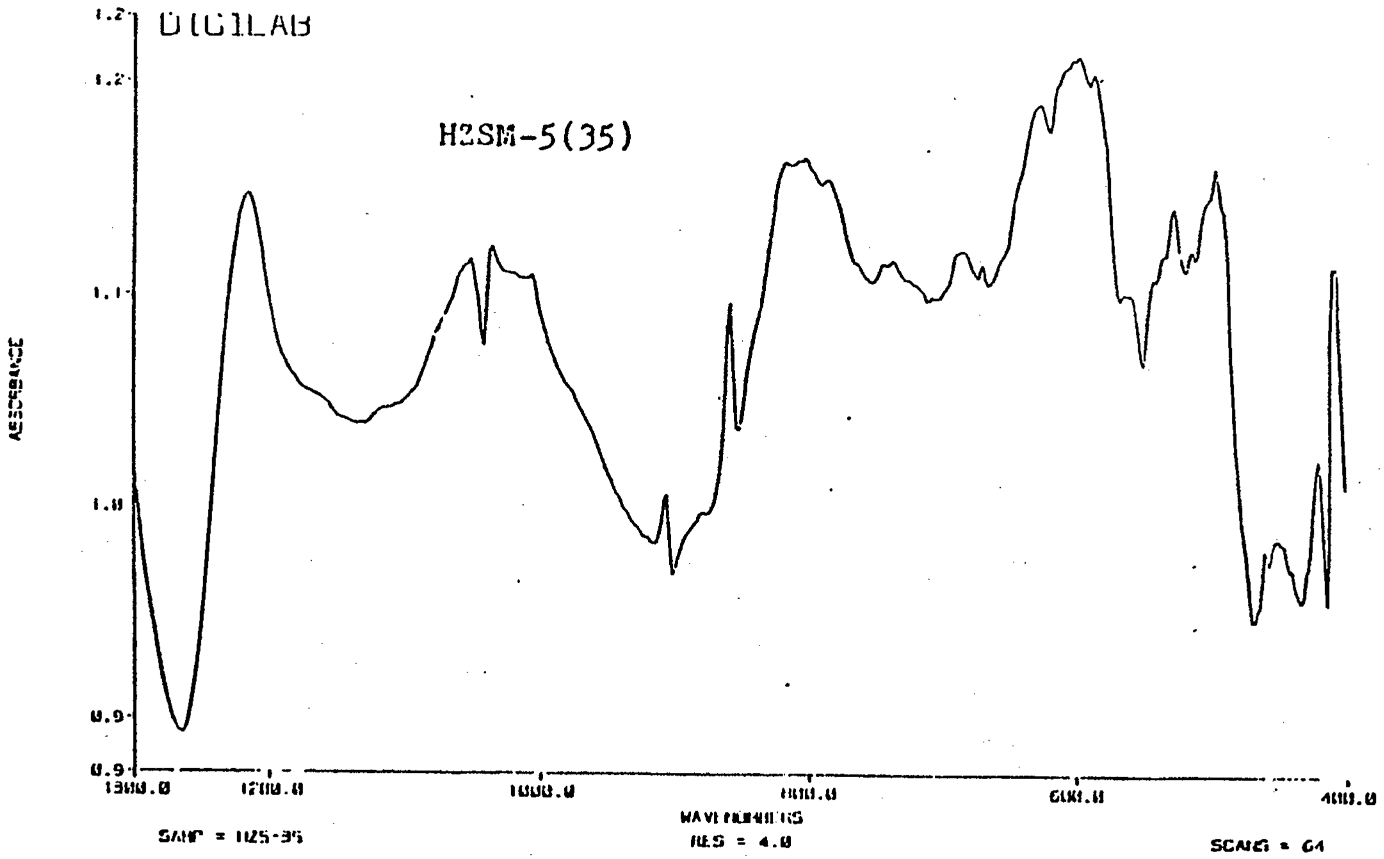
800.0
600.0
400.0
WAVENUMBERS
SAMP = HZS-8
RES = 4.0
SCANS = 64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1.2
1.1
1.0
0.9
0.9
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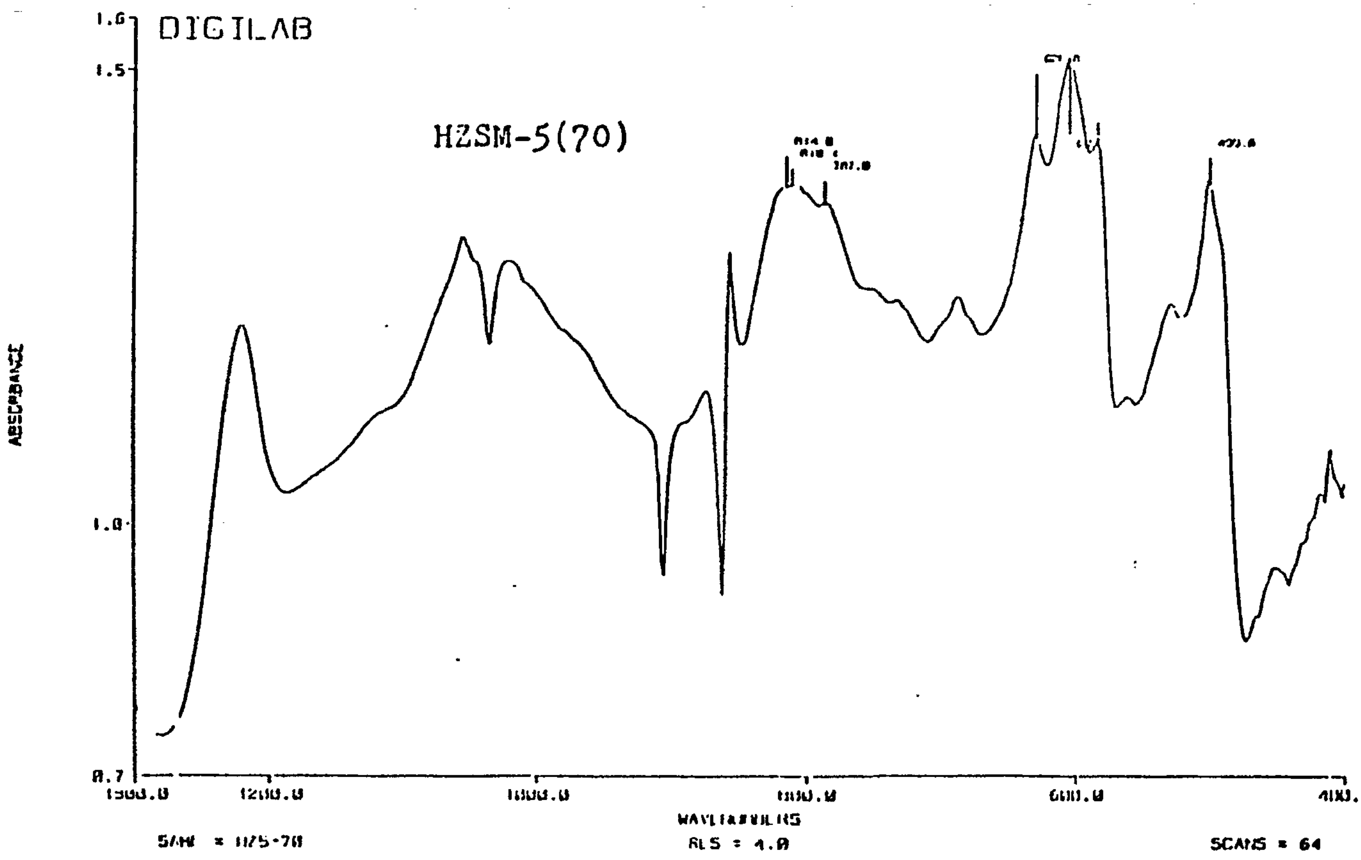
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = H25-35
RES = 4.0
SCANS = 64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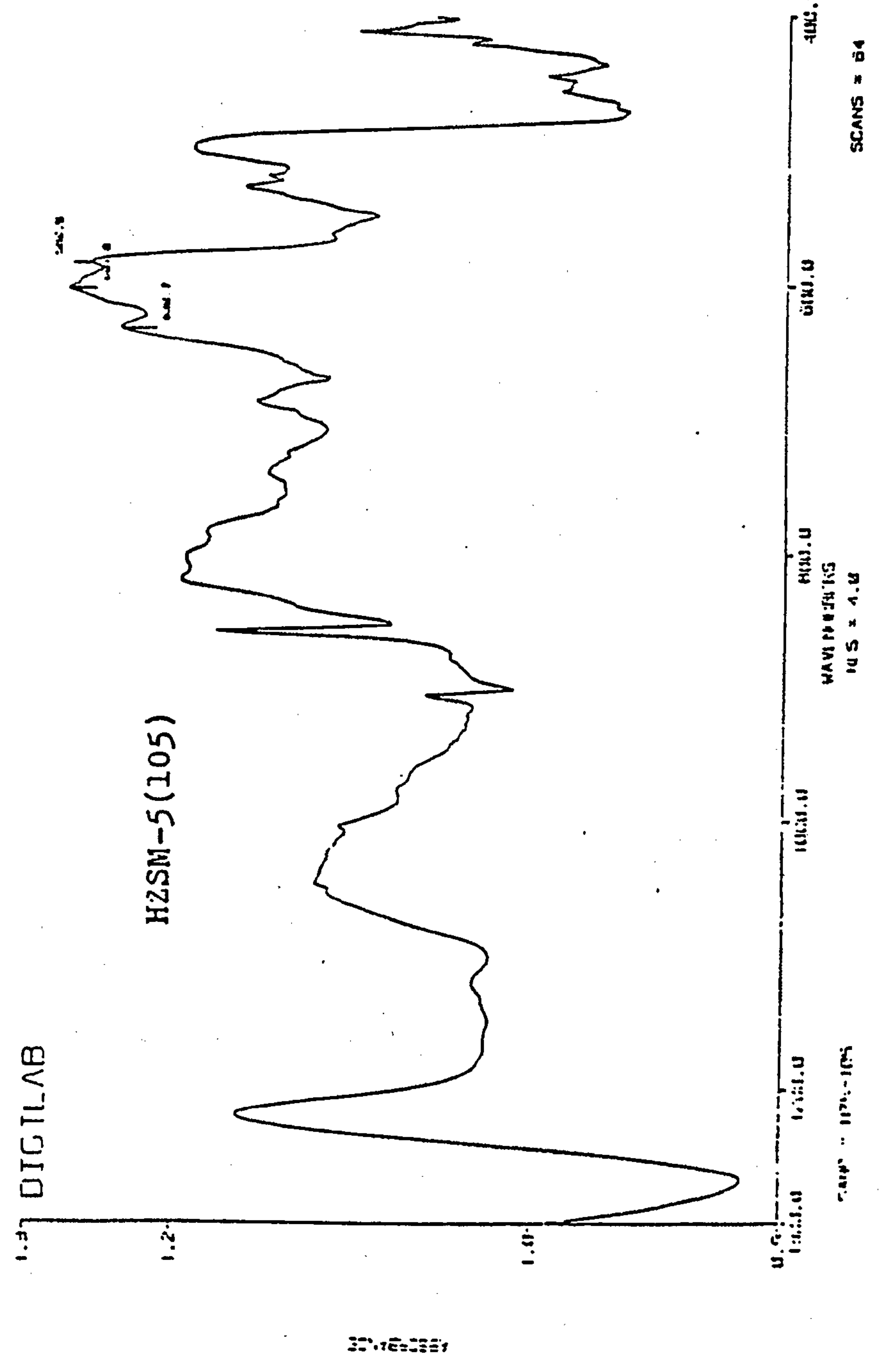
1.5
1.0
0.7
814.0
787.0
1300.0
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAM = 1125-78
RES = 4.0
SCANS = 64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HZSM-5(105)
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1.2
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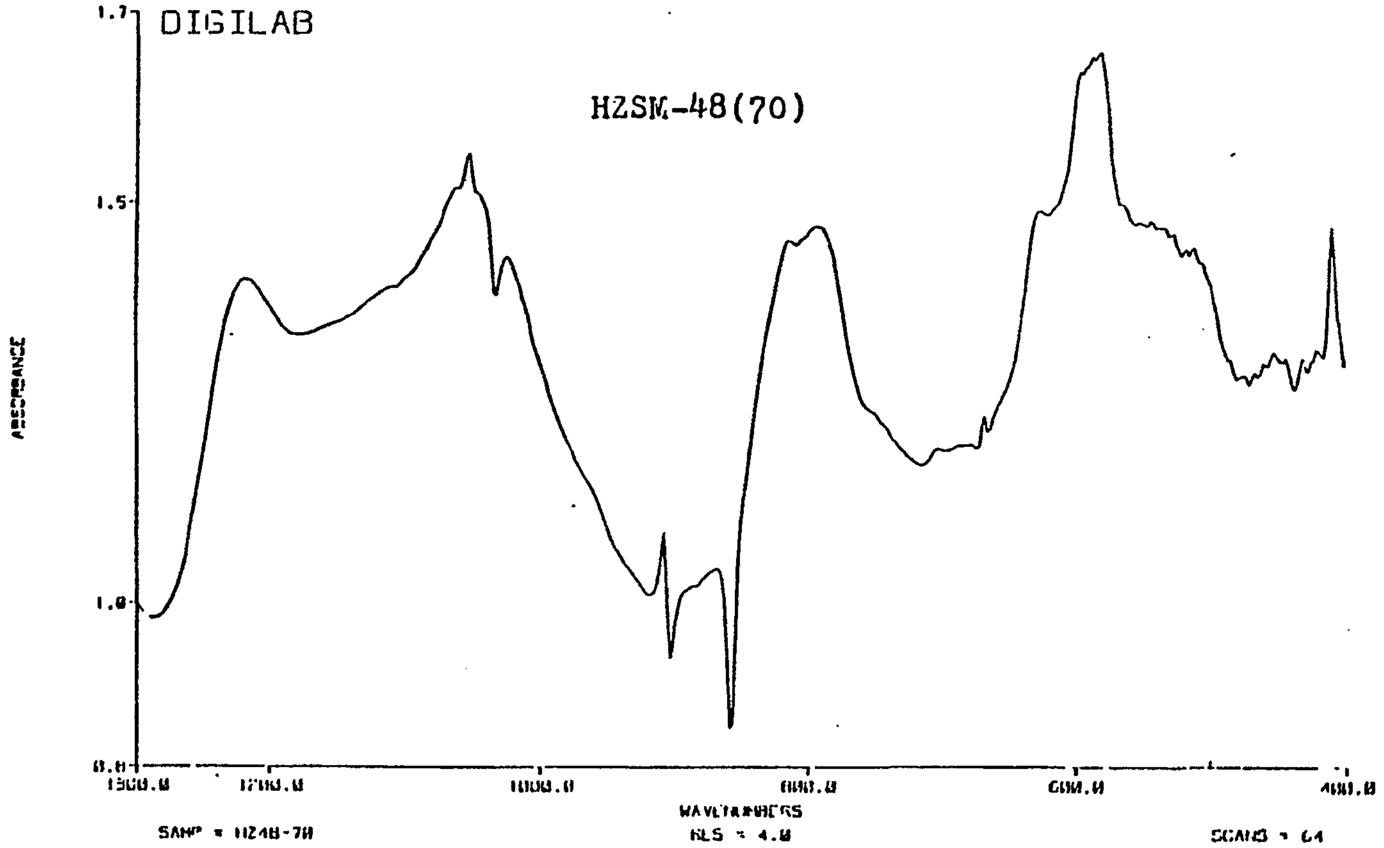
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
RES = 4.0
SCANS = 64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HZSM-48(70)
ABSORBANCE
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1.5
1.0
0.8
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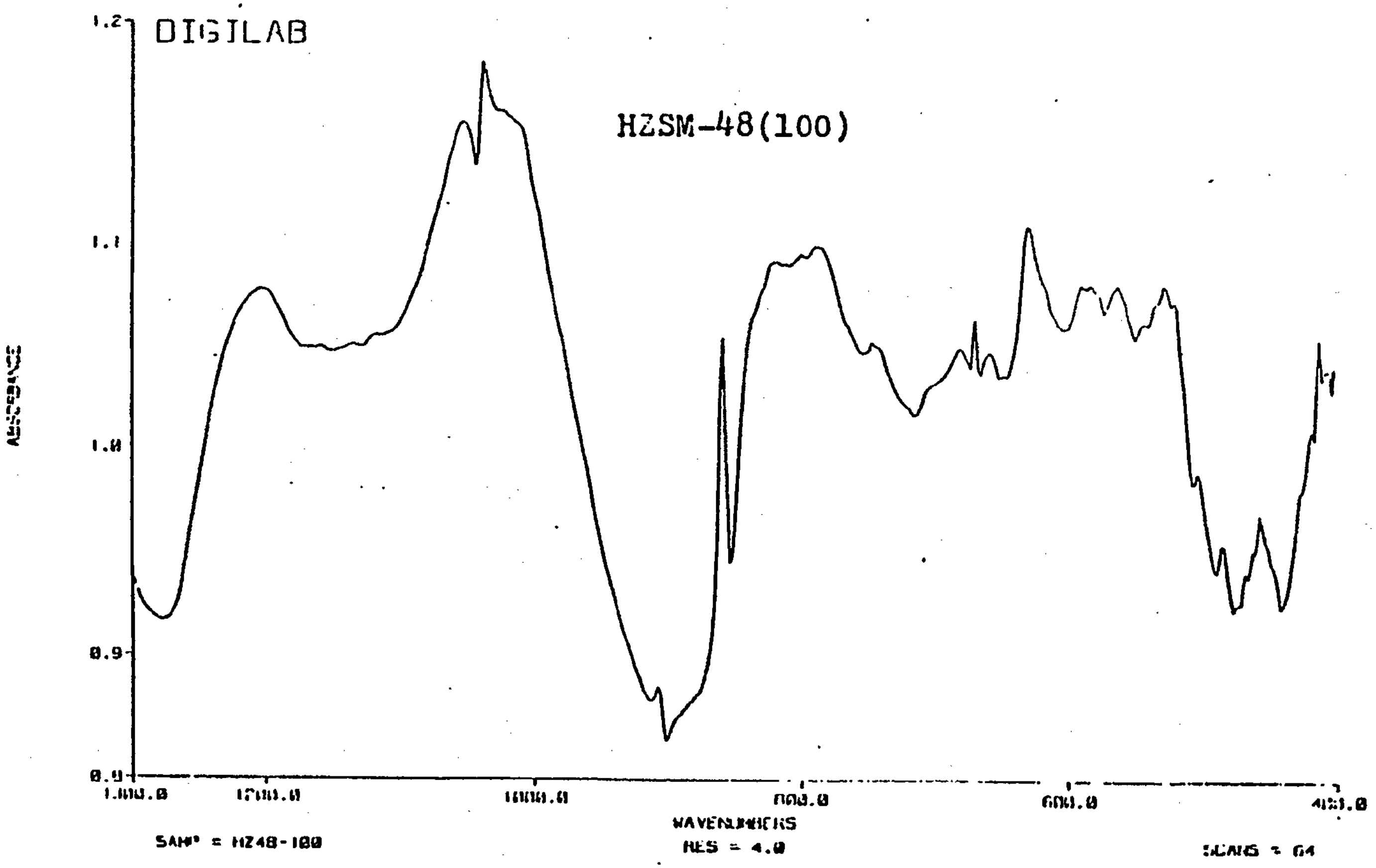
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = HZ48-70
RES = 4.0
SCANS = 64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HZSM-48(100)
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1.1
1.0
0.9
0.8
ABSORBANCE
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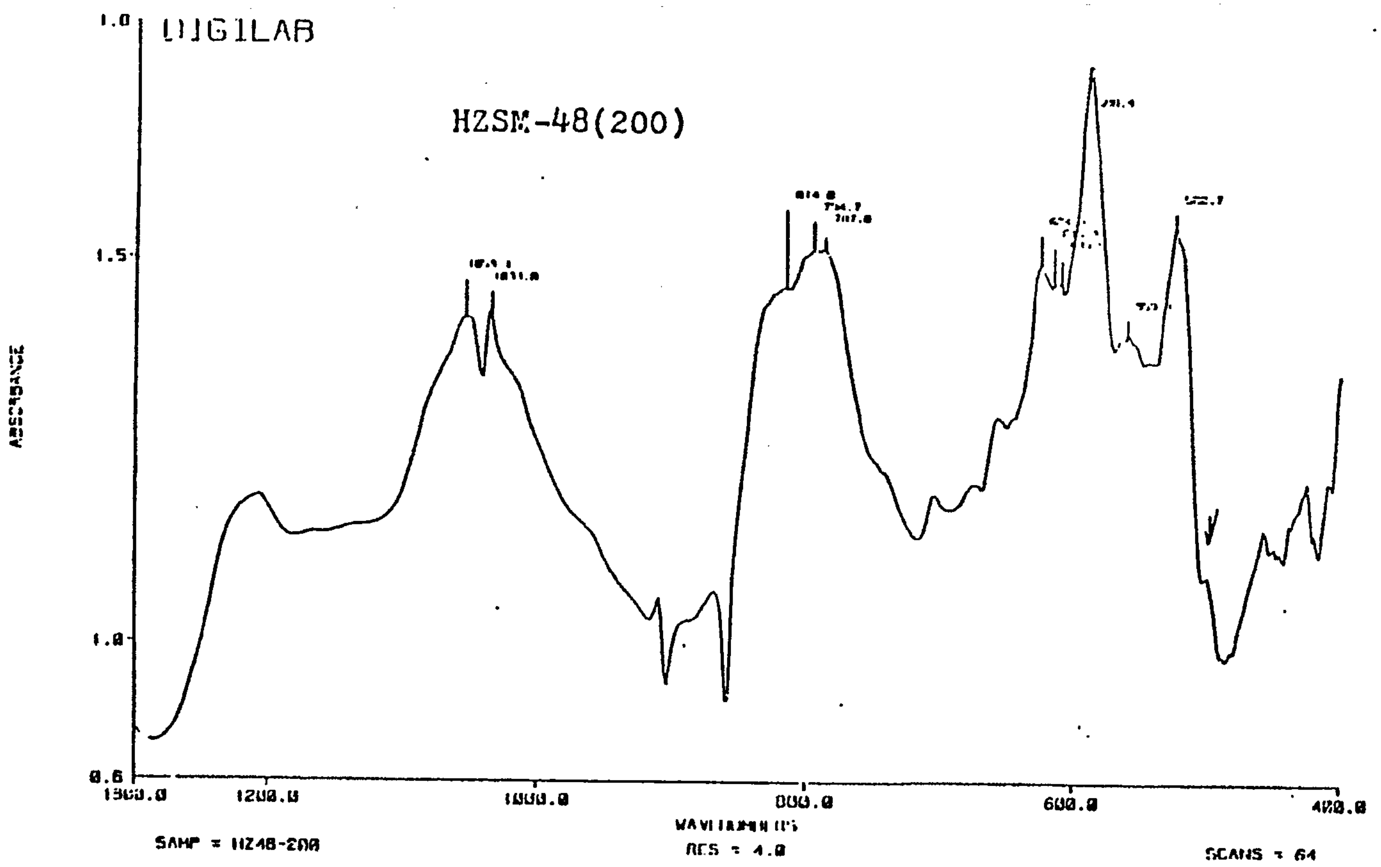
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = HZ48-100
RES = 4.0
SCANS = 64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HZSM-48(200)
ABSORBANCE
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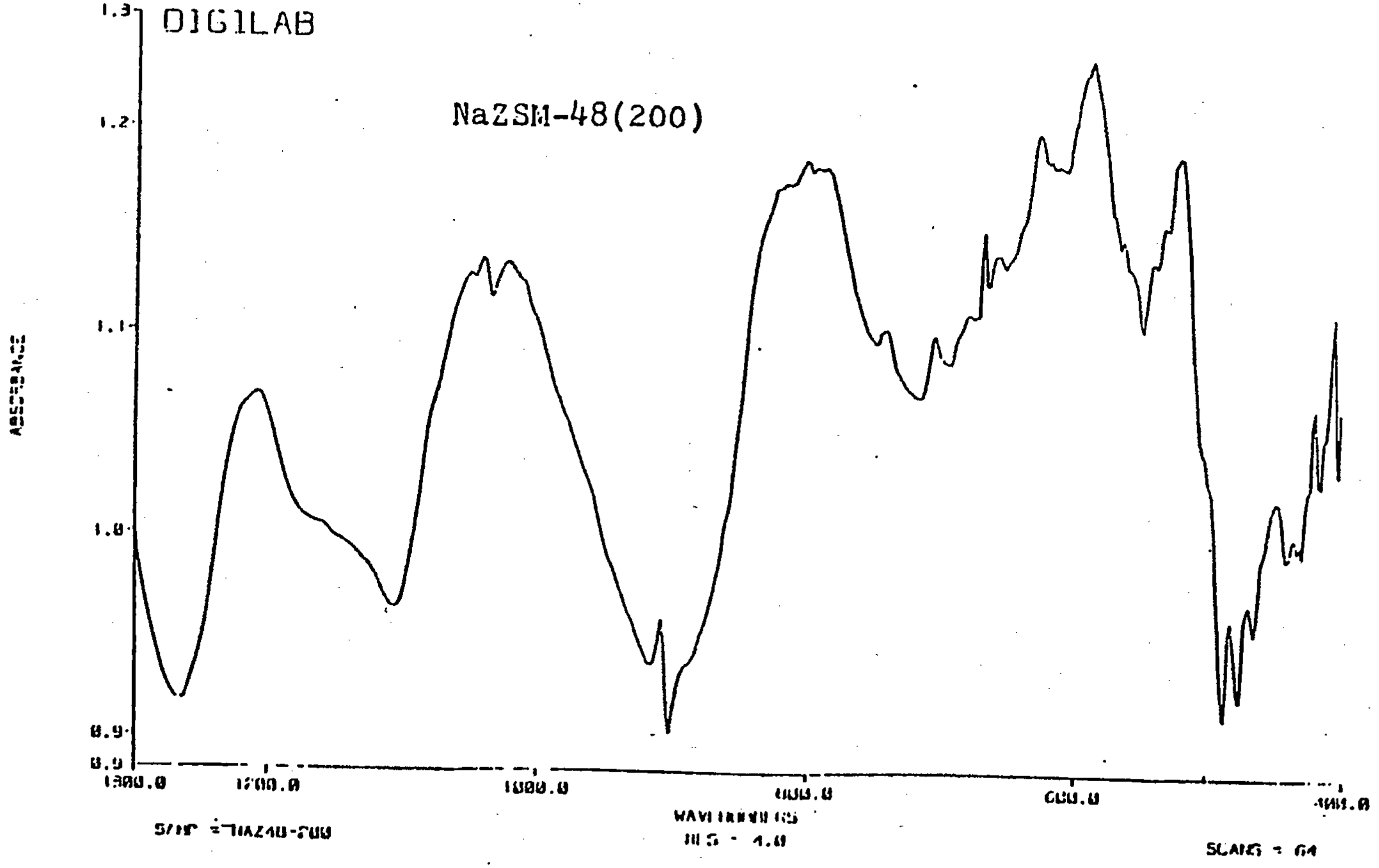
1.0
0.6
1300.0
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
814.0
522.7
SAMP = HZ48-200
RES = 4.0
SCANS = 64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0.9
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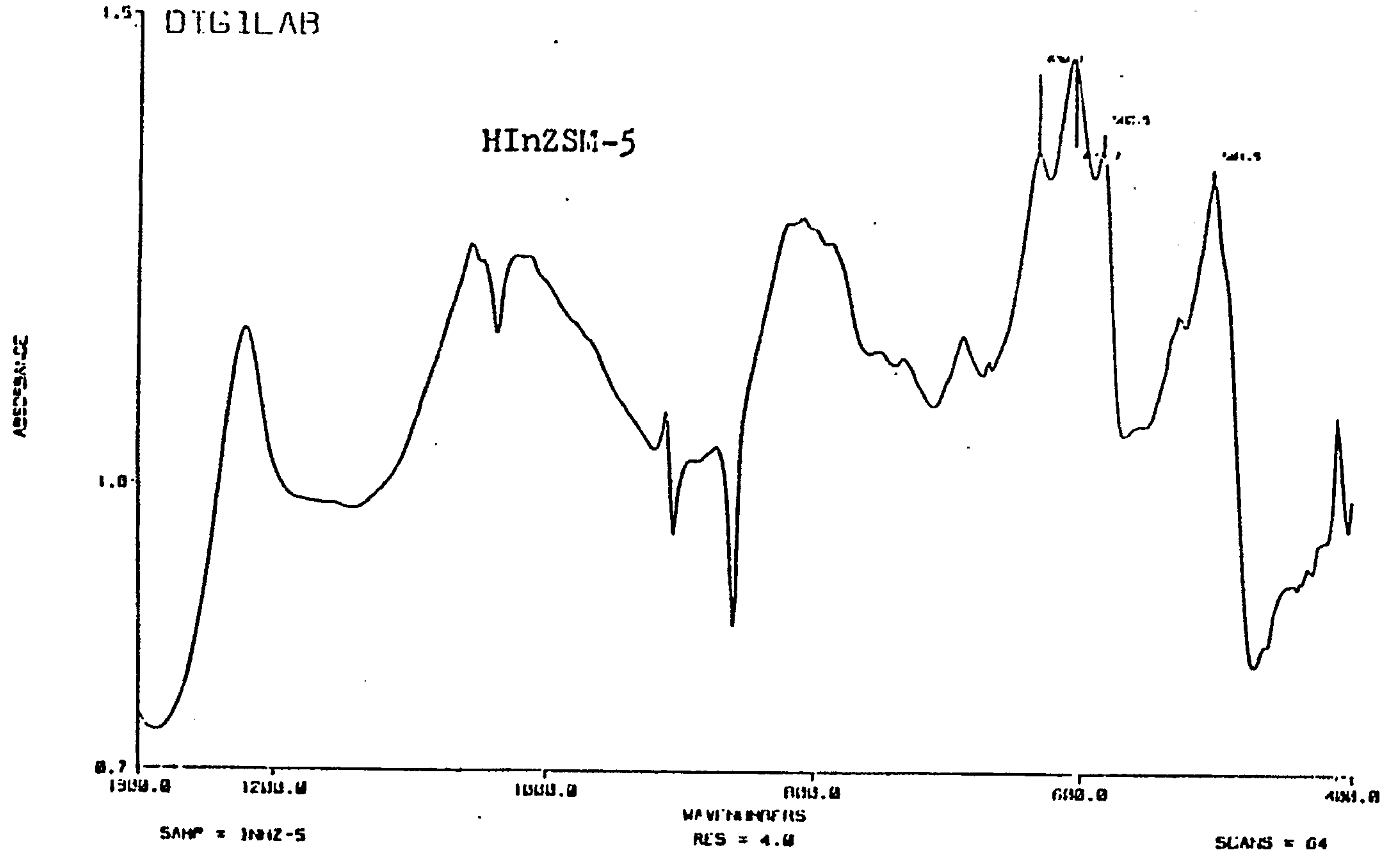
1000.0
800.0
600.0
400.0
WAVENUMBERS
RES = 4.0
SAMP = NAZ48-200
SCANS = 64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HInZSM-5
ABSORBANCE
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1.0
0.7
1300.0
1200.0
1000.0
800.0
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400.0
WAVENUMBERS
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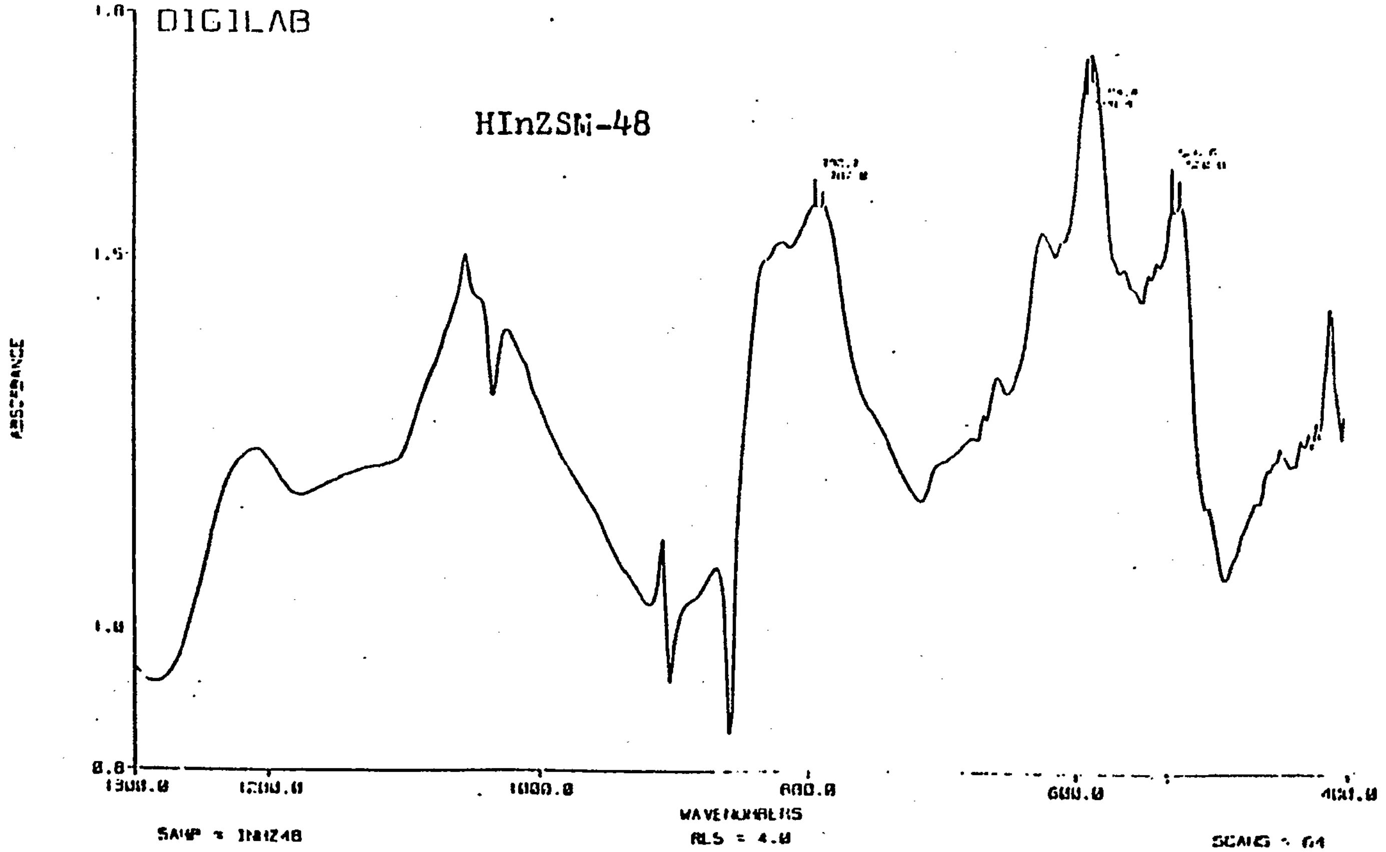
RES = 4.0
SCANS = 64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HInZSM-48
ABSORBANCE
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1.0
0.8
1300.0
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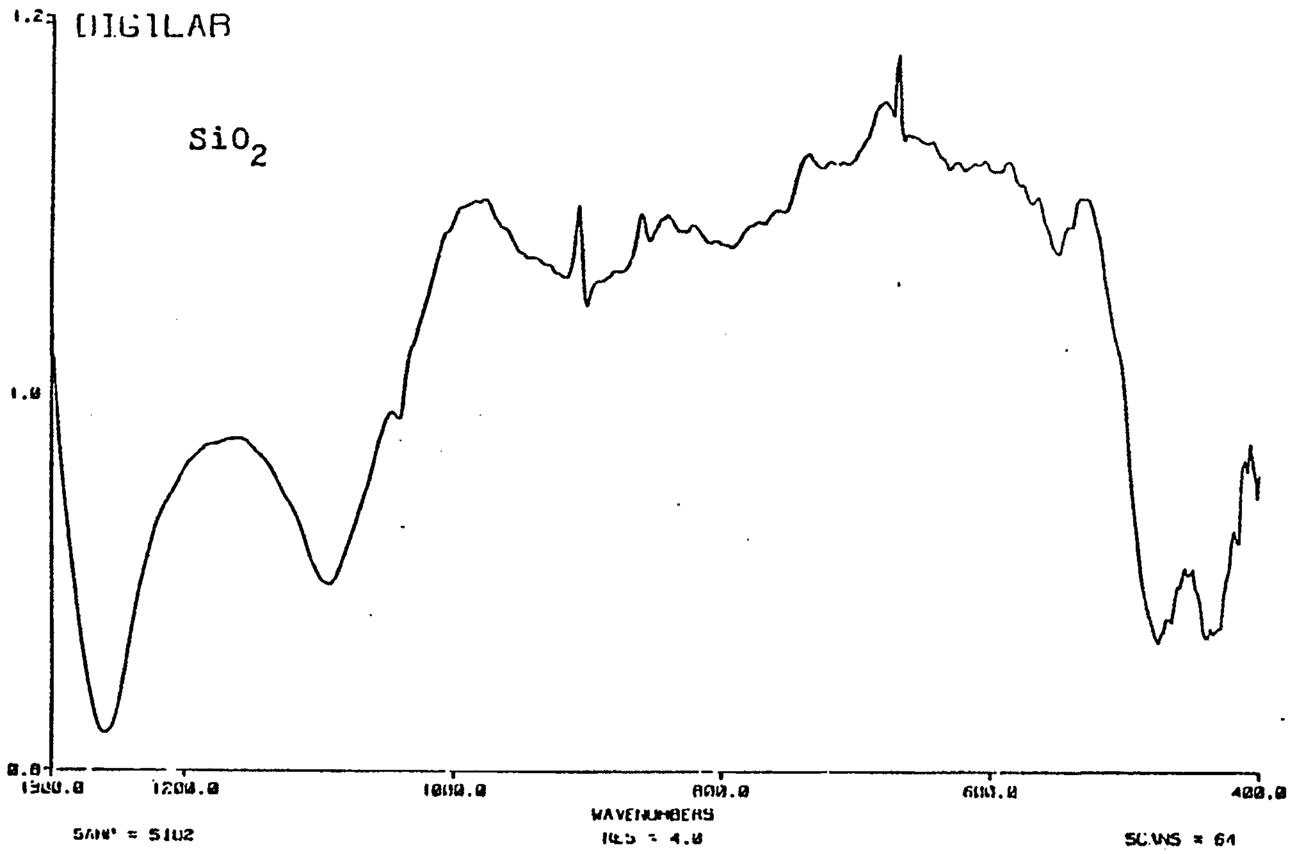
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = INHZ48
RES = 4.0
SCANS = 64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SiO_2
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1.0
0.8
ABSORBANCE
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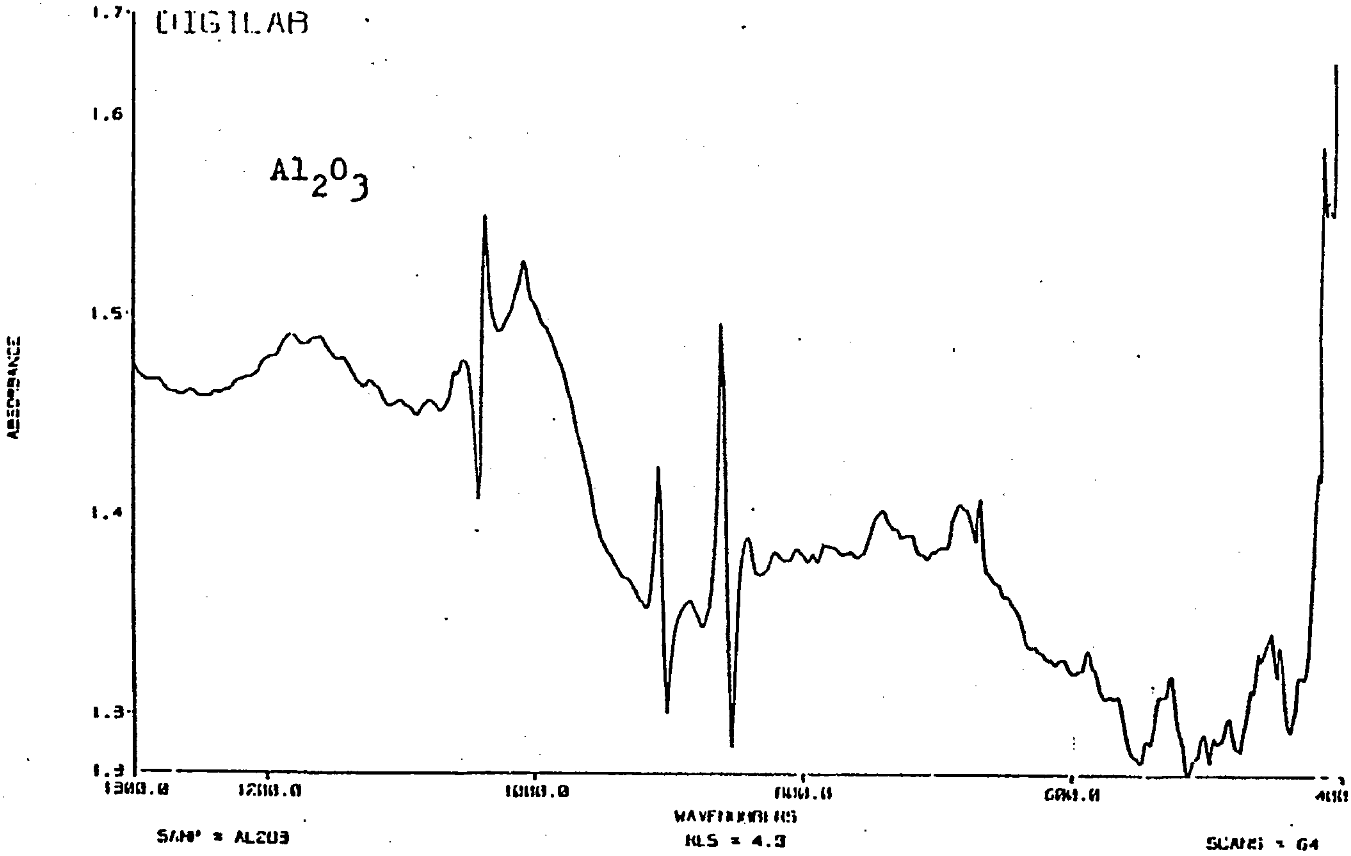
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = SIO2
RES = 4.0
SCANS = 64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Al_2O_3
ABSORBANCE
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1.6
1.5
1.4
1.3
1.3
1300.0
1200.0
1000.0
800.0
600.0
400.0
WAVENUMBERS
SAMP = AL2O3
RES = 4.0
SCANS = 64

APPENDIX B

PRODUCT DISTRIBUTION FOR NORMAL-HEXANE CRACKING OVER SYNTHESIZED ZEOLITES

Cracking of normal-hexane over synthesized zeolites was studied using a fixed-bed continuous flow microreactor operating at atmospheric pressure. Normal-hexane was transported into the reactor from a saturator by means of the helium carrier gas. Product distributions were recorded after ten minutes on stream.

The objective of these experiments was to determine the acidity of the synthesized zeolites. The product distribution obtained with the catalysts used in this study is presented in Table 32.

Table 32

Normal-hexane Cracking over Synthesized Zeolites

	Amorphous SiO_2 Al_2O_3	ZSM-5	ZSM-48	ZSM-48/5
SiO_2/Al_2O_3	-4	70	200	70
Reaction Temp., K	805	481	627	585
Conversion	0.12	0.12	0.17	0.17
Product Distribution, wt%				
$C_1 + C_2$	2.1	1.7	1.4	0.7
C_3	7.7	2.8	6.4	4.0
C_4	2.2	4.5	6.3	7.6
C_5	0.3	3.1	2.6	4.7

APPENDIX C

PRODUCT DISTRIBUTION FOR ALCOHOL REACTIONS OVER SYNTHESIZED ZEOLITES

The reaction of alcohols was studied using a fixed-bed continuous flow microreactor operating at atmospheric pressure. Alcohols were transported into the reactor from a saturator by means of the helium carrier gas. Product distributions were recorded after 40 minutes on stream.

The objective of these experiments was to determine the effect of acidity on the selectivity and activity and to determine the influence of channel structure on selectivity.

Alcohols/He/HZSM-5(35), Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
$C_1 + C_2$	8.9	11.5	9.0	11.4
C_3	21.3	23.1	27.6	29.5
C_4	29.7	29.3	29.4	24.9
C_5	10.2	6.9	5.5	3.5
C_6	8.1	4.7	3.8	3.9
C_7^+ Aliphatics	11.4	9.5	9.1	5.6
A_6	1.4	2.1	2.3	1.8
A_7	4.9	5.9	6.4	4.8
A_8	10.0	8.5	7.9	7.7
A_9^+	0.8	1.2	0.6	1.1

Alcohols/He/HZSM-5(70), Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
$C_1 + C_2$	11.1	27.8	10.4	15.2
C_3	22.1	22.2	31.3	34.0
C_4	29.7	25.9	31.5	29.6
C_5	12.7	9.6	8.5	6.5
C_6	6.3	2.8	4.1	2.1
C_7^+ Aliphatics	4.1	4.3	3.3	2.0
A_6	1.1	1.0	1.4	1.6
A_7	5.5	3.2	5.2	5.5
A_8	6.8	2.8	4.1	3.3
A_9^+	0.6	0.4	0.2	0.2

Alcohols/He/HZSM-5(105), Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
C_1 + C_2	12.0	40.0	8.1	-
C_3	22.3	20.0	35.8	-
C_4	27.1	18.5	29.0	-
C_5	8.3	2.8	3.8	-
C_6	8.6	6.1	6.3	-
C_7^+ Aliphatics	4.9	2.7	3.4	-
A_6	1.1	1.0	1.5	-
A_7	4.6	2.6	4.6	-
A_8	9.8	4.9	6.2	-
A_9^+	1.3	1.5	1.2	-

Alcohols/He/HZSM-5D, Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
C_1 + C_2	9.9	17.8	10.4	13.6
C_3	22.1	23.1	29.8	27.8
C_4	29.7	26.4	28.7	18.4
C_5	9.9	6.0	5.0	2.4
C_6	7.4	5.2	4.6	8.4
C_7^+ Aliphatics	3.6	3.2	2.4	0.7
A_6	1.2	1.9	2.4	6.1
A_7	5.8	7.1	8.8	13.8
A_8	9.6	8.1	7.4	8.6
A_9^+	0.8	1.2	0.5	0.2

Alcohols/He/HZSM-48(70), Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
C_1 + C_2	18.2	70.5	8.0	-
C_3	23.8	11.9	34.3	-
C_4	24.2	6.5	31.0	-
C_5	8.3	0.9	5.0	-
C_6	7.6	1.9	5.4	-
C_7^+ Aliphatics	2.9	0.7	1.9	-
A_6	0.8	0.1	1.4	-
A_7	4.8	2.1	6.6	-
A_8	8.7	4.6	5.9	-
A_9^+	0.7	0.9	0.0	-

Alcohols/He/HZSM-48(200), Temperature = 643 K

	Product Distribution, wt.%			
	Reactant			
	CH_3OH	C_2H_5OH	C_3H_7OH	C_4H_9OH
C_1 + C_2	14.4	75.7	2.7	3.6
C_3	23.7	12.3	52.1	29.8
C_4	26.4	5.2	28.2	42.1
C_5	9.4	0.8	2.4	4.7
C_6	13.1	1.9	6.6	11.1
C_7^+ Aliphatics	6.4	0.7	3.3	3.5
A_6	0.9	0.4	0.9	1.6
A_7	1.2	0.9	0.9	1.3
A_8	3.8	2.1	1.9	1.7
A_9^+	0.7	0.0	0.0	0.6

Methanol/He/HZSM-5(70)

	Product Distribution, wt.%			
	Reaction Temperature, K			
	594	648	710	752
$C_1 + C_2$	23.3	15.4	21.7	33.6
C_3	17.5	27.6	34.1	34.3
C_4	0.0	17.8	16.0	11.2
C_5	23.0	15.2	9.4	4.2
C_6^+ Aliphatics	32.6	13.0	6.2	2.3
A_6	0.6	1.1	1.6	1.4
A_7	0.9	4.3	4.8	4.7
A_8	1.8	5.0	5.7	7.6
A_9^+	0.3	0.6	0.5	0.7

Methanol/He/HZSM-48(200)

	Product Distribution, wt.%			
	Reaction Temperature, K			
	597	648	710	759
$C_1 + C_2$	17.9	16.9	19.6	34.5
C_3	31.8	36.1	50.3	44.1
C_4	0.0	8.2	4.1	0.0
C_5	14.1	9.8	0.5	1.8
C_6^+ Aliphatics	33.7	23.7	18.6	7.9
A_6	1.4	0.9	1.0	1.1
A_7	0.5	1.2	1.5	2.5
A_8	0.6	3.1	4.2	7.6
A_9^+	0.0	0.1	0.2	0.5
Conversion, wt.%	87.0	95.0	95.2	96.0

Methanol/H_2/HZSM-5(70)

	Product Distribution, wt.%			
	Reaction Temperature, K			
	597	648	710	762
$C_1 + C_2$	21.5	15.6	27.1	37.8
C_3	22.4	36.9	46.2	43.8
C_4	0.0	0.0	0.1	0.1
C_5	23.8	21.1	10.8	5.0
C_6^+ Aliphatics	29.6	16.1	4.0	1.3
A_6	0.0	1.3	1.5	1.6
A_7	1.5	4.6	5.0	5.0
A_8	1.1	3.8	5.1	5.2
A_9^+	0.1	0.6	0.2	0.2

Methanol/H_2/HZSM-48(200)

	Product Distribution, wt.%			
	Reaction Temperature, K			
	598	649	711	769
$C_1 + C_2$	19.2	19.7	20.9	29.5
C_3	30.2	34.3	40.3	39.9
C_4	0.0	18.1	20.2	15.7
C_5	21.6	11.2	8.3	4.4
C_6^+ Aliphatics	26.7	14.2	7.2	4.3
A_6	1.4	0.0	0.8	1.1
A_7	0.4	0.9	0.9	2.3
A_8	0.4	1.5	1.4	2.8
A_9^+	0.0	0.1	0.0	0.0

APPENDIX D

INTERPOLATION OF CAPSULE CALIBRATION AND CHEMISORPTION ISOTHERM COMPUTER PROGRAM

It was convenient to calculate the isotherms on the computer whenever a large number of adsorption isotherms were determined for a single catalyst. However, the use of the computer required interpolation of the precision pressure gage capsule calibration data in a form readily usable in the program.

Interpolation of Capsule Calibration Data

The pressure was calculated using the following equations. For angles of rotation in the range

$$0 < \text{Deg} < 1$$

the pressure was calculated from the following expression

$$\text{Pressure} = \text{B1L} * \text{Deg} \qquad \text{(D-1)}$$

where B1L is the tube constant in Torr deg^{-1} supplied by Texas Instruments, Incorporated, for the pressure range 0 to 40 Torr. For angles of rotation in the range

$$1 < \text{Deg} < 999.9$$

the pressure was calculated from the following expression

$$\text{Pressure} = \text{C} + \text{B1} * \text{Deg} + \text{B2} * (\text{Deg})^2 \qquad \text{(D-2)}$$

where C, B1, and B2 are constants. The calibration data supplied by Texas Instruments, Incorporated, was fit by least-squares polynomials using an orthogonal polynomial method. The data were fit to second through fifth order polynomials with an index of determination of 0.9999992 and a standard error of estimate for y (i.e., pressure) of 0.2258019.

The precision pressure gage was purchased with two quartz Bourdon tube capsules. The cell and least squares constants were as follows:

Bourdon tube serial number	4741	5083
B1L	8.05082	8.14762
C	-0.0859211	-0.4245883
B1	8.086858	8.160982
B2	0.00008718	-0.0001544

A program was written in IBM Fortran IV language to generate a table of pressures as a function of degrees of rotation for use in hand calculating adsorption isotherms. The program is reproduced below with appropriate comment cards to explain its use.

```
$WATFIV
C     THIS PROGRAM GENERATED A TABULATION OF PRESSURES IN UNITS OF CM OF
C     HG AS A FUNCTION OF THE DEGREES OF ROTATION READ FROM TI PRECISION
C     PRESSURE GAGE. THE CALIBRATION DATA SUPPLIED BY TEXAS INSTRUMENTS,
C     INC FOR THE QUARTZ SPIRAL BOURDON TUBES WERE FIT BY A LEAST SQUARE
C     POLYNOMIAL METHOD. THE SECOND ORDER POLYNOMIAL FIT WAS SELECTED TO
C     CORRELATE THE DATA FROM 1.0 TO 102.0 DEGREES, THAT IS, P(I) = C +
C     B1*DEG + B2*DEG*DEG WHERE C WAS THE INTERCEPT, B1 WAS COEFFICIENT
C     OF THE FIRST ORDER TERM AND B2 WAS COEFFICIENT OF THE SECOND ORDER
C     TERM. THE PRESSURE FROM 0.0 TO 1.0 WAS CORRELATED BY P(I) = B1L*
C     DEG WHERE B1L WAS THE TUBE CONSTANT IN TORR PER DEG FROM THE ORIG-
C     INAL CALIBRATION.  THE PRESSURES WERE PRINTED OUT FOR EVERY 0.002
C     DEGREES OF ROTATION.  QUARTZ SPIRAL BOURDON CAPSULE NO. 5083.
      DIMENSION H(20),PRESS(20)
      CK=0.000000
C     CARD 3   INTERCEPT C WAS READ
      C  = -0.4245883
C     CARD 4   COEFFICIENT OF FIRST ORDER TERM B1 WAS READ
      B1 = 8.160982
C     CARD 5   COEFFICIENT OF SECOND ORDER TERM B2 WAS READ
      B2 = -0.0001544
C     CARD 6   TUBE CONSTANT B1L WAS READ
      B1L = 8.14762
      DO 20 I=1,10
      H(I)=0.0+0.002000*FLOAT(I-1)
   20 PRESS(I)= 0.0000
      DO 90 N=1,203
   35 WRITE(6,40)N
   400FORMAT(20X,'TEXAS GAGE CALIBRATION, F. V. HANSON, 27 FEBRUARY 1987
    4',30X,'PAGE',I7///)
      WRITE(6,45) (H(N1),N1=1,10)
   45 FORMAT(29X,F8.3,9F9.3)
      WRITE(6,47)
   470FORMAT(23X,'******************************************************
     4************************************')
      DO 80 K=1,25
      DEGI = FLOAT(N-1)*0.5000+FLOAT(K-1)*0.0200
      DO 62 I=10
      DEG = DEGI + H(I)
      IF(DEG-1.0)64,65,65
   64 PRESS(I)=B1L*DEG
      GO TO 62
   65 PRESS(I)= C+DEG*B1+DEG*DEG*B2
   62 CONTINUE
   660WRITE(6,67)DEGI,PRESS(1),PRESS(2),PRESS(3),PRESS(4),PRESS(5),PRESS
     4(6),PRESS(7),PRESS(8),PRESS(9),PRESS(10)
   67 FORMAT(20X,F7.3,'*',F8.3,9F9.3/)
   80 CONTINUE
      WRITE(6,85)
   85 FORMAT(1H1)
   90 CONTINUE
```

```
      STOP
      END
$DATA
$STOP
/*
```

Adsorption Isotherm Computer Program

The adsorption isotherm computer program was also written in IBM Fortran IV language and was based on the isotherm calculation procedure outlined in Section VII. The program was adapted from an original program written by Dalla Betta.[52] The input data included helium calibration pressures, P_1, P_2, and P_3, and temperatures T_1, T_2, and T_3, and isotherm data points, that is, pressures $P_1(n)$ and $P_2(n)$ and temperatures $T_1(n)$. The mass of catalyst was also included to permit calculation of the amount adsorbed per unit mass of catalyst; however, isotherms computed on this basis must be corrected to a dry catalyst basis. The program will accept up to 10 calibration data points and up to 20 isotherm data points. As many as five isotherms can be calculated in a single computation.

The program is reproduced below and the use of the various options are explained on the comment cards. A typical adsorption isotherm printout for the 0.53 percent platinum on silica gel catalyst is presented following the program.

```
$WATFIV
C     THIS PROGRAM CALCULATED THE DOSER AND CELL VOLUMES AND THE ADSORP-
C     TION ISOTHERM FROM PRESSURE DATA, IN UNITS OF DEGREES, OBTAINED
C     WITH A TEXAS INSTRUMENTS PRECISION PRESSURE GAGE IN A CONSTANT VOL-
C     UME ADSORPTION APPARATUS.  THE PROGRAM CONVERTED THE DATA TO PRESS-
C     URE IN CM OF HG, THEN CALCULATED THE VOLUME ADSORBED IN CC / GRAM
C     AND THE AMOUNT ADSORBED IN MICROMOLES PER GRAM.  THE PROGRAM CALCU-
C     LATED UP TO FIVE ISOTHERMS AT A TIME.  QUARTZ SPIRAL BOURDON CAP-
C     SULE NO 5083.
C     DATA DECK WAS ARRANGED AS FOLLOWS
C     1ST CARD    EXPERIMENT IDENTIFICATION INCLUDING LSAC CATALYST
C                 CODE AND ISOTHERMS OBTAINED - UP TO 80 ALPHANUMERIC
C                 CHARACTERS
C     2ND CARD    N YY.YYYY ZZ.ZZ
C                 WHERE N WAS AN INTEGER-0, 1 OR 2 THAT DEFINES THE
C                 STATUS OF THE CALIBRATED BULB, VBULB.
C                 N=0  STANDARD BULB WAS CLOSED TO THE DOSER VOLUME,
C                 N=1  STANDARD BULB WAS OPEN TO THE DOSER VOLUME AND
                       WAS INCLUDED AS PART OF THE DOSER VOLUME
C                 N=2  STANDARD BULB WAS VARIABLE, THAT IS, EITHER
C                      OPENED OR CLOSED FOR EACH ISOTHERM POINT.
C                 Y (FREE FORM) WAS THE MASS OF THE CATALYST CHARGED
C                 TO ADSORPTION CELL, GRAMS
C                 Z (FREE FORM) WAS CELL TEMPERATURE IN DEG CENTIGRADE
C     3RD CARD    CELL VOLUME CALIBRATION DATA, P1, T1, P2, T2, P3, T3
C                 (FREE FORM, SEPARATED BY A SINGLE SPACE) IN THE FORM
C                 UUU.UUU VV.VV WWW.WW XX.XX YYY.YYY ZZ.ZZ
C                 WHERE U=P1 WAS THE PRESSURE IN CALIBRATED DOSER
C                 VOLUME MEASURED AT THE AMBIENT TEMPERATURE V=T1,
C                 W = P2 WAS THE PRESSURE IN THE CALIBRATED DOSER VOL-
C                 UME PLUS THE CONNECTING STOPCOCK VOLUME AFTER EXPAN-
C                 SION MEASURED AT THE AMBIENT TEMPERATURE X = TZ, Y =
C                 P3 WAS THE PRESSURE IN THE DOSER VOLUME PLUS THE
C                 CELL AFTER THE SECOND EXPANSION MEASURED AT THE AM-
C                 BIENT TEMPERATURE Z = T3 WITH THE CELL IMMERSED IN
C                 THE CONSTANT TEMPERATURE BATH, P1, P2, AND P3 WERE IN
C                 DEGREES AND T1, T2, AND T3 WERE IN DEGREES CENTIGRADE
C     4TH CARD    LAST CARD OF CALIBRATION DATA, SAME FORM AS DATA EX-
                  CEPT UUU.UUU WAS 999.9 OR LARGER, THAT IS, FINAL
C                 CARD SHOULD READ
C                 999.9 999.9 999.9 999.9 999.9 999.9
C     5TH CARD    ISOTHERM TITLE - UP TO 80 ALPHANUMERIC CHARACTERS
C     6TH CARD    ADSORPTION ISOTHERM DATA, P1, T1, P2, T2
C                 (FREE FORM, SEPARATED BY A SINGLE SPACE) IN THE FORM
C                 WWW.WWW XX.XX YYY.YYY ZZ.ZZ
C                 WHERE W = P1 WAS THE PRESSURE IN THE DOSER VOLUME AT
C                 AMBIENT TEMPERATURE X = T1, Y = P2 WAS THE PRESSURE
C                 IN THE DOSER VOLUME PLUS THE CELL AFTER EXPANSION AT
C                 AMBIENT TEMPERATURE Z = T2.
C                 THE PROGRAM ACCEPTED 1 TO 20 SETS OF ISOTHERM DATA
C     7TH CARD    LAST CARD OF ISOTHERM DATA, SAME FORM AS DATA EXCEPT
```

```
    C                 UUU.UUU WAS USED TO TERMINATE ISOTHERM CALCULATION
    C                 OR TO SET THE MODE FOR CONTINUATION OF CALCULATION
    C                 OF SUBSEQUENT ISOTHERM, THE FORM OF FINAL CARD WAS
    C                 UUU.UUU 999.9 999.9 999.9
    C                 WHERE IF UUU.UUU =  999.9 TERMINATION OF CALCULATION
    C                       IF UUU.UUU = 1002.0 ANOTHER ISOTHERM TO FOLLOW
    C                                           WHICH INCLUDED A NEW SET
    C                                           OF CELL VOLUME CALIBRATION
    C                                           DATA
    C                 IF N WAS EQUAL TO 2 ON SECOND CARD (STANDARD BULB IN
    C                 VARIABLE MODE) THEN THE ADSORPTION ISOTHERM DATA,
    C                 6TH CARD WAS OF FORM
    C      6TH CARD   WWW.WWW XX.XX YYY.YY ZZ.ZZ M
    C                 WHERE W, X, Y, AND Z WERE THE SAME AS ABOVE
    C                 IF M = 0, STANDARD BULB WAS NOT INCLUDED IN DOSER
    C                           VOLUME
    C                 IF M = 1, STANDARD BULB WAS INCLUDED IN DOSER VOLUME
1          DIMENSION TIT(80),CP1(10),CP2(10),CP3(10)
2          DIMENSION PISOI(100),PISOF(100),DCP1(100),DCP2(100),DCP3(100)
3          DIMENSION RSC(10),RCELL(10),TIC(100),TFC(100),TI(100),TF(100)
4          DIMENSION T1(10),T2(10),T3(10),TK1(10),TK2(10),TK3(10)
5          DIMENSION DPISOF(100),TIT2(80,5),DPISOI(100),NVSB(100),L(5)
6        1 CONTINUE
    C      THE QUARTZ BOURDON TUBE CALIBRATION CONSTANTS C, B1, B2 AND B1L
    C      WERE READ AT THIS POINT.  THE PRESSURE FROM 1.0 TO 102.0 DEGREES
    C      WAS CALCULATED FROM THE EQUATION P(I) = C + B1*DEG + B2*DEG*DEG
    C      WHERE THE CONSTANTS WERE DEFINED AS FOLLOWS, C WAS THE INTERCEPT,
    C      B1 WAS THE COEFFICIENT OF THE FIRST ORDER TERM AND B2 WAS THE
    C      COEFFICIENT OF THE SECOND ORDER TERM.  THE PRESSURE FROM 0.0 TO 1.0
    C      DEGREE WAS CALCULATED FROM THE EQUATION P(I) = B1L*DEG WHERE B1L
    C      WAS THE TUBE CONSTANT IN TORR DEGREE FROM THE ORIGINAL CALIBRATION
    C      IT WAS NECESSARY TO CHANGE THESE CARDS WHEN CAPSULE WAS CHANGED.
    C      ALSO THE CALIBRATED DOSER VOLUME WAS RECALIBRATED WHEN CAPSULE WAS
    C      CHANGED, THAT IS, NEW VALUE OF V1 REQUIRED (PROGRAM CARD NO. 12)
7          B1 = 8.160982
8          B2 = -0.0001544
9          C = -0.4245883
10         B1L= 8.14762
11         VBULB = 49.0548
12         V1 = 6.2890
13         MODE=1
14         NK=0
15         XMULT=0.0
16         ARSC=0.0
17         ARCELL=0.0
18         READ(5,25) (TIT(I),I=1,80)
19      25 FORMAT(80A1)
20         READ, IFSB, WTSAMP, TCELL
21         TC= 273.16 + TCELL
22         N=0
23       3 N=N+1
```

```
      READ, DCP1(N),T1(N),DCP2(N),T2(N),DCPE(N),T3(N)
      TK1(N) = 273.16 + T1(N)
      TK2(N) = 273.16 + T2(N)
      TK3(N) = 273.16 + T3(N)
      IF(DCP1(N)-999.9)100,5,5
  100 CP1(N) = (C + B1*DCP1(N) + B2*DCP1(N)*DCP1(N))/10.0
      CP2(N) = (C + B1*DCP2(N) + B2*DCP2(N)*DCP2(N))/10.0
      CP3(N) = (C + B1*DCP3(N) + B2*DCP3(N)*DCP3(N))/10.0
      RSC(N) = (CP1(N)/TK1(N)-CP2(N)/TK2(N))*TK2(N)/CP2(N)
      RCELL(N)=(CP2(N)/TK2(N)-CP3(N)/TK3(N))*TC/CP3(N)
      ARSC=ARSC+RSC(N)
      ARCELL=ARCELL+RCELL(N)
      GO TO 3
    5 N=N-1
      ARSC=ARSC/FLOAT(N)
      ARCELL=ARCELL/FLOAT(N)
      AVSC=ARSC*V1
      AVCELL=ARCELL*(V1+AVSC)
      NIFSB=IFSB+1
  152 NK=NK+1
      L(NK)=20*(NK-1)
  153 READ(5,25) (TIT2(I,NK),I=1,80)
    9 L(NK)=L(NK)+1
      M=L(NK)
      GO TO (55,55,56),NIFSB
   56 CONTINUE
      READ, DPISOI(M),DPISOF(M),NVSB(M)
      GO TO 59
   55 CONTINUE
      READ,DPISOI(M),TIC(M),DPISOF(M),TFC(M)
   59 IF(DPISOI(M)-999.9)15,20,20
   20 IF(DPISOI(M)-1000.0)53,53,21
   21 MODE=IFIX(DPISOI(M)-1000.0)
      GO TO (53,152,53),MODE
   15 IF(DPISOI(M) - 1.0)16,17,17
   16 PISOI(M) = B1L*DPISOI(M)/10.0
      GO TO 18
   17 PISOI(M) = (C + B1*DPISOI(M) + B2*DPISOI(M)*DPISOI(M))/10.0
   18 CONTINUE
      TI(M) = 273.16 + TFC(M)
      TF(M) = 273.16 + TIC(M)
   22 IF(DPISOF(M) - 1.0)23,24,24
   23 PISOF(M) = B1L*DPISOF(M)/10.0
      GO TO 51
   24 PISOF(M) = (C + B1*DPISOF(M) + B2*DPISOF(M)*DPISOF(M))/10.0
   51 CONTINUE
   52 GO TO 9
   53 VDOSER=V1+AVSC+BULB*FLOAT(IFSB)
      WRITE (6,27)
   27 FORMAT ('1')
      WRITE(6,28)(TIT(I),I=1,80)
```

```
   28 FORMAT(1X,80A1)
      WRITE(6,10)
   10 FORMAT(/43H      P(DEG)      P(CM)       RATIO)
      DO 6 I=1,N
    60WRITE(6,7) DCP1(I),CP1(I),TK1(I),DCP2(I),CP2(I),TK2(I),RSC(I),DCP3
     4(I),CP3(I),TK3(I),RCELL(I)
    70FORMAT(F10.3,F13.3,1H(,F6.2,1H)/F10.3,F13.3,1H(,F6.2,1H),F14.6/
     4F10.3,F13.3,1H(,F6.2,1H),F14.6/)
      WRITE(6,32)ARSC,ARCELL
   32 FORMAT(35X,9H---------/30X,F14.6/30X,F14.6)
      WRITE(6,8)AVSC,AVCELL
    8 FORMAT(1X,12HAVE FSC    =,F10.4/1X,12HAVE VCELL =,F10.4)
      GO TO (70,70,71),NIFSB
   70 WRITE(6,80)VDOSER
      GO TO 72
   71 WRITE(6,81)
   80 FORMAT(1X,12HVDOSER     =,F10.4)
   81 FORMAT(1X,22HVDOSER     = VARIABLE)
   72 IF(WTSAMP)154,154,34
   34 XMULT = 1.0/(76.0*WTSAMP)
      WRITE(6,31)WTSAMP
   31 FORMAT(1X,12HDRY WEIGHT =,F10.4)
  154 DO 155 NL=1,NK
      SPVADS=0.0
      SUMADS=0.0
      OPVLEF=0.0
   35 WRITE(6,28) (TIT2(I,NL),I=1,80)
      IF(NL-1)98,98,99
   98 WRITE(6,11)
  110 FORMAT(/77H P(DEG)      P(CM)        PV(ADSORB)  V ADS(CC/G)
     4SUM VADS    MOLES E-6)
   99 L(NL)=L(NL)-1
      M1=L(NL)-(NL-1)*20
      DO 13 I1=1,M1
      I=I1+(NL-1)*20
      PRINT,VDOSER,AVCELL
      PVIEFT=PISOF(I)*AVCELL
      GO TO (60,60,58),NIFSB
   58 VDCSER=V1+AVSC+VBULB*FLOAT(NFSB(1))
   60 PVADS = ((PISOI(I)/TI(I)-PISOF(I)/TF(I))*VDOSER + OPVLEF/TC-
     4PVLEFT/TC)*273.16
      PRINT,PISOI(I),TI(I),PISOF(I),TF(I),VDOSER,OPVLEF,PVLEFT
      SPVADS=SPVADS+PVADS
      OPVLEF=PVLEFT
   30 ADSG=PVADS*XMULT
   33 SUMADS=SUMADS+ADSG
      XMOLES=SUMADS/0.022414
      GO TO (64,64,62),NIFSB
   62 WRITE(6,63)I1,DPISOI(I),PISOI(I),VDOSER
   63 FORMAT(I3,1H),F7.3,F9.3,4X,8HVDOSER =,F10.4)
      GO TO 13
```

```
   64 WRITE(6,19)I1,DPISOI(I),PISOI(I),TI(I)
   19 FORMAT(13,1H),F7.3F9.3,1H(F6.2,1H))
   13 WRITE(6,26) DPISOF(I),PISOF(I),TF(I),PVADS,ADSG,SUMADS,XMOLES
   26 FORMAT(F11.3,F9.3,1H(,F6.2,1H),4(F12.4)/)
  155 CONTINUE
      GO TO (150,150,1),MODE
  150 CONTINUE
      STOP
      END
$DATA
$STOP
/*
```

```
TAR-11---H2, O2, AND TITRATION ISOTHERMS, PLATINUM/SILICA GEL CATALYST

       P(DEG)             P(CM)                          RATIO
      83.593             68.070( 27.00)
      76.633             62.407( 27.05)                 0.090921
      31.235             25.433( 27.10)                 1.419770

      84.266             68.617( 24.95)
      77.248             62.907( 25.05)                 0.091132
      31.357             25.533( 25.15)                 1.439332

      84.560             68.856( 25.45)
      77.507             63.118( 25.50)                 0.091097
      31.636             25.760( 25.60)                 1.423842

      83.386             67.901( 26.10)
      76.457             62.264( 26.20)                 0.090909
      31.159             25.371( 26.30)                 1.424306
                                                        ---------
                                                        0.091015
                                                        1.426812
AVE VSC     =  0.5724
AVE VCELL   =  9.7899
VDOSER      =  6.8614
DRY WEIGHT  =  0.5030
OXYGEN ADSORPTION ISOTHERM AT 20 C--400 C RED, 400 C EVAC 8 HOUR(REPEAT)

   P(DEG)    P(CM)              PV(ADSORB)         V ADS(CC/G)  SUM VADS    MOLES E-6
1)  8.845     7.175( 25.7)
    3.199     2.568( 26.35)     5.3662             0.1404       0.1404      6.2666

2) 13.342    10.843( 26.3)
    7.260     5.882( 26.70)     0.7369             0.0193       0.1597      7.1272

3) 20.140    16.387( 26.8)
   12.452    10.117( 26.95)     0.4799             0.0126       0.1722      7.6877

4) 25.676    20.901( 26.9)
   17.765    14.451( 27.40)     0.5617             0.0147       0.1869      8.3437

5) 30.126    24.529( 27.4)
   22.724    18.495( 27.70)     0.5906             0.0154       0.2023      9.0333

6) 36.289    29.553( 27.6)
   28.183    22.945( 27.80)     0.4518             0.0118       0.2142      9.5610

CORE USAGE  OBJECT CODE =      6552 BYTES,ARRAY AREA=  7180 BYTES, TOTAL
COMPILE TIME=     0.57 SEC,EXECUTION TIME =     0.18 SEC, WATFIV - VERSION 1
```

APPENDIX E

REACTOR MASS BALANCE COMPUTER PROGRAMS

A. Program for Product Analysis for the Catalytic Cracking of Kerosene

The Fortran program, MASSBAL2, was written to process the data from the analyses of the products produced in the catalytic cracking of kerosene. A sample input and output are included. The input data was taken from the analyses of the gas and liquid products produced in Run number 44.

Table E-1

Program Listing for MASSBAL2

```
C     Program to calculate the product yield from the cracking of
C  kerosene. The program can be easily modified to calculate
C  product yield for the cracking of diesel boiling range material,
C  simply by increasing the product slate to include the highest
C  boiling carbon number below the initial boiling point of diesel. The
C  highest boiling point carbon number which boiled below the initial
C  boiling point of the kerosene for which this program was written was
C  C9.
C     The input is obtained from gas chromatographic analyses of the
C  gas and liquid products. The gas product data is cast in the
C  form of adjusted weight percents (the sum of all the weight
C  percents must equal 100 %). The liquid product data is input as
C  relative weight percents, obtained directly from the analyses of the
C  liquid product. The mass of the liquid, the mass of the gas and the
C  average molecular weight are input in free formatted form. The
C  names of each chemical species and the amounts in the liquid and gas
C  products are also input in a set format.
C     The program calculates the weight percent and mole percent for
C  each species present in the products. The program also
C  calculates the number of moles of each product produced per
C  100 moles of feed converted. In addition the program also
C  computes the following:
C   1)   the weight percent of the feed that was converted,
C   2)   the weight percent yield to aromatics,
C   3)   the number of moles of double bonds in aromatics,
C   4)   the number of moles of double bonds in monounsaturates
C        (olefins + naphthenes),
C   5)   the ratio of accounted double bonds to theoretical
C        double bonds based on the change of the number of moles
C        during the reaction, this value should equal unity when
C        there is no hydrogenation or dehydrogenation and the
C        product analysis is accurate,
C   6)   the hydrogen to carbon ratio of the products, and
```

```
C  7)  the number of moles of product produced for every
C       hundred moles of feed converted.
C
C                             Variables
C   MLIQ---------mass of liquid product
C   MVAP---------mass of vapor product
C   MWAVGF------average molecular weight of feed
C   FRAC---------ratio of accounted unsaturations to theoretical
C                unsaturations
C   HSUM---------the number of moles of hydrogen present in the
C                products
C   CSUM---------the number of moles of carbon present in the
C                products
C   HCRAT-------hydrogen to carbon ratio of the products
C   CENSUM------number of moles of product produced for every
C                hundred moles of feed converted
C   MOLEO--------the number of moles of feed into the reactor
C   MOLEFN------the number of moles of product
C   TUNSAT------the theoretical number of unsaturations produced
C                = MOLEFN - MOLEO
C   OUNSAT------the number of moles of unsaturations present as
C                olefins and naphthenes
C   AUNSAT------the number of unsaturations present in aromatics
C
C                           Arrays
C   NAME---------contains the names of each species in the
C                reactor products
C   MW-----------molecular weight of each species
C   WT-----------relative weight percent of products in liquid
C                feed replaced by absolute weight percent of
C                products in the total liquid and gas product
C   WTG----------absolute weight percent of products in gas
C                product
C   H------------moles of hydrogen atoms/mole of each species
C   C------------moles of carbon atoms/mole of each species
C   MOL----------mole percent of each species in the products
C   CEN----------moles of each product produced per one hundred
C                moles of feed cracked
C
C-----------------------------------------------------------------
C  Variable and array declarations
C
    REAL MLIQ,MVAP,SUMWT,SUM,SUMOL,MWAVGF,FRAC
    REAL WT(42),ADJWT(42),WTLIQ(42),WTG(42),MW(42)
    REAL AUNSAT,OUNSAT,TUNSAT,MOLEO,MOLEFN,H(42),C(42)
    REAL MOL(42),MOLIQ(42),MOLGAS(42),WTGAS(42),FEED(22)
    REAL HSUM,CSUM,HCRAT,CENSUM,CEN(42)
```

```
      INTEGER I
      CHARACTER*14, NAME(42)
C
C  Input the data
      PRINT *,' Input names of species and molecular wts,',
     # ' wt. % of liquid products, wt. % of gas products,',
     # ' moles of H and moles of C in mole of species.'
      DO 10 I=1,42
        READ(5,11)NAME(I),MW(I),WT(I),WTG(I),H(I),C(I)
        WRITE(6,11)NAME(I),MW(I),WT(I),WTG(I),H(I),C(I)
 11     FORMAT(1X,A14,1X,F5.0,1X,F7.3,1X,F7.3,1X,F4.0,1X,F4.0)
 10   CONTINUE
C
      PRINT *, ' Input the total wt. of liquid product (g.).'
      READ *, MLIQ
      WRITE(6,12)MLIQ
 12    FORMAT(2X,F7.2)
      PRINT *, ' Input average molecular weight of feed.'
      READ *, MWAVGF
      WRITE(6,12)MWAVGF
      PRINT *, ' Input the total wt. of gas product (g.).'
      READ *, MVAP
      WRITE(6,12)MVAP
C
C   Normalize the adjusted weight percents in the liquid to
C   absolute weight percents, and determine the number of moles
C   of each species in the product stream.
      SUM= 0.
      DO 14 I=1,42
        SUM= SUM + WT(I)/100.
 14   CONTINUE
C
C
      DO 20 I=1,42
        ADJWT(I)=WT(I)/SUM
        WTLIQ(I)= ADJWT(I)*MLIQ/100.
        MOLIQ(I)= WTLIQ(I)/MW(I)
 20   CONTINUE
      DO 21 I=1,13
        WTGAS(I)=WTG(I)*MVAP/100.
       MOLGAS(I)=WTGAS(I)/MW(I)
 21   CONTINUE
C  Determine absolute weight and liquid fractions.
C
      SUMOL= 0.
      DO 25 I=1,42
        MOL(I)= MOLGAS(I) + MOLIQ(I)
```

```
          SUMOL= SUMOL + MOL(I)
          WT(I)= MOL(I)*MW(I)*100./(MLIQ+MVAP)
 25   CONTINUE
      DO 26 I=1,42
        MOL(I)= MOL(I)*100./SUMOL
 26   CONTINUE
C
C     Calculate conversions (based on weight percent of product).
C     Xa is a dummy variable initially, then it becomes the
C     total conversion. Xd is conversion to aromatics.
      XA= 0.
      DO 28 I=1,19
        XA= XA + WT(I)
 28   CONTINUE
      XD= 0.
      DO 30 I=36,42
          XD= XD + WT(I)
 30   CONTINUE
      XA= (XA+XD)
C     Calculate moles of unsaturations.
C     Aunsat is moles of unsaturations in aromatics.
C     Ounsat is number of unsaturations in naphthenes and
C     olefins (assuming no cycloolefins or diolefins).
      AUNSAT= SUMOL/100.*(4.*(MOL(36)+MOL(37)+MOL(38)
     #  + MOL(39)+MOL(40)+MOL(41) + MOL(42)) )
      OUNSAT= SUMOL/100.*(MOL(2)+MOL(4)+MOL(8)+MOL(11)+MOL(13)
     # +MOL(15)+MOL(17)+MOL(19)+MOL(21)+MOL(23)+MOL(25) )
C
C     Calculate number of theoretical unsaturations by delta
C     moles during reaction.
      MOLEO= (MLIQ+MVAP)/MWAVGF
      MOLEFN= SUMOL
      TUNSAT= MOLEFN - MOLEO
C
C    Calculate actual unsaturations/theoretical unsaturations
      FRAC= (AUNSAT+OUNSAT)/TUNSAT
C
C    Calculate H/C ratio of products.
      HSUM= 0.
      CSUM= 0.
      DO 35 I=1,19
        HSUM= HSUM + MOL(I)*H(I)
        CSUM= CSUM + MOL(I)*C(I)
 35   CONTINUE
      DO 36 I=36,42
        HSUM= HSUM + MOL(I)*H(I)
        CSUM= CSUM + MOL(I)*C(I)
```

```
36   CONTINUE
       HCRAT=HSUM/CSUM
C     Calculate the number of moles of each species for every one
C     hundred moles cracked.
C
      CENSUM = 0.
      TMOL= (MLIQ+MVAP)*(XA)/(100.*MWAVGF)
      DO 37 I=1,42
         IF( (I.GE.20).AND.(I.LE.35) )GO TO 37
         CEN(I)= WT(I)*(MLIQ+MVAP)/(MW(I)*TMOL)
         CENSUM= CENSUM + CEN(I)
37   CONTINUE
      WRITE(6,39)
39   FORMAT('1',1X)
      PRINT *,'------------------------------------------',
     # '-------------------'
      PRINT *,' Product      Mole percent  Wt. percent   Moles/',
     #        '100 Moles'
      PRINT *,'------------------------------------------',
     # '-------------------'
      DO 40 I=1,42
         WRITE(6,41) NAME(I),MOL(I),WT(I),CEN(I)
41        FORMAT(2X,A14,2X,F5.2,3X,F5.2,8X,F7.2)
40   CONTINUE
      PRINT *,'------------------------------------------',
     # '-------------------'
      WRITE(6,42)XA,XD
42   FORMAT(1X,' Total conversion = ',F6.2,/,1X,
     #  ' Conversion to aromatics = ',F6.2,/)
      WRITE(6,51)OUNSAT,AUNSAT,FRAC
51   FORMAT(1X, ' Olefinic and naphthenic unsaturations ',
     # F6.4,/,1X,' Aromatic unsaturations ', F6.4,/,1X,
     # ' Accounted Unsaturations/Theoretical Unsaturations =',
     # 1X,F6.4,/)
      WRITE(6,52)HCRAT
52   FORMAT(1X,' Hydrogen/Carbon Ratio =',1X,F5.2)
      WRITE(6,53)CENSUM
53   FORMAT(1X,' Number of moles produced per 100 moles of',
     #          ' feed cracked = ',F7.2)
      PRINT *,'------------------------------------------',
     # '-----------------'
      STOP
      END
```

Table E-2

Sample Input For MASSBAL2

Since the input for MASSBAL2 is formatted, this data must be input exactly as it appears here. The data in the first column are the names of each species, the data in the second column are their molecular weights, the data in the third column are the relative weight percents of each species in the liquid product and the data in the fourth column are the absolute weight percent of each species in the gas product. The final three numbers in the table are the mass of liquid product collected from the run, the average molecular weight of the feed and the mass of the gas collected from the run, respectively.

C1	16	0	0.07	4	1
C2 olefin	28	0	1.03	4	2
C2	30	0	0.70	6	2
C3 olefin	42	0.0	6.57	6	3
C3	44	0.333	25.14	8	3
Iso C4	58	0.339	20.07	10	4
C4	58	1.727	22.02	10	4
C4 olefin	56	0.524	8.91	8	4
Iso C5	72	3.622	0.15	12	5
C5	72	2.343	5.49	12	5
C5 olefin	70	1.917	8.06	10	5
C6	86	1.878	1.01	14	6
C6 olefin	84	3.406	0.78	12	6
C7	100	0.41	0	16	7
C7 olefin	98	2.05	0	14	7
C8	114	1.07	0	18	8
C8 olefin	112	1.074	0	16	8
C9	128	0.905	0	20	9
C9 olefin	126	0.77	0	18	9
C10	142	4.153	0	22	10
C10 olefin	140	0.0	0	20	10
C11	156	9.795	0	24	11
C11 olefin	154	0.0	0	22	11
C12	170	18.041	0	26	12
C12 olefin	168	0.0	0	24	12
C13	184	14.546	0	28	13
C14	198	11.168	0	30	14
C15	212	6.653	0	32	15
C16	226	3.23	0	34	16
C17	240	3.173	0	36	17
C18	254	1.13	0	38	18
C19	268	0.0	0	40	19
C20	282	0.0	0	42	20
C21	296	0.0	0	44	21
C22	310	0.0	0	46	22
Benzene	78	0.551	0	6	6
Toluene	92	0.76	0	8	7
Xylenes	106	1.081	0	10	8
C9 aromatics	120	0.995	0	12	9
C10 aromatics	134	0.0	0	14	10
C11 aromatics	142	0.0	0	16	11
C12 aromatics	156	0.0	0	18	12

21.95
181.6
4.30

Table E-3

Sample Output from MASSBAL2

This is a sample output resulting from the input data listed in Table B-5. The first page is an output of the input data. The second page presents the results that are calculated from the input data.

```
 Input names of species and molecular wts, wt percent of liquid products, wt percent of gas products,
moles of H and moles of C in mole of species.
C1                16      0.000      0.070     4      1
C2 olefin         28      0.000      1.030     4      2
C2                30      0.000      0.700     6      2
C3 olefin         42      0.000      6.570     6      3
C3                44      0.333     25.140     8      3
Iso C4            58      0.339     20.070    10      4
C4                58      1.727     22.020    10      4
C4 olefin         56      0.524      8.910     8      4
Iso C5            72      3.622      0.150    12      5
C5                72      2.343      5.490    12      5
C5 olefin         70      1.917      8.060    10      5
C6                86      1.878      1.010    14      6
C6 olefin         84      3.406      0.780    12      6
C7               100      0.410      0.000    16      7
C7 olefin         98      2.050      0.000    14      7
C8               114      1.070      0.000    18      8
C8 olefin        112      1.074      0.000    16      8
C9               128      0.905      0.000    20      9
C9 olefin        126      0.770      0.000    18      9
C10              142      4.153      0.000    22     10
C10 olefin       140      0.000      0.000    20     10
C11              156      9.795      0.000    24     11
C11 olefin       154      0.000      0.000    22     11
C12              170     18.041      0.000    26     12
C12 olefin       168      0.000      0.000    24     12
C13              184     14.546      0.000    28     13
C14              198     11.168      0.000    30     14
C15              212      6.653      0.000    32     15
C16              226      3.230      0.000    34     16
C17              240      3.173      0.000    36     17
C18              254      1.130      0.000    38     18
C19              268      0.000      0.000    40     19
C20              282      0.000      0.000    42     20
C21              296      0.000      0.000    44     21
C22              310      0.000      0.000    46     22
Benzene           78      0.551      0.000     6      6
Toluene           92      0.760      0.000     8      7
Xylenes          106      1.081      0.000    10      8
C9 aromatics     120      0.995      0.000    12      9
```

```
C10 aromatics          134        0.000        0.000        14         10
C11 aromatics          142        0.000        0.000        16         11
C12 aromatics          156        0.000        0.000        18         12
  Input the total wt. of liquid product (g.).
     21.95
  Input average molecular weight of feed.
    181.60
  Input the total wt. of gas product (g.).
      4.30
```

Product Species	Mole (%)	Weight (%)	Moles Produced / 100 Moles Cracked
C1	0.08	0.01	0.34
C2 olefin	0.65	0.17	2.85
C2	0.42	0.11	1.81
C3 olefin	2.78	1.08	12.11
C3	10.87	4.40	47.28
Iso C4	6.70	3.58	29.15
C4	9.53	5.09	41.43
C4 olefin	3.70	1.91	16.10
Iso C5	4.72	3.13	20.52
C5	4.38	2.91	19.07
C5 olefin	4.60	2.96	19.99
C6	2.24	1.77	9.74
C6 olefin	3.94	3.04	17.12
C7	0.38	0.35	1.66
C7 olefin	1.95	1.76	8.46
C8	0.87	0.92	3.80
C8 olefin	0.89	0.92	3.88
C9	0.66	0.78	2.86
C9 olefin	0.57	0.66	2.47
C10	2.72	3.56	0.00
C10 olefin	0.00	0.00	0.00
C11	5.84	8.39	0.00
C11 olefin	0.00	0.00	0.00
C12	9.87	15.45	0.00
C12 olefin	0.00	0.00	0.00
C13	7.35	12.46	0.00
C14	5.25	9.56	0.00
C15	2.92	5.70	0.00
C16	1.33	2.77	0.00
C17	1.23	2.72	0.00
C18	0.41	0.97	0.00
C19	0.00	0.00	0.00
C20	0.00	0.00	0.00
C21	0.00	0.00	0.00
C22	0.00	0.00	0.00
Benzene	0.66	0.47	2.86
Toluene	0.77	0.65	3.34
Xylenes	0.95	0.93	4.13
C9 aromatics	0.00	0.00	0.00
C10 aromatics	0.00	0.00	0.00
C11 aromatics	0.00	0.00	0.00
C12 aromatics	0.00	0.00	0.00

```
-----------------------------------------------------------------
Total conversion =  38.44
Conversion to aromatics =    2.90

Olefinic and naphthenic unsaturations 0.0461
Aromatic unsaturations 0.0304
Accounted Unsaturations/Theoretical Unsaturations = 0.7880

Hydrogen/Carbon Ratio =  2.21
Number of moles produced per 100 moles of feed cracked =  274.32
-----------------------------------------------------------------
```

APPENDIX F

DERIVATION OF THE BET EQUATIONS

In order to better understand the nature of the BET equation and its limitations, the equations obtained by Brunauaer, Emmett and Teller[259] are derived here. In addition to the derivation of the BET (A) ('the BET equation'), the derivations of the BET (B), BET (C) and BET (D) equations are also provided.

The Derivation of the BET (A) Equation

The derivation of the BET (A) equation incorporates several basic assumptions:

1) the properties of the adsorptive in the second and higher monolayers are equivalent to the properties of adsorptive in the liquid phase, and;
2) an infinite number of monolayers can be formed.

In the derivation that follows s_1, s_2, s_3, . . . , s_i represent the area covered by the 1st, 2nd, 3rd, . . . , ith layers of adsorptive adsorbed on the surface of the adsorbent. The term s_0 will represent the bare or uncovered surface of the adsorbent.

At equilibrium the area of uncovered surface, s_0, remains constant. That is, the rate of uncovering of bare surface by desorption from the first monolayer is equivalent to the rate of bare surface being covered by adsorption from the gas phase.

First equate the rate of adsorption in the first monolayer on the bare adsorbent surface and the rate of desorption from the first monolayer which exposes the bare adsorbent surface:

$$a_1 p s_0 = b_1 s_1 \exp\left(\frac{-E_1}{RT}\right) \qquad \text{(F-1)}$$

where

a_1 is the rate constant for adsorption;

p is the partial pressure of adsorptive;

s_0 is the area of adsorbent surface available for adsorption;

b_1 is the rate constant for desorption;

s_1 is the surface area covered by the first monolayer; and

E_1 is the heat of adsorption of adsorptive in the first monolayer.

A similar expression can be written for the second adsorbed monolayer at equilibrium.

$$a_2 p s_1 + b_1 s_1 \exp\left(\frac{-E_1}{RT}\right) = b_2 s_2 \exp\left(\frac{-E_2}{RT}\right) + a_1 p s_0 \qquad \text{(F-2)}$$

where:

a_2 is the rate constant for adsorption of the second adsorbed monolayer;

b_2 is the rate constant for desorption of the second adsorbed monolayer;

s_2 is the surface area covered by the second adsorbed monolayer; and

E_2 is the heat of adsorption of adsorptive in the second adsorbed monolayer.

The first term on the left represents the rate of adsorption on the first monolayer as it is covered with adsorptive to form the second adsorbed monolayer. The second term is the rate of desorption from the first monolayer to uncover the bare adsorbent surface. The first term on the right is the rate of formation of the first monolayer due to desorption from the second adsorbed monolayer, the second term on the right is the rate of formation of the first monolayer due to adsorption of adsorptive on the bare surface. If Equation (F-1) is subtracted from Equation (F-2) we obtain the following expression:

$$a_2ps_1 = b_2s_2 \exp\left(\frac{-E_2}{RT}\right) \tag{F-3}$$

This procedure can be extended to an infinite number of monolayers to generate the following set of equations:

$$a_3ps_2 = b_3s_3 \exp\left(\frac{-E_3}{RT}\right)$$

$$\begin{matrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{matrix}$$

$$a_ips_{i-1} = b_is_i \exp\left(\frac{-E_i}{RT}\right) \tag{F-4}$$

The total surface area of the adsorbent is obtained from the summation of the exposed surface areas of all the monolayers formed from the bare surface or zeroth monolayer up to the highest monolayer:

$$A = \sum_{i=0}^{\infty} s_i \tag{F-5}$$

The total volume of adsorptive adsorbed in all monolayers is given by Equation F-6.

$$v = v_0 \sum_{i=0}^{\infty} is_i \tag{F-6}$$

where:

v_0 is the volume of gas required to cover a unit area of the bare surface, cm^3;

s_i is the surface area covered by the i^{th} monolayer, m^2; and

i in the summation represents the sum of the monolayers covered by the i^{th} monolayer.

It follows that:

$$\frac{v}{Av_0} = \frac{v}{v_m} = \frac{\sum_{i=0}^{\infty} i s_i}{\sum_{i=0}^{\infty} s_i} \tag{F-7}$$

where:

v_m is the volume of gas adsorbed when the entire adsorbent surface is covered with a complete unimolecular monolayer of adsorptive.

It is assumed that the heats of adsorption of the second and higher monolayers of adsorbent are identical to the latent heat of condensation of the adsorptive. It is also assumed that the adsorption/desorption properties of the second and higher monolayers are equal. These two assumptions can be expressed as follows:

$$E_2 = E_3 = \ldots E_i = E_L \tag{F-8}$$

and

$$\frac{b_2}{a_2} = \frac{b_3}{a_2} = \ldots \frac{b_i}{a_i} = g \tag{F-9}$$

The fraction of the surface covered by the first monolayer, s_1, can be calculated from Equation (F-1):

$$s_1 = \frac{a_1}{b_1} p s_0 \exp\left(\frac{E_1}{RT}\right) \tag{F-10}$$

or

$$s_1 = ys_o \qquad \text{where } y = \frac{a_1}{b_1}\, p \exp\left(\frac{E_1}{RT}\right) \tag{F-11}$$

The fraction of the surface covered by the second monolayer, s_2, can be calculated from Equation (F-3).

$$s_2 = \frac{a_2 p s_1}{b_2} \exp\left(\frac{E_2}{RT}\right) = \frac{p s_1}{g} \exp\left(\frac{E_L}{RT}\right) \tag{F-12}$$

or

$$s_2 = xs_1 \qquad \text{where } x = \frac{p}{g} \exp\left(\frac{E_L}{RT}\right) \tag{F-13}$$

This analysis can be extended to subsequent monolayers:

$$s_3 = xs_2 = x^2 s_1 \tag{F-14}$$

or for the i^{th} monolayer we have:

$$s_i = xs_{i-1} = x^{i-1}s_1 = x^{i-1}ys_o = cx^i s_o \tag{F-15}$$

where

$$c = \frac{y}{x} \tag{F-16}$$

$$c = \frac{a_1}{b_1}\, g \exp\left[\frac{(E_1 - E_L)}{RT}\right] \tag{F-17}$$

The substitution of Equation (F-15) into Equation (F-7) gives:

$$\frac{v}{v_m} = \frac{\sum_{i=0}^{\infty} is_i}{\sum_{i=0}^{\infty} s_i} = \frac{\sum_{i=0}^{\infty} i(cx^i s_0)}{s_0 + \sum_{i=1}^{\infty} (cx^i s_0)} \qquad \text{(F-18)}$$

Since c and s_o are constant, they can be moved out of the summations. When i = 0, the first term in the upper summation vanishes, thus,

$$\frac{v}{v_m} = \frac{cs_0 \sum_{i=1}^{\infty} ix^i}{s_0 + cs_0 \sum_{i=1}^{\infty} x^i} = \frac{c \sum_{i=1}^{\infty} ix^i}{1 + c \sum_{i=1}^{\infty} x^i} \qquad \text{(F-19)}$$

When x is less than 1, the summation in the denominator can be written as:

$$\sum_{i=1}^{\infty} x^i = \frac{x}{1-x} \qquad \text{(F-20)}$$

Equation (F-20) may be substituted into Equation (F-19) to obtain:

$$\frac{v}{v_m} = \frac{c \sum_{i=1}^{\infty} ix^i}{[1 + \frac{cx}{(1-x)}]} \qquad \text{(F-21)}$$

Consider the expansion of the summation in the numerator:

$$ix^i = x + 2x^2 + 3x^3 + 4x^4 \ldots \qquad \text{(F-22)}$$

which may be rewritten as:

$$\sum_{i=1}^{\infty} ix^{i} = x\frac{d(x)}{dx} + x\frac{d(x^{2})}{dx} + x\frac{d(x^{3})}{dx} + \frac{d(x^{4})}{dx} \quad \ldots \tag{F-23}$$

We can rewrite Equation (F-23) as:

$$\sum_{i=1}^{\infty} ix^{i} = x\frac{d}{dx}\left(\sum_{i=1}^{\infty} x^{i}\right) \tag{F-24}$$

Substituting Equation (F-20), for the summation reduces the summation to an algebraic expansion:

$$\sum_{i=1}^{\infty} ix^{i} = x\frac{d}{dx}\left(\frac{x}{(1-x)}\right) = x\left(\frac{x}{(1-x)^{2}}\right) \tag{F-25}$$

$$\sum_{i=1}^{\infty} ix^{i} = \frac{x}{(1-x)^{2}} \tag{F-26}$$

If we substitute Equation (F-26) into Equation (F-21), we obtain:

$$\frac{v}{v_m} = \frac{\dfrac{cx}{(1-x)^{2}}}{1 + \dfrac{cx}{(1-x)}} = \frac{cx}{(1-x)^{2}\left(1 + \dfrac{cx}{(1-x)}\right)} \tag{F-27}$$

$$\frac{v}{v_m} = \frac{cx}{(1-x)(1-x+cx)} \tag{F-28}$$

Adsorption on a free surface at the saturation pressure of the adsorptive, p_0, results in the formation of an infinite number of monolayers. If $v = \infty$ and $p = p_0$, then:

$$\frac{v}{v_m} = \infty = \frac{cx}{(1-x)(1-x+cx)} \qquad \text{(F-29)}$$

which requires x = 1 for finite values of c.

Then

$$x = 1 = \frac{p_o}{g} \exp(\frac{E_L}{RT}) \qquad \text{(F-30)}$$

or

$$\frac{1}{g} \exp(\frac{E_L}{RT}) = \frac{1}{p_o}$$

and

$$\frac{p}{p_o} = p\frac{1}{g} \exp(\frac{E_L}{RT}) \qquad \text{for all p}$$

$$\frac{p}{p_o} = x \qquad \text{(F-31)}$$

The substitution of Equation (F-31) into Equation (F-29) gives:

$$\frac{v}{v_m} = \frac{c(\frac{p}{p_o})}{(1 - \frac{p}{p_o})(1 + \frac{p}{p_o} + \frac{cp}{p_o})}$$

$$v = \frac{v_m cp}{(po-p)\,[1 + (c-1)\frac{p}{p_o}]} \qquad \text{(F-32)}$$

$$\frac{1}{v_m c}\left[1 + (c-1)\frac{p}{p_o}\right] = \frac{p}{v(p_o - p)}$$

$$\frac{p}{v(p_o - p)} = \frac{1}{v_m c} + \frac{(c-1)p}{v_m c \; p_o} \qquad \text{(F-33)}$$

Equation (F-33) is known as the BET (A) equation.

There are three other BET equations which relieve assumptions that were included as part of the derivation of the BET (A) equation. The BET (B) equation relieves the assumption that an infinite number of monolayers form. Adsorption in the pores of solid adsorbents permits the formation of a limited number of monolayers. Consequently, at higher dimensionless pressures, the pores of the catalyst limit the formation of additional monolayers and the actual adsorption is less than the adsorption predicted by the BET (A) equation. This normally occurs above dimensionless pressures greater than x = p/po greater than 0.35, but it can occur at lower dimensionless pressures in materials with small pore diameters.

The BET (C) equation relieves the assumption that $E_2 = E_L$, that is, that the heat of adsorption of the second monolayer is equal to the heat of condensation of liquid adsorptive.

The BET (D) equation relieves the assumption in the BET (B) equation that the pores are all of equal size.

Each of the equations are derived below.

The Derivation of the BET (B) Equation

The BET (B) equation assumes that an infinite number of monolayers is formed. The derivation of the BET (A) equation and the BET (B) equations are identical until that assumption is applied in the derivation of the BET (A) equation. Equation (F-19) is the starting point for the derivation of the BET (B) equation. Since only n monolayers are formed, the maximum limit of the summation is n and not infinity.

$$\frac{v}{v_m} = \frac{c \sum_{i=1}^{n} i x^i}{1 + c \sum_{i=1}^{n} x^i} \qquad \text{(F-19)}$$

The summations can be expanded as follows:

$$\frac{v}{v_m} = \frac{c \left[\sum_{i=1}^{\infty} i x^i - \sum_{i=n+1}^{\infty} i x^i \right]}{1 + c \left[\sum_{i=1}^{\infty} x^i - \sum_{i=n+1}^{\infty} x^i \right]} \qquad \text{(F-34)}$$

Substituting Equation (F-26) for the first summation that appears in Equation (F-34) and substituting Equation (F-20) for the first summation in the denominator of Equation (F-34) yields:

$$\frac{v}{v_m} = \frac{c \frac{x}{(1-x)^2} - \sum_{i=n+1}^{\infty} i x}{\left[1 + \frac{cx}{(1-x)} - c \sum_{i=n+1}^{\infty} x^i \right]} \qquad \text{(F-35)}$$

The summations with limits of n+1 and infinity must be converted to closed algebraic expressions.

The summation in the denominator can be converted to a closed algebraic expression by factoring out x^n so that its lower limit is one. The resulting summation has the closed algebraic form that appeared in the derivation of the BET (A) equation.

$$\sum_{i=n+1}^{\infty} x^i = x^n \sum_{i=1}^{\infty} x^i = x^n \frac{x}{(1-x)^2} = \frac{x^{n+1}}{(1-x)^2} \qquad \text{(F-36)}$$

or:

$$\sum_{i=n+1}^{\infty} x^i = \frac{x^{n+1}}{(1-x)^2} \qquad \text{(F-37)}$$

The summation in the numerator of Equation (F-35) can be converted to a closed algebraic form by the same method with which the equivalent summation was converted in the derivation of the BET (A) equation. The summation in the numerator of Equation (F-35) can be expressed as the following:

$$\sum_{i=n+1}^{\infty} ix^i = x \frac{d}{dx} \left[\sum_{i=n+1}^{\infty} x^i \right]$$

Substituting Equation (F-37) for the summation term yields:

$$\sum_{i=n+1}^{\infty} ix^i = x \frac{d}{dx} \left[\frac{x^{n+1}}{(1-x)} \right]$$

$$\sum_{i=n+1}^{\infty} ix^i = x \frac{[(n+1)x^n - nx^{n+1}]}{(1-x)^2}$$

$$\sum_{i=n+1}^{\infty} ix^i = \frac{(n+1)x^{n+1} - nx^{n+2}}{(1-x)^2} \qquad \text{(F-38)}$$

Substituting (F-38) and (F-37) into (F-35) gives the following:

$$\frac{v}{v_m} = c\,\frac{\left[\frac{x}{(1-x)^2} - \frac{(n+1)x^{n+1} - nx^{n+2}}{(1-x)^2}\right]}{1 + c\left[\frac{x}{(1-x)} - \frac{x^{n+1}}{(1-x)}\right]} \qquad \text{(F-39)}$$

Factoring and cancelling give:

$$\frac{v}{v_m} = \frac{cx\,[1 - (n+1)x^n + nx^{n+1}]}{(1-x)(1 - x + cx - cx^{n+1})}$$

or:

$$v = \frac{cv_m x\,[1 - (n+1)x^n + nx^{n+1}]}{(1-x)\,[1 + (c-1)x - cx^{n+1}]} \qquad \text{(F-40)}$$

Equation (F-40) is known as the BET (B) equation. For the special case of n = 1, this equation reduces to the Langmuir equation by the following transformation:

$$v = \frac{cv_m x\,(1 - 2x + x^2)}{(1-x)\,[1 + (c-1)x - cx^2}$$

Factoring yields:

$$v = \frac{cv_m x\,(1-x)^2}{(1-x)(1-x)(1+cx)}$$

Cancelling terms yields:

$$v = \frac{cv_m x}{(1 + cx)} \qquad \text{(F-41)}$$

If c/po is set equal to b, the result is:

$$\frac{v}{v_m} = \frac{\left[\frac{c}{p_0}\right] p}{\left(1 + \frac{cp}{p_0}\right)} = \frac{bp}{(1 + bp)} \qquad \text{(F-42)}$$

which is the Langmuir equation.

The Derivation of the BET (C) Equation

The derivation of the BET (C) equation relaxes two assumptions employed in the derivation of the BET (A) equation, that is:

(1) the heat of adsorption of the second monolayer is equal to the heat of condensation of the liquid adsorptive; and

(2) the packing of the molecules in the first monolayer is the same as the packing of the molecules in the liquid state.

The derivation of the BET (C) equation is the same as the derivation of the BET (A) equation up until the point that assumptions 1 and 2 above are applied. Starting with Equation (F-7):

$$\frac{v}{Av_0} = \frac{v}{v_m} = \frac{\sum_{i=0}^{\infty} i s_i}{\sum_{i=0}^{\infty} s_i} \qquad \text{(F-7)}$$

When i = 0, the first term in the upper summation is equal to 0, which yields:

$$\frac{v}{Av_0} = \frac{v}{v_m} = \frac{\sum_{i=1}^{\infty} is_i}{\sum_{i=0}^{\infty} s_i} \qquad \text{(F-43)}$$

The heats of adsorption of the third and higher monolayers are assumed to be equal to the heat of condensation of the adsorptive, so the following is true,

$$E_3 = E_4 = \ldots. = E_i = E_L \qquad \text{(F-44)}$$

and

$$\frac{b_3}{a_3} = \frac{b_4}{a_4} \; . \; . \; . \; . \; . = \frac{b_i}{a_i} = g \qquad \text{(F-45)}$$

From Equation (F-11), the following is known:

$$s_1 = ys_0 \qquad \text{where } y = \frac{a_1}{b_1} p \exp\left(\frac{E_1}{RT}\right) \qquad \text{(F-11)}$$

Since $E_2 = E_L$, a new quantity, z, is defined:

$$s_2 = zs_1 = zys_0; \qquad \text{where } z = \frac{a_2}{b_2} p \exp\left[\frac{D_2}{RT}\right] \qquad \text{(F-46)}$$

$$s_3 = xs_2 = xzs_1 = xzys_0; \qquad \text{where } x = \frac{a_3}{b_3} p \exp\left[\frac{E_3}{RT}\right] \qquad \text{(F-47)}$$

or:

$$x = \frac{p}{g} \exp\left[\frac{E_L}{RT}\right]$$

For the fourth monolayer:

$$s_4 = xs_3 = x^2s_2 = x^2zs_1 = x^2zys_0 \tag{F-48}$$

For the ith monolayer:

$$s_i = xs_{i-1} = x^{i-2}zs_1 = x^{i-2}zys_0 \quad i \geq 2 \tag{F-49}$$

Equation (F-49) does not apply for i=1. However, for s_1, the following is true:

$$s_1 = cxs_0 \tag{F-50}$$

The variable c is defined as it was in Equation (F-16) in the derivation of the BET (A) equation. Since $E_2 = E_L$, an additional variable, b, is also defined as follows:

$$b = \frac{z}{x} = \frac{a_2}{b_1} g \exp\left[\frac{(E_2 - E_L)}{RT}\right] \tag{F-51}$$

Substituting (F-16) and (F-51) into (F-49) gives:

$$s_i = x^{i-2}zys_0 = x^ibcs_0 \tag{F-52}$$

Equation (F-44) can be rewritten as:

$$\frac{v}{v_m} = \frac{\delta s_1 + \sum_{i=2}^{\infty} is_i}{s_0 + s_1 + \sum_{i=2}^{\infty} s_i} \tag{F-53}$$

δ is defined as the ratio of the volume of adsorptive required to form the first monolayer to the volume of adsorptive required to form subsequent monolayers:

$$\delta = \frac{v_{m,1}}{v_m} \tag{F-54}$$

δ allows for the possibility that molecules of adsorptive packed into the first monolayer are in an adsorbed state which is packed more densely than adsorptive molecules in the liquid phase but less densely than adsorptive molecules in the solid phase. Since $v_{m,1}$, the volume of adsorptive required to form a monolayer on the bare surface, is greater than v_m for any other subsequent monolayer o should be greater than one, but it should not exceed the ratio of the solid density to the liquid density raised to the 2/3 power.

Substituting (F-11) and (F-52) into (F-53) gives:

$$\frac{v}{v_m} = \frac{\delta y s_0 + \sum_{i=2}^{\infty} b c s_0 (i x^i)}{s_0 + c s_0 x + \sum_{i=2}^{\infty} b c s_0 (x^i)}$$

$$\frac{v}{v_m} = \frac{\delta c x s_0 + b c s_0 \sum_{i=2}^{\infty} i x^i}{s_0 + c s_0 x + b c s_0 \sum_{i=2}^{\infty} x_i} \tag{55}$$

s_0 and c can be factored out of the numerator to give:

$$\frac{v}{v_m} = \frac{cs_0\ (\delta x + b \sum_{i=2}^{\infty} ix^i}{s_0\ (1 + cx + bc \sum_{i=2}^{\infty} x^i)} \qquad \text{(F-56)}$$

The summations with the limits 2 and infinity can be converted to summations with limits of 1 and infinity.

$$\frac{v}{v_m} = \frac{c\ (\delta x + b \sum_{i=1}^{\infty} ix^i - bx)}{(1 + cx + bc \sum_{i=1}^{\infty} x^i - bcx)} \qquad \text{(F-57)}$$

Substituting (F-20) and (F-22) into (F-57) yields:

$$\frac{v}{v_m} = \frac{c\ (\delta x + b \dfrac{x}{(1-x)^2} - bx)}{(1 + cx + \dfrac{bcx}{(1-x)} - bcx)} \qquad \text{(F-58)}$$

Factoring $\frac{x}{(1-x)^2}$ out of the numerator and $\frac{1}{(1-x)}$ out of the denominator yields:

$$\frac{v}{v_m} = \frac{\dfrac{cx}{(1-x)^2}\ [\delta(1-x)^2 + b - b(1-x)^2]}{\dfrac{1}{(1-x)}\ [(1-x) + cx(1-x) + \dfrac{bcx}{(1-x)} - bcx(1-x)]}$$

Expanding and distributing yields:

$$\frac{v}{v_m} = \frac{cx}{(1-x)}\ [\frac{\delta(1-2x+x^2) + b - b(1-2x+x^2)}{1 - x + cx - cx^2 + bcx - bcx + bcx^2}]$$

Consolidation of terms in the numerator finally yields:

$$v = \frac{v_m cx}{(1-x)} \left[\frac{\delta + (b-\delta)(2x-x^2)}{1 + (c-1)x + (b-1)cx^2} \right] \qquad \text{(F-59)}$$

Equation (F-59) is the BET (C) equation.

The BET (D) equation requires no lengthy derivation, but it is included here for purposes of completeness. The BET (D) equation results form the derivation of the BET (B) equation In the derivation of the BET (B) equation, it was assumed that the pores were all of uniform size so that only n monolayers could form in any pore. When there is a wide distribution of pore sizes, the BET (B) equation will not suitably predict the data.

Equation (F-40) is the BET (B) equation:

$$v = \frac{cv_m x \, [1 - (n+1)x^n + nx^{n+1}]}{(1-x) \, [1 + (c-1)x - cx^{n+1}]} \qquad \text{(F-40)}$$

The left hand term of the right hand side is not a function of the pore size distribution and it will not be manipulated to derive the BET (D) equation. The right hand term of the right hand side is a function of the pore size distribution as manifest in the variable n. Each set of pores with the same pore size distribution has the same diameter and consequentially the same value for n. For each set of pores with the same pore size, the right hand term of the right hand side can be written as follows:

$$\frac{1 - (n+1)x^n + nx^{n+1}}{1 + (c-1)x - cx^{n+1}} \qquad \text{(F-60)}$$

The fraction of the surface that is contained in each set of pores can be multiplied in the front of each expression equivalent to Equation (F-60). Summing for all pores gives the BET (D) equation.

$$v = \frac{v_m c x}{(1-x)} \sum_{i=1}^{\infty} \beta_n \left[\frac{1 - (n+1)x^n + nx^{n+1}}{1 + (c-1)x - cx^{n+1}}\right] \qquad \text{(F-61)}$$

β_n here is the fraction of the total surface contained in pores that can contain no more than n monolayers.

The procedure for using the BET (B), BET (C), and BET (D) equations is to first use the BET (A) equation to determine v_m and c, and then to use subsequent equations to determine the respective variables that give the best fit of a plot of the curve with the data.

The BET (A) equation is used far more often than the other three equations combined, but they are useful in various applications and can provide insights to the nature of an adsorbent.

APPENDIX G

BET SURFACE AREA COMPUTER PROGRAM

A. Program for the Calculation of BET Surface Areas

BET1 is a Fortran program written to process data obtained from the BET equipment described in Section VII. Sample input and output for this program are included here. The data presented was taken from run number 7 in which a complete adsorption/desorption isotherm was determined for a sample of HZSM-5 catalyst (sample 6).

Table G-1

Program Listing for BET1

```
C   A program to calculate Vadsorbed from BET data, and to
C  perform a linear regression on the data to determine the surface
C  area and the heat of adsorption, (E1-EL).
C   Inputs include the vapor pressure of nitrogen at the
C  temperature of the cell, the temperature of the cell, the
C  temperature of the doser manifold, the volume of the doser
C  manifold, the volume of the cell at liquid nitrogen
C  temperature, the volume of the cell at ambient temperature,
C  the mass of the sample and the number of data points that were
C  taken. Additional information includes the number of points to
C  be used to determine the monolayer volume and whether or not
C  to use the Langmuir or BET equation to determine the monolayer
C  volume. Finally the data points obtained from the adsorption
C  equipment are needed. With each set of data points the volume
C  of the dosing manifold is needed. If zero is input then the
C  volume that is used in the mass balance is the volume that was
C  used in the last step of the mass balance. This allows for the
C  possibility that the operator of the adsorption/desorption equipment
C  can use different dosing volumes to facilitate the determination of
C  the adsorption/desorption isotherm.
C   The method is to calculate the amount of gas adsorbed at
C  each adsorptive pressure and to fit a set of points to a straight
C  line by least squares. The slope and y-intercept of the line will
C  be related to the monolayer volume and the heat of adsorption
C  of adsorbate on the surface. Data points below a dimensionless
C  pressure of P/Po of 0.01-0.05 are not included in the least
C  squares because such points do not fit the theory of the
C  Langmuir or BET equations very well. Since this program was
C  used almost exclusively to calculate the surface area of
C  zeolites, P/Po ≤ 0.01 were not used. For larger pore adsorbents
C  the higher value than P/Po = 0.01 should be used in this program.
```

```
C   Outputs are the surface area per unit mass of sample, the
C  monolayer volume, the slope and y-intercept of the line that
C  was used in the least squares approximation. A coefficient is
C  also printed which is the average percentage deviation of each
C  point from the least squares approximation. The points used
C  for the least squares method are also printed.
C   If the Langmuir equation is used to determine the monolayer
C  volume then the straight line is generated from it and the 'b-
C  value' is included in the output. If the BET equation is used
C  then the 'c-value' is included in the output. Output includes
C  the volume (STP) of adsorbent adsorbed at various pressures
C  and dimensional pressures (P/Po).
C
C                    Variables
C      PO--------the partial pressure of nitrogen at the
C               temperature of the sample in the cell
C      TM--------the temperature of the dosing manifold
C      TC--------the temperature of the cryogenic portion of the
C               cell
C      VCC-------the volume of the cell at cryogenic temperature
C      VCH-------the volume of the cell at ambient temperature
C      NAVAN2----the surface area covered by a mole of nitrogen
C               molecules, in m2
C      C---------the 'c-value' of the BET equation or the 'b-
C               value of the Langmuir equation
C      E1--------the (E1-EL) of the BET equation, or the heat of
C               adsorption of the Langmuir equation
C      R---------Gas Constant, 1.9869 cal./gmol.K
C      ASMPL-----surface area of sample per unit mass
C      VMONO-----monolayer volume
C      BETA1,BETA2,ALPHA1,ALPHA2----quantities of the least
C              squares method
C      S--------fit coefficient, average percentage deviation
C              from least squares approximation
C      M--------slope of line generated by least squares method
C      B--------y-intercept of the line generated by least
C              squares
C      N--------the number of data points corresponding to the
C              number of points taken to determine the
C              adsorption/desorption isotherm
C      NO-------the number of points to be disregarded for the
C              linear regression because they were taken at
C              too low of a pressure, see 'the BET paper'.
C      NBET-----the cutoff of points to be considered for the
C              linear regression
C      ASKM-----character work variables for asking questions to
C              the user
```

```
C            Arrays
C       P1-------contains the initial pressures of the dosing
C                volume before it was opened to the sample
C       P2-------contains the equilibrium pressures in the
C                dosing manifold and sample cell
C       PE-------contains the pressure in the sample cell
C                which is equal to P2 of the previous data
C                point
C       VADS-----contains the volume of adsorbent (STP) adsorbed
C                on the sample at each data point in cc./unit
C                mass
C       X,Y------contains the points to be used for the least
C                squares approximation
C       VM-------the volume of the dosing manifold for each point
C       VMAYBE---work array used with VM
C
C Variable declarations
      REAL P1(60),P2(60),PE(60),VADS(60),X(60),Y(60)
      REAL PO,TM,TC,VCC,VCH
      INTEGER I,N,NO
      CHARACTER*1 ASKM
C
      REAL BETA1,BETA2,ALPHA1,ALPHA2,S,M,B
      INTEGER NBET
C
      REAL NAVAN2,VM(60),VMAYBE(60)
      REAL C,E1,R,ASMPL,MSMPL,VMONO
C
C Input data
 5    PRINT *,'Input PO,VCH,VCC.'
      READ *, PO,VCH,VCC
      WRITE(6,6)PO,VCH,VCC
 6     FORMAT(2X,F5.1,', ',F6.3,', ',F6.3)
      PRINT *, ' Input TM and TC.'
      READ *, TM,TC
      WRITE(6,7)TM,TC
 7     FORMAT(2X,F6.2,', ',F6.2)
      PRINT *, ' Mass of sample?'
      READ *, MSMPL
      WRITE(6,8)MSMPL
 8     FORMAT(2X,F8.5)
C
C Initialize data
      NAVAN2= 9.7556 *(10**4)
      R= 1.9869
C
C Input data
```

```
      PRINT *, 'No. of points?'
      READ *, N
      WRITE(6,9)N
 9     FORMAT(2X,I2)
C
      PRINT *, ' Use BET or Langmuir equation? '
      READ(5,70)ASKM
 70    FORMAT(1X,A1)
      WRITE(6,21)ASKM
 21    FORMAT(2X,A2)
C
      PRINT *, ' Input P1"s and P2"s, and VM.'
      DO 10 I=1,N
        READ *, P1(I),P2(I),VMAYBE(I)
        IF(VMAYBE(I) .NE. 0.)THEN
           VM(I)= VMAYBE(I)
        ELSE
           VM(I)= VM(I-1)
        ENDIF
 10    CONTINUE
C
C Calculate mass balance
      PE(1)= 0.
      VADS(1)= (273.15/760.)*( VM(1)/TM*(P1(1)-P2(1)) +
     #  (VCC/TC+VCH/TM)*(PE(1)-P2(1)) )/MSMPL
C
      DO 20 I=2,N
         PE(I)= P2(I-1)
         VADS(I)= VADS(I-1) + (273.15/760.)*( VM(I)/TM*
     #        (P1(I)-P2(I)) + (VCC/TC+VCH/TM)*(PE(I)-P2(I)) )/MSMPL
 20    CONTINUE
C
C Send data from mass balance to be put in the particular
C   equation to get points for least squares approximation
      IF( ASKM .EQ. 'L' )THEN
          CALL LANGMU(VADS,P2,N,X,Y)
      ELSE
          CALL BET(VADS,P2,PO,N,NO,X,Y)
      ENDIF
C
      DO 40 I=1,N
         WRITE(6,41) P1(I),P2(I),VADS(I),X(I),Y(I)
 41       FORMAT(2X,F8.2,2X,F8.2,2X,F8.3,2X,F7.4,2X,F12.8)
 40    CONTINUE
C
C Perform linear regression using the least squares method
      PRINT *, ' How many points for the BET? '
```

```
      READ *, NBET
      WRITE(6,42)NBET
 42    FORMAT(1X,I2)
      IF( NBET .LE. (NO+2))THEN
        PRINT *,' ERROR!, More points are needed for the',
     #          ' linear regression.'
        STOP
      ENDIF
      WRITE(6,9)
C
      BETA1= 0.
      BETA2= 0.
      ALPHA1= 0.
      ALPHA2= 0.
      DO 60 I= NO+1, NBET
        BETA1= BETA1 + X(I)*Y(I)
        BETA2= BETA2 + (X(I)**2)
        ALPHA1= ALPHA1 + X(I)
        ALPHA2= ALPHA2 + Y(I)
 60    CONTINUE
C
      B= (ALPHA2- ALPHA1*(BETA1/BETA2))/( REAL(NBET) -
     #    (ALPHA1**2)/BETA2 )
      M= (BETA1-B*ALPHA1)/BETA2
C
      S= 0.
      DO 61 I= NO+1, NBET
        S= S + ( ((Y(I) - (M*X(I) + B))**2)**0.5 )/
     #      (M*X(I)+B)
 61    CONTINUE
        S= 100.*S/REAL(NBET-NO)
C
C Calculate monolayer volume, heat of adsorption, and surface
C     area
      IF(ASKM .EQ. 'L')THEN
        VMONO= 1./M
        C= 1./(VMONO*B)
        E1= 0.
      ELSE
        VMONO= 1./(M+B)
        C= (M+B)/B
        IF( C .LE. 0. )THEN
          PRINT *, ' ERROR! Intercept is less than zero.'
          E1= -1.
          GO TO 63
        ENDIF
        E1= R*TC*ALOG(C)
```

```
 63   ENDIF
     ASMPL= VMONO*NAVAN2/22400.
     IF( ASKM .EQ. 'L' )THEN
        VMONO= 1./M
        C= (M+B)/B
        IF( C .LE. 0. )THEN
           PRINT *,' ERROR! Intercept is less than zero. '
           GO TO 64
        ENDIF
        E1= R*TC*ALOG(C)
 64   ENDIF
     ASMPL= VMONO*NAVAN2/22400.
C  Print results
     WRITE(6,65)ASMPL,VMONO
 65    FORMAT(2X,'ASMPL= ',F7.2,2X,'Monolayer volume cc.,(STP)=',
    # F7.2)
     WRITE(6,67)C,E1
 67    FORMAT(2X,'C= ',F8.2,2X,'E1-EL= ',F8.2)
     WRITE(6,68)M,B,S
 68    FORMAT(6X,'Linear Equation from Least Squares',
    # ' Approximation',/,2X,'y = ',1PE11.4,'x + ';1PE11.4,/,
    # 2X,'S= ',G10.4,' %')
     STOP
     END
C
C
C
     SUBROUTINE LANGMU(VADS,P,N,X,Y)
     REAL VADS(60),P(60),X(60),Y(60)
     INTEGER I,NLANG
C
     PRINT *, ' No. of points for the Langmuir eqn.?'
     READ *, NLANG
C
     DO 10 I=1,NLANG
       Y(I)= P(I)/VADS(I)
       X(I)= P(I)
 10   CONTINUE
     PRINT *,'        P1         P2        VADS        P',
    # '     P/V'
     PRINT *,'----------------------------------------',
    # '------------'
     DO 20 I=2,NLANG
        DELTA= (Y(I)-Y(I-1))/(X(I)-X(I-1))
        PRINT *, DELTA
 20   CONTINUE
     RETURN
```

```
      END
C
C
C
      SUBROUTINE BET(VADS,P,PO,N,NO,X,Y)
      REAL VADS(60), P(60), X(60), Y(60), PO
      INTEGER I,N,NO
C
      NO= 1
      DO 10 I=1,N
         X(I)= P(I)/PO
         IF( X(I).LE. 0.001 )THEN
           NO= I
         ENDIF
         Y(I)= P(I)/( VADS(I)*(PO-P(I)) )
 10   CONTINUE
      PRINT *, '     P1          P2     VADS        P/PO',
     #   '     P/V(PO-P)'
      PRINT *, '-------------------------------------',
     #   '-----------------'
      RETURN
      END
```

Table G-2

Sample Input for BET1

This table contains a sample input for Fortran program BET1. Since the program is free formatted it does not require that the data be input in a specific format.

The first line of data contains the vapor pressure of nitrogen at the temperature of the sample, the volume of the sample cell at ambient temperature and the volume of the sample cell at liquid nitrogen temperatures. The volumes must be input in units of cubic centimeters. The terms in the second line are the ambient temperature and the temperature of the cryogenic bath, both must be in degrees Kelvin. The third line is the mass of the sample in grams. The fourth line is the number of sets of data points for which the mass balance is to be calculated. The fifth line tells the computer that the BET (A) equation is to be used to calculate the surface area. The other choice is 'L' which tells the computer to use the Langmuir equation to calculate the surface area. The following lines each contain three data points. The first data point is the initial pressure in the dosing manifold before the dosing volume and the sample cell were allowed to come to equilibrium. The second data point is the pressure in the dosing volume after the dosing volume and the sample cell pressure had come to equilibrium. The final point is the volume of the dosing volume if the dosing volume is different than in the taking of the previous data point, if not, the third data point is zero. The very last point tells the program how many points are to be used for calculating the BET surface area. BET1 automatically eliminates points taken at pressures less than $p/p_o < 0.01$. then it does the linear regression up to the n^{th} data point taken. Where n is the integer specified in the last data point.

```
655.8,2.512,4.981
299.6,76.1
.06045
42
 B
410.6,0.06,9.57
31.5,0.12,0.
33.9,1.,0.
37.5,5.2,0.
9.2,5.9,0.
23.3,9.1,0.
35.7,14.5,0.
38.5,19.7,0.
54.7,27.7,0.
70.,37.6,0.
80.4,47.7,0.
112.7,63.4,0.
154.,86.2,0.
284.5,138.5,0.
323.5,189.1,0.
365.7,238.2,0.
374.7,276.2,0.
455.6,326.3,0.
518.5,379.1,0.
516.4,415.8,0.
605.3,465.3,0.
658.1,512.9,0.
589.5,563.1,60.84
652.3,621.5,0.
706.3,640.0,9.57
677.9,646.8,0.
672.8,650.4,0.
685.5,651.9,0.
684.4,654.,0.
717.2,655.3,0.
721.2,655.7,0.
510.2,650.1,0.
490.0,628.4,0.
269.1,530.7,0.
344.5,477.3,0.
243.4,410.4,0.
199.7,350.6,0.
137.1,304.9,0.
63.1,264.6,0.
112.9,157.5,60.84
1.5,115.6,9.57
22.2,91.3,0.
9
```

Table G-3

Sample Output from BET1

This table contains a sample output from BET1. The output is clearly explained except the very last term, 'S', which is the average percentage deviation of all the points used in the linear regression from the value predicted based on the slope and y-intercept of the least squares fit of those points.

```
Input PO,VCH,VCC.
 655.8,  2.512,  4.981
 Input TM and TC.
 299.60,  76.10
 Mass of sample?
  0.06045
No. of points?
 42
 Use BET or Langmuir equation?
  B
 Input P1's and P2's, and VM (manifold volume).

      P1            P2           VADS         P/PO         P/V(PO-)

    410.60         0.06         77.942       0.0001       0.00000117
     31.50         0.12         83.875       0.0002       0.00000218
     33.90         1.00         89.737       0.0015       0.00001702
     37.50         5.20         94.027       0.0079       0.00008500
      9.20         5.90         94.347       0.0090       0.00009622
     23.30         9.10         95.639       0.0139       0.00014713
     35.70        14.50         97.294       0.0221       0.00023239
     38.50        19.70         98.582       0.0300       0.00031415
     54.70        27.70        100.198       0.0422       0.00044014
     70.00        37.60        102.005       0.0573       0.00059626
     80.40        47.70        103.781       0.0727       0.00075583
    112.70        63.40        106.251       0.0967       0.00100725
    154.00        86.20        109.118       0.1314       0.00138688
    284.50       138.50        113.886       0.2112       0.00235091
    323.50       189.10        117.197       0.2884       0.00345730
    365.70       238.20        119.856       0.3632       0.00475905
    374.70       276.20        121.881       0.4212       0.00596984
    455.60       326.30        124.443       0.4976       0.00795779
    518.50       379.10        127.737       0.5781       0.01072572
    516.40       415.80        130.731       0.6340       0.01325236
    605.30       465.30        135.589       0.7095       0.01801416
    658.10       512.90        142.268       0.7821       0.02522861
    589.50       563.10        152.104       0.8586       0.03993594
    652.30       621.50        163.653       0.9477       0.11071908
    706.30       640.00        168.123       0.9759       0.24093276
    677.90       646.80        171.044       0.9863       0.42016417
    672.80       650.40        173.718       0.9918       0.69333816
    685.50       651.90        179.441       0.9941       0.93153632
    684.40       654.00        184.292       0.9973       1.97152102
    717.20       655.30        195.477       0.9992       6.70461702
    721.20       655.70        207.741       0.9998      31.57103160
    510.20       650.10        183.630       0.9913       0.62109768
    490.00       628.40        166.872       0.9582       0.13743640
    269.10       530.70        160.081       0.8092       0.02650034
```

```
      344.50         477.30          158.303        0.7278          0.01689130
      243.40         410.40          155.957        0.6258          0.01072330
      199.70         350.60          153.551        0.5346          0.00748125
      137.10         304.90          141.746        0.4649          0.00613005
       63.10         264.60          121.170        0.4035          0.00558209
      112.90         157.50          114.339        0.2402          0.00276437
        1.50         115.60          111.064        0.1763          0.00192678
       22.20          91.30          108.608        0.1392          0.00148917

How many points for the BET?
9

ASMPL=  418.07  Monolayer volume cc.,(STP)=  95.99
C=  7677.11  E1-EL=  1352.66
    Linear Equation from Least Squares Approximation
y =  1.0416E-02x +  1.3569E-06
S= 0.7458     %
```

C. Program for the Prediction of Adsorption Isotherms

Because of the narrow pores of ZSM-5 zeolite the BET(A) equation can only predict the amount of nitrogen adsorbed on the zeolite at dimensionless pressures $p/p_o < 0.1$. The BET(B) equation relieves the infinite pore diameter assumption used in the derivation of BET(A) equation. The BET(D) equation relieves the homogenous pore diameter assumption used in derivation of the BET(B) equation. Consequently a Fortran language program was written to predict the adsorption of nitrogen (or any other adsorptive) on a adsorbent whose pore properties are known or estimated. This program was used to find the right combination of pore properties which would permit an estimation of the adsorption of nitrogen on ZSM-5 zeolite. The derivation of the various BET equations are found in Appendix A.

Table G-4

Program Listing for BETD

```
                  Program Listing for BETD
C     Program to predict nitrogen adsorption data based on a
C   special form of the BET (D) equation (below). The BET(D)
C   equation is found in the original paper by Brunauer, Emmett
C   and Teller. That equation has been modified here to allow c
C   to vary according to pore size. For pores larger than 10-20
C   angstroms the heat of adsorption of adsorbate which appears
C   in c is fairly constant. While for micropores (less than
C   10-20 angstroms) the apparent heat of adsorption is higher.
C     Since this program was written mainly for estimating the
C   adsorption isotherms of zeolites which are microporous the
C   above modification of the BET (D) equation was necessary.
C     For each adsorbent, vm, the monolayer volume, needs to be
C   input.
C     The adsorption isotherm for an adsorbent with as many as
C   five different pore sizes can be estimated here. For each
C   type of pore the heat of adsorption (E1-EL) needs to be
C   input. In addition the fraction of the total surface area in
C   those pores needs to be input. The size of each pore is input
C   as n which is the number of monolayers of adsorbent which can
C   be adsorbed in that pore. n can be any real number.
C     The amount of adsorption adsorbate is calculated for p/po
C   from zero to (1-0.2delx) where delx is the increment by which
C   p/po is increased along the curve of vadsorbed vs. p/po. delx
C   is also an input variable.
C     The output data are the points of the adsorption curve,
C   vadsorbed vs. p/po.
C                 Variables
C    VM       monolayer volume
C    R        ideal gas constant
C    T        temperature of adsorbent, is set equal to 76.1 K
C             in this program. It can be changed for other
C             adsorbents than nitrogen
C    X        dimensionless pressure, p/po
C    VADS     the volume of adsorbent adsorbed at a given
C             dimensionless pressure x. VADS is in the same units
C             as VM
C    I        do variable
C    K        number of different pore types in the adsorbent,
C             must not exceed five
C
C                 Arrays
C    C        contains the BET equation 'c-values' for each pore
C             type
```

```
C     BET    the ß-values in the BET(D) equation, that is, the
C            fraction of the total adsorbent surface that is
C            contained in the pores of a certain type
C     N      the number of monolayers that can be formed in a
C            pore of a certain size
C     E1     the heat of adsorption of the first monolayer of
C            adsorbate minus the heat of condensation of liquid
C            adsorbate for each pore size. The values in the
C            array C are calculated from this value. BETD allows
C            this value to be different for different pore
C            sizes. E1 is to be in cal./gmole.
C
C
C
      REAL VM,C(5),BET(5),N(5),E1(5),R,T,VADS,X
      INTEGER I,K
C
      R= 1.9869
      T= 76.1

 1    WRITE(6,20)
 20   FORMAT(2X, ' Input number of types of pores and Vm.')
      READ(5,*)K, VM
      IF( K .GT. 5 )THEN
        PRINT *,' ERROR! K cannot be greater than 5.'
        GO TO 1
      ENDIF
      WRITE(6,2) K,VM
 2    FORMAT(2X,I2,2X,F7.2)
C
      DO 3 I=1,K
       WRITE(6,21)I
 21    FORMAT(2X,/, ' Input BETA and N for pore type ',I1)
       READ(5,*)BET(I),N(I)
       WRITE(6,4)BET(I),N(I)
 4       FORMAT(2X,F5.3,2X,F6.2)
 3    CONTINUE
C
      DO 5 I=1,K
       WRITE(6,22)I
 22      FORMAT(2X,/,' Input E1-EL for pore type ',I1)
       READ(5,*)E1(I)
       WRITE(6,6)E1(I)
 6       FORMAT(2X,F5.0)
       C(I)= EXP( E1(I)/(R*T) )
 5    CONTINUE
C
      WRITE(6,23)
```

```
 23  FORMAT(2X,/, ' Input delta p/po.')
     READ(5,*)DELX
     WRITE(6,24)DELX
 24   FORMAT(2X,F7.3)
     WRITE(6,25)
 25  FORMAT('1','----------------------------',/,
    # 2X,'p/po',6X,'Vads',/)
C
     X= 0.
  9  VADS= 0.
     DO 10 I=1,K
        VADS= VADS + BET(I)*C(I)*X/(1.-X) *
    #          ( 1. - (N(I)+1.)*(X**N(I)) +
    #          N(I)*(X**(N(I)+1.)) )/
    #          ( 1. + (C(I)-1.)*X - C(I)*(X**(N(I)+1.)) )
 10  CONTINUE
        VADS= VM*VADS
     IF(X .EQ. 0.)THEN
       WRITE(6,13)X,VADS
 13    FORMAT('+',1X,F6.4,',',F7.2,',')
     ELSE
       WRITE(6,12)X,VADS
 12    FORMAT(2X,F6.4,',',F7.2,',')
     ENDIF
     X= X + DELX
     IF( (X .GE. 1.) .AND. (Z .NE. 1.) )THEN
       Z= 1.
       X= X - 0.2*DELX
     ENDIF
     IF(X .GE. 1)STOP
     GO TO 9
     END
```

Table G-5

Sample Input for BETD

This table contains a sample input for the Fortran program BETD, which estimates the amount of adsorptive that is adsorbed on a material, where adsorption on that material can be described by the BET(D) equation.

The first line contains the number of different pore diameters in the adsorbent and the monolayer volume of adsorptive on the sample, in cm^3.(STP)/g. The next three data points contain the fraction of surface area contained in each pore type and the number of monolayers that can be formed in each type of pore. Specifying the number of monolayers that can be formed in each type of pore is equivalent to specifying the diameter of pore type.

The next three lines are the differential heats of adsorption of adsorptive in each pore type. The last line states the increments for which data points are to be calculated in terms of dimensionless pressure, p/p_o.

3,100.
0.47,1.2
0.50,1.95
0.03,30.
1500.
900.
800.
0.02

Table G-6

Sample Output from BETD

This table contains the output generated by BETD. It is obvious what each term represents. The volume adsorbed is in cm^3 (STP)/g of adsorbent.

```
 Input number of types of pores and Vm.
  3    100.00

Input BETA and N for pore type 1
 0.470     1.20

Input BETA and N for pore type 2
 0.500     1.95

Input BETA and N for pore type 3
 0.030    30.00

Input E1-EL for pore type 1
 1500.

Input E1-EL for pore type 2
  900.

Input E1-EL for pore type 3
  800.

Input delta p/po.
   0.020
```

```
-----------------------------
p/po      Vads
0.0000,   0.00,
0.0200,  94.99,
0.0400,  99.32,
0.0600, 101.64,
0.0800, 103.35,
0.1000, 104.78,
0.1200, 106.05,
0.1400, 107.22,
0.1600, 108.31,
0.1800, 109.33,
0.2000, 110.31,
0.2200, 111.25,
0.2400, 112.15,
0.2600, 113.02,
0.2800, 113.86,
0.3000, 114.69,
0.3200, 115.49,
0.3400, 116.27,
0.3600, 117.04,
0.3800, 117.80,
0.4000, 118.55,
0.4200, 119.29,
0.4400, 120.02,
0.4600, 120.75,
0.4800, 121.48,
0.5000, 122.22,
0.5200, 122.95,
0.5400, 123.70,
0.5600, 124.46,
0.5800, 125.23,
0.6000, 126.02,
0.6200, 126.84,
0.6400, 127.69,
0.6600, 128.58,
0.6800, 129.53,
0.7000, 130.53,
0.7200, 131.62,
0.7400, 132.80,
0.7600, 134.11,
0.7800, 135.56,
0.8000, 137.21,
0.8200, 139.08,
0.8400, 141.24,
0.8600, 143.74,
0.8800, 146.62,
0.9000, 149.92,
```

0.9200, 153.67,
0.9400, 157.83,
0.9600, 162.33,
0.9800, 167.05,
0.9960, 172.59,

APPENDIX II

DATA BASE MANAGEMENT SYSTEM FOR THE SURVEYED LITERATURE FROM THE HIGH DENSITY AVIATION FUEL PROJECT

The LITERATURE DATABASE FILES are created to match the needs of the research project for which the literature survey is to be complied. Then, each pertinent literature citation/reference can be stored as a record in the relative data files by utilizing the DATA TRANSITION function. The data transition process includes three independent modes: record addition, record editing, and record deletion. The MAINTENANCE routine is performed after each batch of citations has been transmitted, to confirm that no duplicated entries exist and to insure that the format of the input record is correct. Any error found in the records should be corrected by the use of the DATA TRANSITION routine. The literature in the database files can be searched and retrieved by using the author's name, journal name, year, or index as a search parameter in the SEARCHING routine. Multiple parameter searching is also included.

The structures of the related database files and the programs for the database management are already created and stored on the disk. The performance of the data (record) transition routine is supported by the general dBASE III software commands. The performance of searching and maintenance is supported by the 'SM' program.

Start Procedure

1 > Insert the system disk in disk drive A.

2 > Turn on power.

3 > Type the date and time; wait for the A> prompt.

4 > Insert dBASE III disk in drive A.

5 > Type dBASE ↵ (↵ means hit the return key).

6 > Wait until . prompt appears (The . prompt means the computer is under control of the dBASE III system.

Major Commands

1 > USE: open file.

2 > LIST: list all the files on the screen.

3 > DISPLAY: list the file or parts of the files on the screen.

4 > BROWSE: list the file and each record in one line.

5 > COPY: duplicate the structure or file to other file.

6 > APPEND: add the record at the end of file.

7 > EDIT: correct the existing record.

8 > DELETE: temporarily delete the record.

9 > PACK: permanently delete the record.

10 > GOTO: point to the desired record.

11 > SKIP: point to the next record.

12 > DO: execute the program.

13 > QUIT: return to DOS.

EXAMPLE:

```
USE TT

. LIST

Record#     AUTHOR1          AUTHOR2          AUTHOR3          AUTHOR4
AUTHOR5
                  AUTHOR6                    JOURNAL              VOL
                    YEAR INDEX1                 INDEX2            INDEX3
            INDEX4            INDEX5              TITLE
      1      Hanson, F.V.   Bensen, J.E.
                                          J. Catal.          31, 471
                    73   Pump                Gas Circulation
                                              An Inexpensive Noncontaminat
ing Gas Recirculation Pump

      2      Hanson, F.V.   Boudart, M.
                                          J. Catal.          53, 56
                    78   Pt                 Hydrogen          Oxygen
                                              The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

      3      Hanson, F.V.   Miller, J.D.   Oblad, A.G.
                                          U.S. Pat.           4,3337,14
3                   82   Tar Sand
                                              Process for Obtaining Produc
ts from Tar Sand

      4
                                          J. Catal.          53, 56
                    78
```

```
. DISPLAY ALL

Record#     AUTHOR1          AUTHOR2          AUTHOR3          AUTHOR4
AUTHOR5
                 AUTHOR6                 JOURNAL              VOL
                   YEAR INDEX1             INDEX2           INDEX3
          INDEX4           INDEX5            TITLE
     1  · Hanson, F.V.   Bensen, J.E.
                                          J. Catal.            31, 471
                   73   Pump                 Gas Circulation
                                              An Inexpensive Noncontaminat
ing Gas Recirculation Pump

     2    Hanson, F.V.   Boudart, M.
                                          J. Catal.            53, 56
                   78   Pt                  Hydrogen          Oxygen
                                              The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

     3    Hanson, F.V.   Miller, J.D.   Oblad, A.G.
                                          U.S. Pat.            4,3337,14
3                  82   Tar Sand
                                              Process for Obtaining Produc
ts from Tar Sand

Record#     AUTHOR1          AUTHOR2          AUTHOR3          AUTHOR4
AUTHOR5
                 AUTHOR6                 JOURNAL              VOL
                   YEAR INDEX1             INDEX2           INDEX3
          INDEX4           INDEX5            TITLE
     4
                                          J. Catal.            53, 56
                   78
```

```
. BROWSE

Record No.       2    TT
AUTHOR1-------- AUTHOR2-------- AUTHOR3-------- AUTHOR4--------
Hanson, F.V.    Bensen, J.E.
Hanson, F.V.    Boudart, M.
Hanson, F.V.    Miller, J.D.    Oblad, A.G.


Record No.       2    TT
AUTHOR5-------- AUTHOR6-------------- JOURNAL------------------
                                              J. Catal.
                                              J. Catal.
                                              U.S. Pat.
                                              J. Catal.


Record No.       2    TT
VOL------------ YEAR INDEX1---------------- INDEX2----------------
31, 471          73  Pump                   Gas Circulation
53, 56           78  Pt                   Hydrogen
4,3337,143       82  Tar Sand
53, 56           78
```

After the BROWSE command, each record appears on the screen at one line. The right-side fields of the records can be seen by hitting the Control → keys. Screen editing can be done in the BROWSE mode; hit Control-End when complete.

Function Keys

The function keys at the left side of the keyboard can execute the special functions. They can be redefined by using some commands. (For details, see the dBASE III manual).

The function keys are defined as follows:

Function key F1: help
Function key F2: assist
Function key F3: list
Function key F4: dir
Function key F5: display structure
Function key F6: display status
Function key F7: display memory
Function key F8: display
Function key F9: append
Function key F10: edit

Data File Structure

The data file structures of the following are used for the surveyed literatures.

TT.DBF: database files of the surveyed literatures for practice purpose.

```
Structure for database  :    C:TT.dbf
Number of data records :    4
Date of last update     :    01/01/80
Field  Field name    Type            Width          Dec
   1   AUTHOR1       Character         15
   2   AUTHOR2       Character         15
   3   AUTHOR3       Character         15
   4   AUTHOR4       Character         15
   5   AUTHOR5       Character         25
   6   AUTHOR6       Character         25
   7   JOURNAL       Character         25
   8   VOL           Character         30
   9   YEAR .        Character          2
  10   INDEX1                  Character          20
  11   INDEX2                  Character          20
  12   INDEX3                  Character          20
  13   INDEX4                  Character          20
  14   INDEX5                  Character          20
  15   TITLE         Character        120
** Total **                           388
```

STDJOUR.DBF: database file for the standard journal name.

```
Structure for database   : C:STDJOUR.dbf
Number of data records  : 3
Date of last update       : 01/01/80
Field  Field name    Type           Width  Dec
   1   VJOUR                 Character         25
** Total **                             26
```

Create Data File Structure

1 > Use the CREATE command to create the desired file. (For details, see the dBASE III manual.)

2 > Use the COPY command to create the file structure from the existing files.

Example:

XXX.DBF: existing file

YYY.DBF: created file

```
.USE XXX ↵

.COPY STRUCTURE TO YYY.DBF ↵
```

Then, YYY.DBF has the same structure as the XXX.DBF.

or

```
.USE XXX ↵

.COPY TO YYY.DBF ↵
```

Then YYY.DBF has the same structure and the same data as the XXX.DBF.

Data Transition

Make sure the database file is in 'USE' before data transition.

1 > Add Record:

```
APPEND

Record No.          5
AUTHOR1
AUTHOR2
AUTHOR3
AUTHOR4
AUTHOR5
AUTHOR6
JOURNAL
VOL
YEAR
INDEX1
INDEX2
INDEX3
INDEX4
INDEX5
TITLE
```

The record appended at the current file appears on the screen. Input the data and hit Control-End when complete.

2 > Edit Record:

```
. EDIT 1

Record No.       1
AUTHOR1     Hanson, F. V.
AUTHOR2     Bensen, J. E.
AUTHOR3
AUTHOR4
AUTHOR5
AUTHOR6
JOURNAL     J. Catal.
VOL         31, 471
YEAR        73
INDEX1           Pump
INDEX2           Gas Circulation
INDEX3
INDEX4
INDEX5
TITLE       An Inexpensive Noncontaminating Gas Recirculation Pump
```

The edited record appears on the screen. Correct the errors and hit Control-End when complete.

Screen editing can also be done if several records having errors are found. For details, see the example of the BROWSE command in the "Major Commands" section.

3 > Deleted Record:

Use the following commands:

```
GOTO n ↵
DELETE ↵
```

The record of record number 'n' is temporarily deleted from the file. The deleted record can be recalled. (For details, see the dBASE III manual.)

Use the commands

```
GOTO n ↵
DELETE ↵
PACK   ↵
```

The record of record number 'n' is permanently deleted from the file.

You can use either the 'LIST' or the 'DISPLAY ALL' command to list the current file in order to confirm that the record has been deleted.

Data Searching and Maintenance

The searching and maintenance functions are executed with the ‘SM’ program as explained in the following figures.

An example performance of the 'SM' program is listed as follows.

```
DO SM





*****************************************************************
*                                                               *
*   THIS IS A SEARCHING AND MAINTENANCE PROGRAM FOR THE    *
*LITERATURE SURVEY, FINISHED UNDER THE AIR FORCE PROJECT.  *
*              Contract No. F33615-85-C-2567               *
*                                                               *
*  AUTHOR, JOURNAL NAME, YEAR, AND INDEX CAN BE USED AS    *
*  THE SEARCHING PARAMETERS; THE COMBINED SEARCHING ALSO   *
*                   CAN BE SELECTED.                       *
*                                                               *
*   THIS PROGRAM IS USED UNDER THE DBASE III SOFTWARE.     *
*                                                               *
*        THE PROGRAM IS WRITTEN BY KIEN-RU CHEN            *
*                                    NOVEMBER, 1985             *
*                                    FUELS ENGINEERING DEPT.    *
*                                    UNIVERSITY OF UTAH         *
*                                                               *
*****************************************************************

Press any key to continue.
```

```
INPUT THE FILE NAME INCLUDING THE EXTENSION(.DBF) TT.DBF
```

```
***************** MAIN MENU ******************
*                                            *
*   1> AUTHOR                4> INDEX        *
*   2> JOURNAL               5> MULTIPLE     *
*   3> YEAR                  6> MAINTENANCE  *
*                                            *
*            type Q to quit                  *
*                                            *
**********************************************

 INPUT THE SELECTION:
```

```
               ***************** MAIN MENU ******************
               *                                            *
               *   1> AUTHOR              4> INDEX          *
               *   2> JOURNAL             5> MULTIPLE       *
               *   3> YEAR                6> MAINTENANCE    *
               *                                            *
               *            type Q to quit                  *
               *                                            *
               **********************************************


                INPUT THE SELECTION:   1

                 INPUT THE AUTHOR NAME:      Hanson, F.V.


   SEARCHING PARAMETER:  Hanson, F.V.

Record#       AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4       AUTHOR5
                        AUTHOR6                   JOURNAL                 VOL
                           YEAR INDEX1                INDEX2             INDEX3
               INDEX4               INDEX5                TITLE
      1       Hanson, F.V.    Bensen, J.E.
                                                  J. Catal.               31, 471
                           73   Pump                  Gas Circulation
                                                          An Inexpensive Noncontaminat
ing Gas Recirculation Pump

      2       Hanson, F.V.    Boudart, M.
                                                  J. Catal.               53, 56
                           78   Pt                    Hydrogen           Oxygen
                                                          The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

      3       Hanson, F.V.    Miller, J.D.    Oblad, A.G.
                                                  U.S. Pat.               4,3337,14
3                          82   Tar Sand
                                                          Process for Obtaining Produc
ts from Tar Sand


AUTHOR SEARCHING COMPLETE !

Press any key to continue...
```

```
               ***************** MAIN MENU *****************
               *                                           *
               *   1> AUTHOR              4> INDEX         *
               *   2> JOURNAL             5> MULTIPLE      *
               *   3> YEAR                6> MAINTENANCE   *
               *                                           *
               *            type Q to quit                 *
               *                                           *
               *********************************************


                INPUT THE SELECTION:   2

                 INPUT THE JOURNAL NAME:     J. Catal.



   SEARCHING PARAMETER:  J. Catal.

Record#       AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4       AUTHOR5
                        AUTHOR6                  JOURNAL                  VOL
                           YEAR INDEX1              INDEX2              INDEX3
               INDEX4              INDEX5              TITLE
      1       Hanson, F.V.    Bensen, J.E.
                                                 J. Catal.                31, 471
                           73   Pump                Gas Circulation
                                                       An Inexpensive Noncontaminat
ing Gas Recirculation Pump

      2       Hanson, F.V.    Boudart, M.
                                                 J. Catal.                53, 56
                           78   Pt                  Hydrogen              Oxygen
                                                       The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

      3
                                                 J. Catal.                53, 56
                           78


JOURNAL NAME SEARCHING COMPLETE !

Press any key to continue...
```

```
              ***************** MAIN MENU ******************
              *                                            *
              *   1> AUTHOR               4> INDEX         *
              *   2> JOURNAL              5> MULTIPLE      *
              *   3> YEAR                 6> MAINTENANCE   *
              *                                            *
              *           type Q to quit                   *
              *                                            *
              **********************************************


               INPUT THE SELECTION:   3


              *************** YEAR SEARCHING MENU *****************

                   1> EQUAL THE INPUT YEAR
                   2> BEFORE THE INPUT YEAR (INCLUDING THE YEAR)
                   3> AFTER THE INPUT YEAR (INCLUDING THE YEAR)

                   INPUT THE SELECTION:    1

                   INPUT THE YEAR:   78


   TYPE SELECTION (1 =, 2 <=, 3 >=):   1
   SEARCHING         PARAMETER:  78

Record#       AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4        AUTHOR5
                        AUTHOR6                   JOURNAL                   VOL
                           YEAR INDEX1               INDEX2               INDEX3
               INDEX4             INDEX5                 TITLE
    1         Hanson, F.V.    Boudart, M.
                                                  J. Catal.                 53, 56
                           78    Pt                  Hydrogen             Oxygen
                                                         The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

    2
                                                  J. Catal.                 53, 56
                           78


YEAR SEARCHING COMPLETE !

Press any key to continue...
```

```
               ***************** MAIN MENU ******************
               *                                            *
               *   1> AUTHOR              4> INDEX          *
               *   2> JOURNAL             5> MULTIPLE       *
               *   3> YEAR                6> MAINTENANCE    *
               *                                            *
               *            type Q to quit                  *
               *                                            *
               **********************************************


                INPUT THE SELECTION:   4

         INPUT THE INDEX NAME:   Tar Sand


   SEARCHING PARAMETER:  Tar Sand


Record#       AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4        AUTHOR5
                        AUTHOR6                   JOURNAL                  VOL
                           YEAR INDEX1               INDEX2              INDEX3
               INDEX4               INDEX5                TITLE
      1       Hanson, F.V.    Miller, J.D.    Oblad, A.G.
                                                  U.S. Pat.                4,3337,14
3                          82   Tar Sand
                                                         Process for Obtaining Produc
ts from Tar Sand


INDEX SEARCHING COMPLETE !

Press any key to continue...
```

```
***************** MAIN MENU ******************
*                                            *
*   1> AUTHOR               4> INDEX         *
*   2> JOURNAL              5> MULTIPLE      *
*   3> YEAR                 6> MAINTENANCE   *
*                                            *
*            type Q to quit                  *
*                                            *
**********************************************

 INPUT THE SELECTION:   5
```

```
************ MULTIPLE SEARCHING MENU *************

   1> AUTHOR                4> INDEX
   2> JOURNAL               5> RETURN TO MAIN MENU
   3> YEAR

      INPUT THE SELECTION
```

```
               ************ MULTIPLE SEARCHING MENU *************

                  1> AUTHOR                 4> INDEX
                  2> JOURNAL                5> RETURN TO MAIN MENU
                  3> YEAR

                     INPUT THE SELECTION     1


               INPUT THE AUTHOR NAME:  Hanson, F.V.


   SEARCHING PARAMETER: Hanson, F.V.

Record#       AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4       AUTHOR5
                        AUTHOR6                   JOURNAL                   VOL
                           YEAR INDEX1                 INDEX2             INDEX3
               INDEX4               INDEX5                 TITLE
      1       Hanson, F.V.    Bensen, J.E.
                                                  J. Catal.                 31, 471
                           73   Pump                   Gas Circulation
                                                           An Inexpensive Noncontaminat
ing Gas Recirculation Pump

      2       Hanson, F.V.    Boudart, M.
                                                  J. Catal.                 53, 56
                           78   Pt                     Hydrogen           Oxygen
                                                           The Reaction Between Hydroge
n and Oxygen over Supported Platinum Catalysts

      3       Hanson, F.V.    Miller, J.D.    Oblad, A.G.
                                                  U.S. Pat.                 4,3337,14
3                          82   Tar Sand
                                                           Process for Obtaining Produc
ts from Tar Sand


AUTHOR SEARCHING COMPLETE !

Press any key to continue...
```

```
              ************ MULTIPLE SEARCHING MENU *************

                 1> AUTHOR                   4> INDEX
                 2> JOURNAL                  5> RETURN TO MAIN MENU
                 3> YEAR

                    INPUT THE SELECTION     4


              INPUT THE INDEX NAME:   Tar Sand


      SEARCHING PARAMETER: Tar Sand

Record#       AUTHOR1          AUTHOR2          AUTHOR3         AUTHOR4         AUTHOR5
                        AUTHOR6                     JOURNAL                    VOL
                           YEAR INDEX1                 INDEX2              INDEX3
               INDEX4                  INDEX5                  TITLE
     1        Hanson, F.V.     Miller, J.D.     Oblad, A.G.
                                                    U.S. Pat.                 4,3337,14
3                          82   Tar Sand
                                                                Process for Obtaining Produc
ts from Tar Sand



INDEX SEARCHING COMPLETE !

Press any key to continue...
```

```
***************** MAIN MENU ******************
*                                            *
*   1> AUTHOR              4> INDEX          *
*   2> JOURNAL             5> MULTIPLE       *
*   3> YEAR                6> MAINTENANCE    *
*                                            *
*            type Q to quit                  *
*                                            *
**********************************************

 INPUT THE SELECTION:   6
```

```
************ MAINTENANCE MENU *************

   1> DUPLICATE CHECK
   2> VERIFY
   3> RETURN TO MAIN MENU

INPUT THE SELECTION
```

```
************ MAINTENANCE MENU *************

   1> DUPLICATE CHECK
   2> VERIFY
   3> RETURN TO MAIN MENU

INPUT THE SELECTION : 1
```

```
THE FOLLOWING TWO RECORDS ARE DUPLICATED

RECORD NO. =            4
RECORD NO. =            2
```

```
Record#      AUTHOR1         AUTHOR2         AUTHOR3         AUTHOR4        AUTHOR5
                       AUTHOR6                     JOURNAL                    VOL
                          YEAR INDEX1                 INDEX2                INDEX3
              INDEX4               INDEX5                 TITLE
     3

                                                   J. Catal.                  53, 56
                          78
```

```
            DUPLICATE CHECKING COMPLETE !

            Press any key to continue...
```

```
************ MAINTENANCE MENU *************

   1> DUPLICATE CHECK
   2> VERIFY
   3> RETURN TO MAIN MENU

INPUT THE SELECTION : 2
```

```
JOURNAL NAME OF THE FOLLOWING RECORD NOT IN THE STANDARD STYLE

RECORD NO. =          3
JOURNAL NAME =        U.S. Pat.

VERIFY COMPLETE !

Press any key to continue...
```

```
             ************ MAINTENANCE MENU *************

                1> DUPLICATE CHECK
                2> VERIFY
                3> RETURN TO MAIN MENU

             INPUT THE SELECTION : 2
```

```
             *********** VERIFY MENU **************

               1> CONTINUE VERIFY
               2> DISCRETE VERIFY
               3> RETURN TO MAINTENANCE MENU

             INPUT   THE   SELECTION:      1

             INPUT THE RECORD NUMBER:      1


JOURNAL NAME OF THE FOLLOWING RECORD NOT IN THE STANDARD STYLE

RECORD NO. =          3
JOURNAL NAME = U.S. Pat.


VERIFY COMPLETE !

Press any key to continue...
```

Printout Procedure

The hard copies from the printer can be obtained by two methods.

1 > hit Ctrl P
The printout can be obtained from the latter data appeared on the screen.
Hit Ctrl P to cancel the hard copies.

2 > hit Shift PrtSc
The printout will be the same as the data on the screen.

Stop Procedure

1 > .QUIT ↵, return to the DOS A > prompt.
2 > Insert the DATABASE FILE BACKUP disk into drive A.
3 > A > COPY C:*.DBF A: ↵
4 > Take the disk from drive A, and keep the disk inside the disk bank.
5 > Turn off power.

```
clear
set Talk off
store ' ' to nul
store 'T' to MORE
store '                    ' to LI
CLEAR
@3,9 say   '***************************************************************** '
@4,9 say   '*    THIS IS A SEARCHING AND MAINTENANCE PROGRAM FOR THE          *'
@5,9 SAY   '*   LITERATURE SURVEY, FINISHED UNDER THE AIR FORCE PROJECT.      *'
@6,9 SAY   '*               Contract No. F33615-85-C-25867                    *'
@7,9 say   '*                                                                 *'
@8,9 SAY   '*     AUTHOR, JOURNAL NAME, YEAR, AND INDEX CAN BE USED AS        *'
@9,9 SAY   '*     THE SEARCHING PARAMETERS; THE COMBINED SEARCHING ALSO       *'
@10,9 SAY  '*     CAN BE SELECTED.                                            *'
@11,9 SAY  '*                                                                 *'
@12,9 SAY  '*     THE PROGRAM IS USED UNDER THE DBASE III SOFTWARE.           *'
@13,9 SAY  '*                                                                 *'
@14,9 SAY  '*     THE PROGRAM IS WRITTEN BY KIEN-RU CHEN                      *'
@15,9 SAY  '*                              NOVEMBER, 1985                     *'
@16,9 SAY  '*                              FUELS ENGINEERING DEPT.            *'
@17,9 SAY  '*                              UNIVERSITY OF UTAH                 *'
@18,9 SAY  '******************************************************************'
@23,5 SAY  'Press any key to continue' get nul
CLEAR
@ 9,3 SAY  'INPUT THE FILE NAME INCLUDING THE EXTENSION(.DBF)' GET LI
READ
Do while MORE = 'T'
clear
@4,16 SAY  '*************************** MAIN MENU ***************************'
@5,16 SAY  '*                                                                *'
@6,16 SAY  '*       1> AUTHOR                   4> INDEX                     *'
@7,16 SAY  '*       2> JOURNAL                  5> MULTIPLE                  *'
@8,16 SAY  '*       3> YEAR                     6> MAINTENANCE               *'
@9,16 SAY  '*                                                                *'
@10,16 SAY '*                      type Q to quit                            *'
@11,16 SAY '******************************************************************'
store ' ' to CHOICE
@13,18 SAY 'INPUT THE SELECTION: ' GET CHOICE
READ
store     '                                  ' TO AUTHOR
store     '                                       ' to JOUR
store     '                                    ' to IX
SET DELETE ON
Do case
   case CHOICE = '1'
      DO AR
   case CHOICE = '2'
      DO JR
   case CHOICE = '3'
      DO YR
   CASE CHOICE = '4'
```

```
      DO IN
   CASE CHOICE = '5'
      DO ML
   CASE CHOICE = '6'
      DO MN
   case UPPER(CHOICE) = 'Q'
      MORE = 'F'
  ENDCASE CHOICE
USE $LI
SET DELETE OFF
RECALL ALL
ENDDO SEARCH
```

```
*THIS IS A SUB PROGRAM FOR AUTHOR SEARCHING
@15,18 SAY 'INPUT THE AUTHOR NAME:  ' GET AUTHOR
READ
 USE $LI
  GOTO TOP
  DO WHILE .NOT. EOF()
   IF ((AUTHOR = AUTHOR1) .OR. (AUTHOR = AUTHOR2)) . OR. AUTHOR = AUTHOR3
    SKIP
   ELSE
    IF ((AUTHOR=AUTHOR4) .OR. (AUTHOR = AUTHOR5)) . OR. AUTHOR = AUTHOR6
     SKIP
    ELSE
     DELETE
     SKIP
    ENDIF
   ENDIF
 ENDDO
?
? '         SEARCHING PARAMETER:  ', AUTHOR
?
?
COPY TO TP.DBF
USE TP
DISPLAY ALL
CLOSE DATABASE
ERASE TP.DBF
?
?
?
? 'AUTHOR SEARCHING COMPLETE !'
?
WAIT
RETURN
C>
```

```
*THIS IS A SUB PROGRAM FOR YEAR SEARCHING
clear
@5,10 say ’******************** YEAR SEARCHING MENU ********************’
@7,10 SAY ’     1> EQUAL THE INPUT YEAR’
@8,10 SAY ’     2> BEFORE THE INPUT YEAR (INCLUDING THE YEAR)’
@9,10 SAY ’     3> AFTER THE INPUT YEAR (INCLUDING THE YEAR)’
STORE ’ ’ TO YRSELECT
@ 12,12 SAY ’INPUT THE SELECTION:   ’ GET YRSELECT
Store ’    ’ to YRINPUT
@ 14,12 SAY ’INPUT   THE   YEAR:   ’ GET YRINPUT
READ
USE $LI
GOTO TOP
do case
 case YRSELECT = ’1’
  DO WHILE .NOT. EOF()
   IF YRINPUT = YEAR
    SKIP
   ELSE
    DELETE
    SKIP
   ENDIF
  ENDOO
CASE YRSELECT = ’2’
 DO WHILE .NOT. EOF()
  IF YEAR >= YRINPUT
   SKIP
  ELSE
   DELETE
   SKIP
  ENDIF
 ENDDO
ENDCASE YRSELECT
?
?’     TYPE SELECTION (1=, 2 <=, 3 >=):       ’, YRSELECT
?’     YEAR     SEARCHING    PARAMETER:     ’, YRINPUT
?
?
copy to tp.dbf
use tp
DISPLAY ALL
CLOSE DATABASE
erase tp.dbf
?
?
?
? ’YEAR SEARCHING COMPLETE !’
?
WAIT
RETURN
```

```
*THIS IS A SUB PROGRAM FOR JOURNAL SEARCHING
@ 15,10 SAY 'INPUT THE JOURNAL NAME:  ' GET JOUR
READ
USE $LI
GOTO TOP
DO WHILE .NOT. EOF()
  IF JOUR = JOURNAL
   SKIP
  ELSE
   DELETE
   SKIP
  ENDIF
ENDDO
?
?'    SEARCHING PARAMETER:  ', JOUR
?
?
copy to tp.dbf
use tp
DISPLAY ALL
CLOSE DATABASE
erase tp.dbf
?
?
?
? 'JOURNAL NAME SEARCHING COMPLETE !'
?
WAIT
RETURN

C>
```

```
*THIS IS A SUB PROGRAM FOR INDEX SEARCHING
@ 15,10 SAY 'INPUT THE INDEX NAME:    ' GET IX
READ
USE $LI
GOTO TOP
DO WHILE .NOT. EOF()
  IF IX = INDEX1 .OR. IX = INDEX2 .OR. IX = INDEX3
    SKIP
  ELSE
    DELETE
    SKIP
  ENDIF
ENDDO
?
?'   SEARCHING PARAMETER: ', IX
?
?
copy to tp.dbf
use tp
DISPLAY ALL
CLOSE DATABASE
erase tp.dbf
?
?
?
? 'INDEX SEARCHING COMPLETE !'
?
WAIT
RETURN

C>
```

```
* THIS IS A MULTIPLE SEARCHING PROGRAM
STORE 'T' TO KEYING
STORE ' ' TO CBSEL
DO WHILE KEYING = 'T'
CLEAR
@4,18 SAY  '*********** MULTIPLE SEARCHING MENU ************'
@6,18 SAY  '   1> AUTHOR          4> INDEX'
@7,18 SAY  '   2> JOURNAL         5> RETURN TO MAIN MENU'
@8,18 SAY  '   3> YEAR'
@10,20 SAY '      INPUT THE SELECTION ' GET CBSEL
READ
DO CASE
   CASE CBSEL = '1'
   DO AR
   CASE CBSEL = '2'
   DO JR
   CASE CBSEL = '3'
   DO YR
   CASE CBSEL = '4'
   DO IN
   CASE CBSEL = '5'
   KEYING = 'F'
ENDCASE
ENDDO
RETURN

C>
```

```
*THIS IS A MAINTENANCE PROGRAM
*set up loop
SET TALK OFF
STORE 'T' To Morel
STORE ' ' TO Selectm
DO WHILE Morel = 'T'
   *set up screen
    clear
    @ 5,17 SAY   '************* MAINTENANCE MENU ***************'
    @ 7,20 SAY   '   1> DUPLICATE CHECK'
    @ 8,20 SAY   '   2> VERIFY'
    @ 9,20 SAY   '   3> RETURN TO MAIN MENU'
    @ 11,18 SAY  '      INPUT NUMBER TO SELECTION :' GET Selectm
    READ
   *perform desired function
    do case
    case Selectm = '1'
   *check for duplicate
    do du
    case selectm = '2'
   *verify new records
    do vr
    case selectm = '3'
   *setup the loop to exit
   store 'F' to Morel
 endcase
enddo
RETURN

C>
```

```
* THIS IS A DUPLICATE CHECKING PROGRAM
store '                                               ' to CVOL
store '                                         ' to CJOUR
store '        ' to CYEAR
store 1 to CC
USE $1i
GOTO BOTTOM
STORE RECNO() TO ALPHA
GOTO CC
DO WHILE .NOT. EOF()
  CVOL = VOL
  CJOUR = JOURNAL
  CYEAR = YEAR
  SKIP
  DO WHILE .NOT. EOF()
   IF ((CVOL = VOL) .AND. (CYEAR = YEAR)) .AND. (CJOUR = JOURNAL)
    ?
    ? 'THE FOLLOWING TWO RECORDS ARE DUPLICATED'
    ?
    ? 'RECORD NO. = ', RECNO()
    ? 'RECORD NO. = ', CC
    ?
   DISPLAY
   SKIP
  ELSE
   SKIP
  ENDIF
 ENDDO
 IF CC < ALPHA
   CC = CC + 1
   GOTO CC
 ELSE
 ENDIF
ENDDO
?
?
?
?  ' DUPLICATE CHECKING COMPLETE !'
?
WAIT
RETURN

C>
```

```
*THIS IS A VERIFY PROGRAM
CLEAR
@6,18 SAY   '******************** VERIFY MENU *************************'
@8,18 SAY   '   1> CONTINUE VERIFY'
@9,18 SAY   '   2> DISCRETE VERIFY
@10,18 SAY  '   3> RETURN TO MAINTENANCE MENU'
STORE ' ' TO VERCHOI
@ 12,18 SAY 'INPUT    THE    SELECTION:    ' GET VERCHOI
STORE '   ' TO PN
@ 14,18 SAY 'INPUT THE RECORD NUMBER:  ' GET PN
READ
STORE 1 TO PT
PT = VAL(PN)
STORE '                                        ' TO JOURN
STORE 0 TO ALPHA
DO CASE
   CASE VERCHOI = '1'
     USE $LI
     GOTO BOTTOM
     STORE RECNO() TO ALPHA
     GOTO PT
     DO WHILE .NOT. EOF()
         JOURN = JOURNAL
         STORE 0 TO CC
         SELECT 2
         USE STDJOUR
         GOTO TOP
         DO WHILE .NOT. EOF()
          IF (VJOUR = JOURN)
           CC = CC+1
           SKIP
          ELSE
           SKIP
          ENDIF
         ENDDO
         IF CC = 0
         ?
         ? 'JOURNAL NAME OF THE FOLLOWING RECORD NOT IN THE STANDARD STYLE'
         ?
         ? 'RECORD NO. = ', PT
         ? 'JOURNAL NAME = ', JOURN
         ENDIF
         IF PT < ALPHA
           PT = PT + 1
           SELECT 1
           GOTO PT
         ELSE
           SELECT 1
           SKIP
         ENDIF
      ENDDO
```

```
   CASE VERCHOI = '2'
    SELECT 1
    USE $LI
    GOTO PT
         JOURN = JOURNAL
         STORE 0 TO CC
         SELECT 2
         USE STDJOUR
         GOTO TOP
         DO WHILE .NOT. EOF()
          IF (VJOUR = JOURN)
           CC = CC+1
           SKIP
          ELSE
           SKIP
          ENDIF
         ENDDO
         IF CC = 0
         ?
         ? 'DISCRETE VERIFY'
         ? 'JOURNAL NAME OF THE FOLLOWING RECORD NOT IN THE STANDARD STYLE'
         ?
         ? 'RECORD NO. = ', PT
         ? 'JOURNAL NAME = ', JOURN
         ENDIF
         SELECT 1
   ENDCASE
?
?
?
? 'VERIFY COMPLETE !'
?
WAIT
RETURN
C>
```

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