THE DEVELOPMENT OF AN AUTOMOTIVE EXHAUST EMISSION TEST FACILITY

By

VIJAY K. AGARWAL

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The many courtesies extended by the personnel of the Fuels and Lubricant Laboratory, National Research Council of Canada, are highly appreciated.

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ABSTRACT

This thesis describes the design, planning and construction of an exhaust emission test facility employing exhaust gas recirculation (EGR) as a control system for reducing NO_x emissions from spark ignition engines. Tests were conducted on a suitably modified CFR engine. The effects of changes in several variables on NO_x emissions are presented: Effectiveness of EGR in reducing NO_x emissions is independent of recycled gas temperature. Two empirical equations have been developed to relate NO_x reduction to percent EGR for rich and lean air-fuel mixtures. It has been found that NO_x emissions are considerably effected by intake air humidity, mixture temperature and exhaust port vacuum.

In the analytical part of the study, the control of nitric oxide by EGR has been evaluated by a digital computer simulation of the engine cycle.

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ABBREVIATIONS

A/F	air-fuel ratio
App.	appendix
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
ATC	after top dead center
BHP	brake horse power
BTC	before top dead center
^oC	degree centigrade
cal.	calorie
cc	cubic centimeter
EGR	exhaust gas recirculation
^oF	degree fahrenheit
ft	foot (feet)
Fig.	Figure(s)
gm	gram(s)
grains	grains per pound of dry air
Hg.	mercury head
IAD	intake air drier
ID	inner diameter
IHP	indicated horse power
in.	inch(es)
lb.	pound(s)
min.	minute(s)

mm	millimeter
no.	number
OD	outer diameter
p	pressure
P_2O_5	phosphorous penta oxide
ppm	parts per million
psig	pounds per square inch gauge
RPM	revolutions per minute
SAE	Society of Automotive Engineers
SC	standard carburetion
SCFH	standard cubic feet per hour
SCFM	standard cubic feet per minute
SOC	standard operating conditions
t	time
T	temperature
TDC	top dead center
Temp.	temperature
T_{mix}	mixture temperature
v	displacement volume
VOC	variable operating conditions
vs.	versus
θ	crank angle

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Chapter 1

INTRODUCTION

The gasoline powered automobile employing an Internal Combustion reciprocating Engine has been known for many years to be a major source of air pollutants in urban area* (1-4). Pollutants from this source can contain toxic compounds and organic materials that may not themselves be objectionable, but which can react in the atmosphere to form photochemical smog. Appendix A details the history and forecast of Emission Standard (5). Much work has been done on Unburned Hydrocarbons (HC) and Carbon Monoxide (CO), compared to that done on Nitrogen Oxides ((NO_x))†. For this reason, the work described herein was undertaken to study NO_x emissions.

Several methods have been suggested (6-11) to decrease NO_x emissions. One such method is to increase the dilution of the intake charge with the product gases. This can be achieved by

(i) Exhaust Gas Recirculation;
(ii) Reducing Compression Ratio;
(iii) Increasing Valve Overlap.

---

* Numbers in the parentheses designate References listed.

† NO plus NO_2

Another method of decreasing NO_x emission is to inject water either directly into the engine cylinder (8) or through the inlet manifold (12-13). These studies revealed NO_x reduction of over 85%.

The scope of the project described in this thesis has been in the following area:

(i) Design and Construction of an Experimental Equipment;
(ii) Acquiring useful data on NO_x emissions;
(iii) Interpreting data and deriving conclusions;
(iv) Making recommendations for the further studies and evaluating further usage of the Test Facility;
(v) Analytical Investigations.

The writer has purposely avoided including in this Introduction a detailed literature survey on the state of exhaust emission research. Excellent summaries of current work are available to the reader in References (14-22). By summarizing from the references, the effect of exhaust recycling on the emission of nitrogen oxides (NO_x) can be described as follows: Addition of exhaust gas, or any inert gas, such as carbon dioxide, water vapor or nitrogen, to the combustible mixture will lower the combustion temperature during the combustion process in the engine cylinder, that is, EGR functions by increasing the heat capacity of the working fluid. Since the amount of nitric oxide produced in the engine cylinder from atmospheric nitrogen and oxygen is an exponential function of combustion temperature, even a moderate decrease in the combustion temperature will result in a significant decrease in nitric oxide production.

Chapter 2

EXPERIMENTAL EQUIPMENT

2.1 GENERAL FEATURES OF THE SYSTEM

A major portion of the study involved the design, planning and construction of the Test Facility† and the procurement of instruments, equipments and control units, etc. The single cylinder CFR engine used in this study was modified, exhaust gas recirculatory system and sampling system were designed and fabricated to incorporate the following aspects:

ENGINE*

(i) A wide range of air fuel ratios may be covered.

(ii) An Intake Air Drier was designed and fabricated to ensure constant humidity intake air to the engine.

(iii) A pressure transducer has been mounted on the cylinder head and connected to the Engine Analyser Oscilloscope. to monitor pressure versus crank angle (p-θ), and pressure versus displacement volume (p-v).

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† Shown in Figures 2.1 and 2.2.

* Selected Specifications are in Appendix B

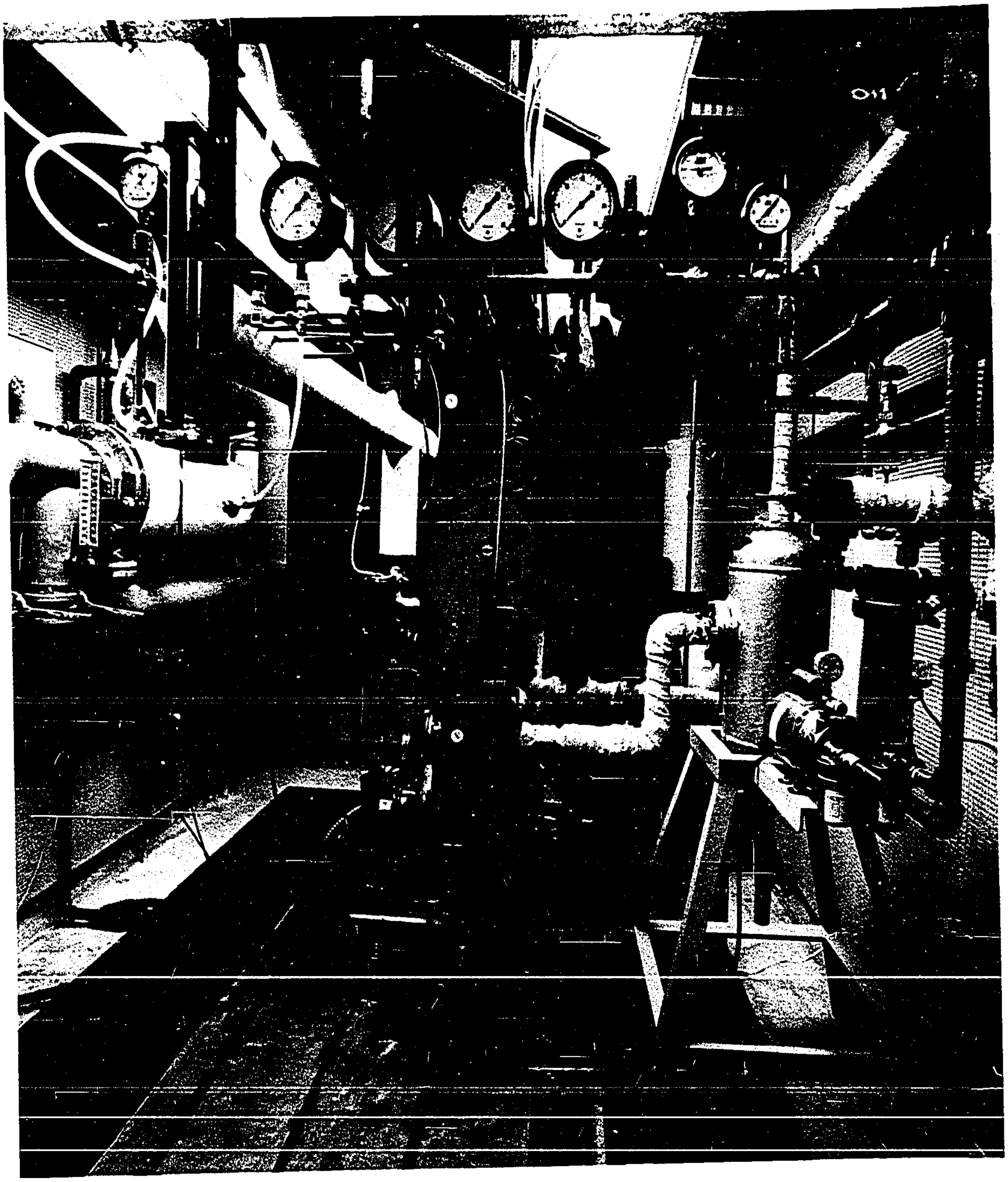

Fig. 2.1 TEST FACILITY (front view)

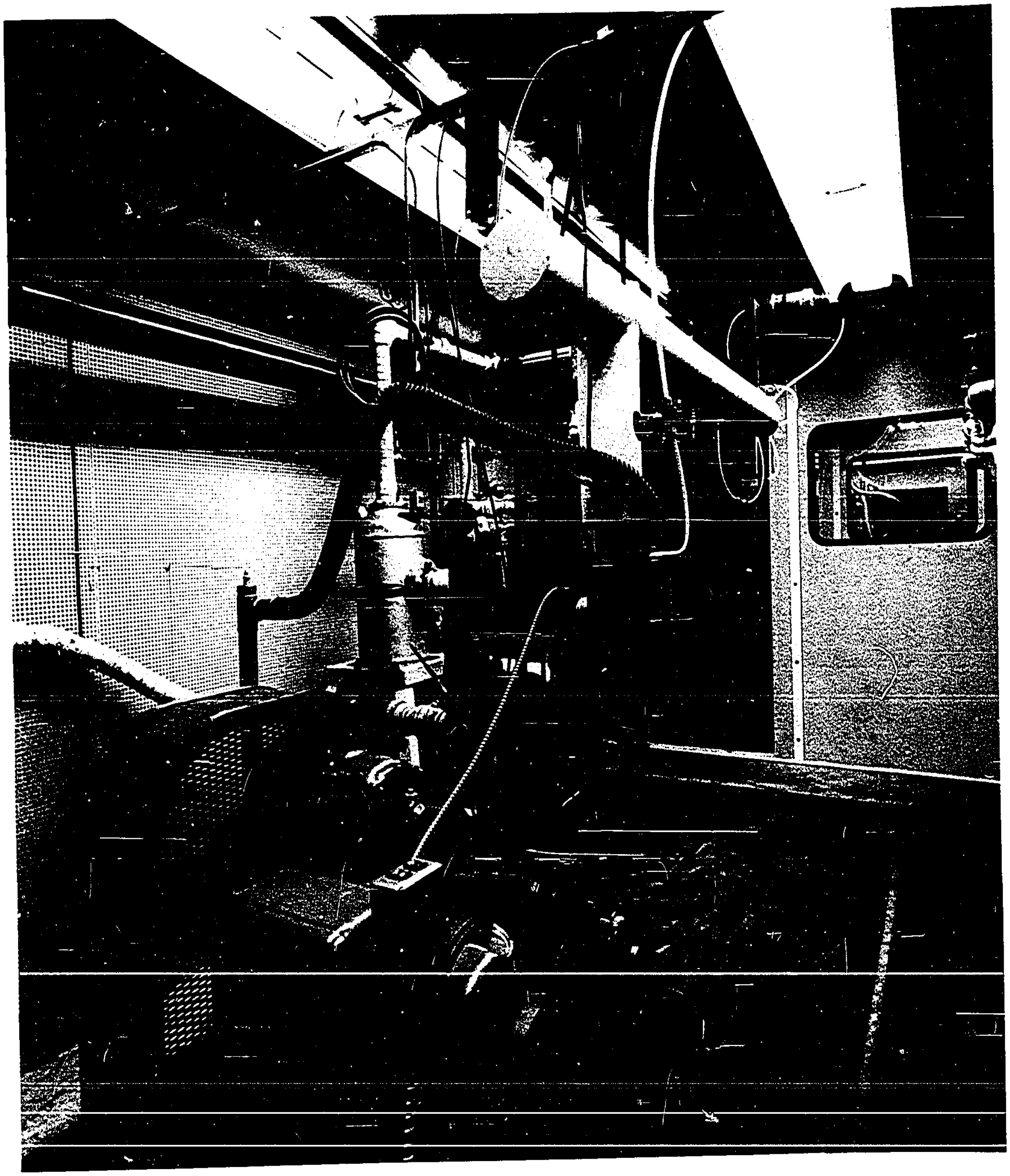

Fig. 2.2 TEST FACILITY (rear view)

EGR SYSTEM

(i) Recirculated exhaust temperature may be varied from room temperature to 500° F.

(ii) To some extent, the humidity can be varied from very dry to maximum moisture present in the exhaust products.

(iii) As much as 90% of the exhaust gas may be recirculated.

(iv) A metered quantity of any other gas (eg., N_2, CO_2, He, A, etc.) may be injected into the combustion chamber.

(v) Exhaust gas may be injected into the engine combustion chamber with any other gas simultaneously.

(vi) The length of the EGR line has been kept minimum so that time lag or hang up is as low as possible.

SAMPLING SYSTEM

(i) Designed with the SAE Recommended Practice (30).

(ii) Both hot and cold sampling are possible.

(iii) Continuous sampling has been adopted and sampling flow control is independent of the EGR flow control.

(iv) With little modification, the system may be used for the analysis of HC and CO.

(v) Response of NO_x analyser is very fast.

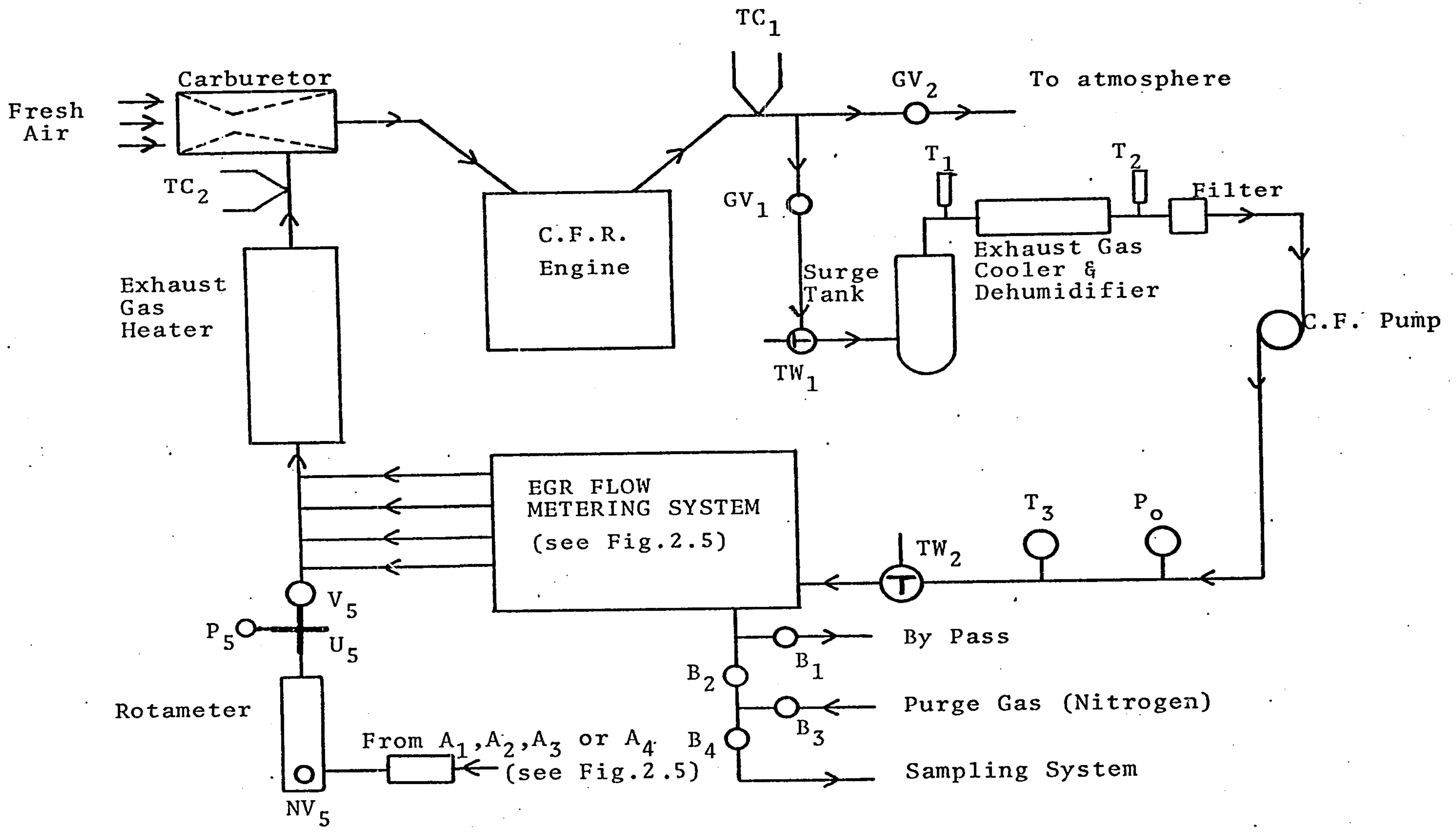

Fig. 2.3 EXPERIMENTAL SET-UP

(vi) Lag time of the sampling line is kept as low as possible.

2.2 ENGINE

The engine installed in the Test Cell was not firing initially. There was no spark at the plug. A complete overhauling of the ignition system as well as of all 15 electrical connection resulted in proper engine operation.

2.2.1 ENGINE DESCRIPTION

A schematic diagram of the experimental set up is shown in Fig. 2.3. A modified single cylinder CFR engine was used in this study. The unit comprises a spark ignition continuously variable compression ratio, variable spark advance (or retard), single cylinder engine with suitable loading and accessory equipments and instruments mounted on a stationary base. The gravity fed fuel system makes use of three carburetor fuel tanks all of which are adjustable in the vertical direction. The vertical movement enables one to vary mixture conditions. A selector valve can engage any one of the three fuel tanks or shut all of them off.

The original intake air equipment was equipped with an ice tower and an intake air-heater. This was modified as described in the section 2.2.2. In addition, a mixture heater element mounted after the carburetor could be used to alter the mixture inlet temperature.

A water-cooled condenser coil is used to maintain constant coolant temperature around the cylinder. A spring loaded dial gauge mounted on the cylinder measures the position of the cylinder head with respect to the piston. A chart (23) is available to relate the dial gauge reading to a compression ratio.

A crankcase oil heater can be used to bring the oil up to operating temperature prior to start up. An adjustable safety switch on the oil line shuts off the ignition coil if the pressure drops below 16 psig.

A reluctance type 550 volt A.C. synchronous electric motor is used to start the engine. It also absorbs the power produced by the engine and maintains a constant speed of 900 ± 9 r.p.m. Coupled with the A.C. motor is a 110 volt D.C. generator which supplies power to the ignition coil.

The control panel (Fig. 2.4) contains the controls for the D.C. generator, mixture heater, intake manifold air heater and ignition control as well as for Start and Stop switches for the synchronous motor. Instrument gauges can monitor the oil pressure, oil temperature, D.C. generator

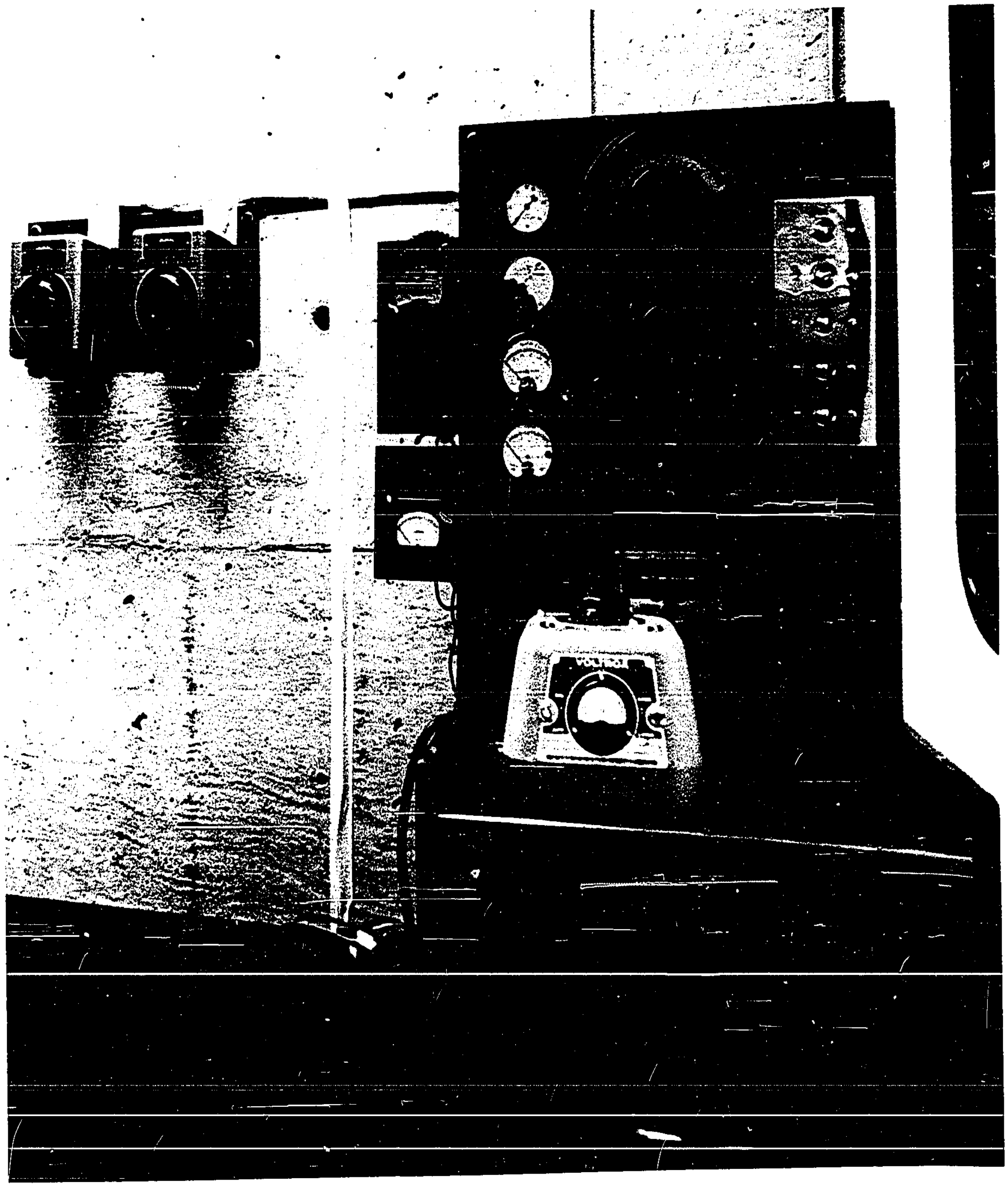

Fig. 2.4 ENGINE CONTROL PANEL

voltage, mixture heater current and air heater current.

2.2.2 ENGINE MODIFICATIONS

Intake airflow rate measurement is essential to determine the air fuel ratio of the mixture. To monitor the intake air flow rate with a Nozzle Meter equipped with surge drum, the intake airline ice tower and intake air surge tank with air heater were removed. Fresh air was drawn through a calibrated Nozzle Meter and an Intake Air Dehumidifier (IAD). The IAD is a suitably jacketed heat exchanger and capable of cooling and dehumidifying air to 10° F dewpoint. Crushed ice with potassium bromide can be used in the cooling jacket. At the IAD exit, if desired, the air can be heated by a heating tape wrapped around the outlet pipe. Air temperature at the IAD exit is monitored by a copper constanton thermocouple. The engine intake air temperature can be controlled by a Temperature Controller with a thermocouple probe (working range of 0° to 250° F and 0.1° F sensitivity).

The initial size of the fuel metering jets of all three bowls was 0.029". These metering jets would have supplied A/F ratios of interest in the present study. However, to have a much wider range of air fuel ratios, two metering jets were changed. On bowl #1 a 0.036" metering jet and on bowl #3 a 0.046" metering jet was installed, bowl #2 was left unchanged. This combination of the metering jets provided a range of air fuel ratios.

The conventional pressure pick up* was replaced by a Tektronix Pressure sensor.

Other modifications, such as a provision to inject exhaust gas or any other gas into the combustion chamber and changes in the exhaust port connections are described in the section 2.3.

2.3 EXHAUST GAS RECIRCULATORY SYSTEM

2.3.1 FUNCTIONS AND OBJECTIVES

The purpose of the system was to recirculate a measured quantity of exhaust gas into the combustion chamber and analyse its effect on exhaust gas composition. The system is capable of recirculating any measured quantity of exhaust gas into the engine while monitoring and controlling desired pressure and temperature at different locations of importance. Depending upon recirculated gas quantity, the gas can be heated as high

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* Originally used in experiments with knock-meter for fuel octane rating tests.

as 500° F before injection into the engine. Thus most of the conceivable parameters like gas temperature, pressure, quantity and to some extent, humidity, can be controlled. The system is designed to supply continuous hot sample and/or cold sample for analysis purposes.

As shown in Fig. 2.3, exhaust gas was drawn from the engine exhaust port through a two inch Globe valve GV_1 and the remaining gas was exhausted to the atmosphere. The gas was pulled by the centrifugal pump through two inch galvanized steel piping, three way valve TW_1, Surge Tank, Exhaust Gas Cooler and Dehumidifier, 40 μ Filter. Then it was pumped into the engine in 3/4 inch piping through another three way valve TW_2, Exhaust Gas Flow Metering system and Exhaust Gas Heater leading to carburetor at a distance of about one inch downstream of the throat.

The centrifugal pump was used as a pressure riser and also to create vacuum upstream of the pump. Gas flow rate and upstream vacuum were controlled by the valve GV_1 and the downstream pressure was controlled by BY PASS valve B_1 shown in Fig. 2.3. Each component of the system is now described in more detail below.

2.3.2 SYSTEM DESCRIPTION

(a) VALVES GV_1 and GV_2: To control the flow of exhaust gas in the EGR System.

(b) VALVE TW_1: Installed to provide hot exhaust gas samples for analysis purposes, if needed.

(c) SURGE TANK: To damp the engine exhaust gas.

(d) EXHAUST GAS COOLER AND DEHUMIDIFIER: This is a shell and tube type heat exchanger. The cooling water enters the shell at 40° F and leaves at 42° F. Flow rate of cooling water is automatically controlled by a spring loaded valve actuated with a thermostat. The valve is preset to a desired exhaust gas temperature by a screw cap; the temperature range of the thermostat being 75° to 135° F. A manual control was also provided to override these temperature limits.

(e) FILTER: A 40 μ filter was used to remove carbon particles, moisture and other impurities, if any. A significant amount of water can be condensed and trapped by this filter which can often require draining of water and cleaning of filter bowl.

(f) CENTRIFUGAL PUMP: Since the exhaust gas gauge pressure is quite small and also a considerable amount of piping is involved between the exhaust port and EGR injection, a significant total pressure drop across the EGR system results. A centrifugal pump has been used as a pressure riser. This pump is capable of producing 20 psig. continuous service or pull a vacuum of 27 inches of mercury and delivering 5.2 C.F.M. at 20 psig. Two pressure gauges mounted on the inlet and outlet of the pump indicate the pull and pressure at the respective ports.

(g) VALVE TW_2: This three way valve was installed to facilitate the injection of any gas other than exhaust gas into the engine and to provide other options to measure the exhaust gas flow rate.

(h) EGR FLOW METERING SYSTEM: Pressurized exhaust gas is carried in 3/4 inch pipe from the pump through the valve TW_2 as shown in Fig 2.5. The EGR flow metering system has four parallel 3/8 inch OD, 1/4 inch ID copper tubes. Each of these lines originates from 3/4 inch pipe and terminates into another 3/4 inch pipe. Each gas flow line consists of two needle valves, one high accuracy pressure gauge mounted on one end of a union cross. The opposite end has a screwed plug. The plug may be removed when flow of gas is desired through a standard flow meter, by letting the gas pass through this end and closing the valve V_1. All four flow lines were identical except that the needle valve of

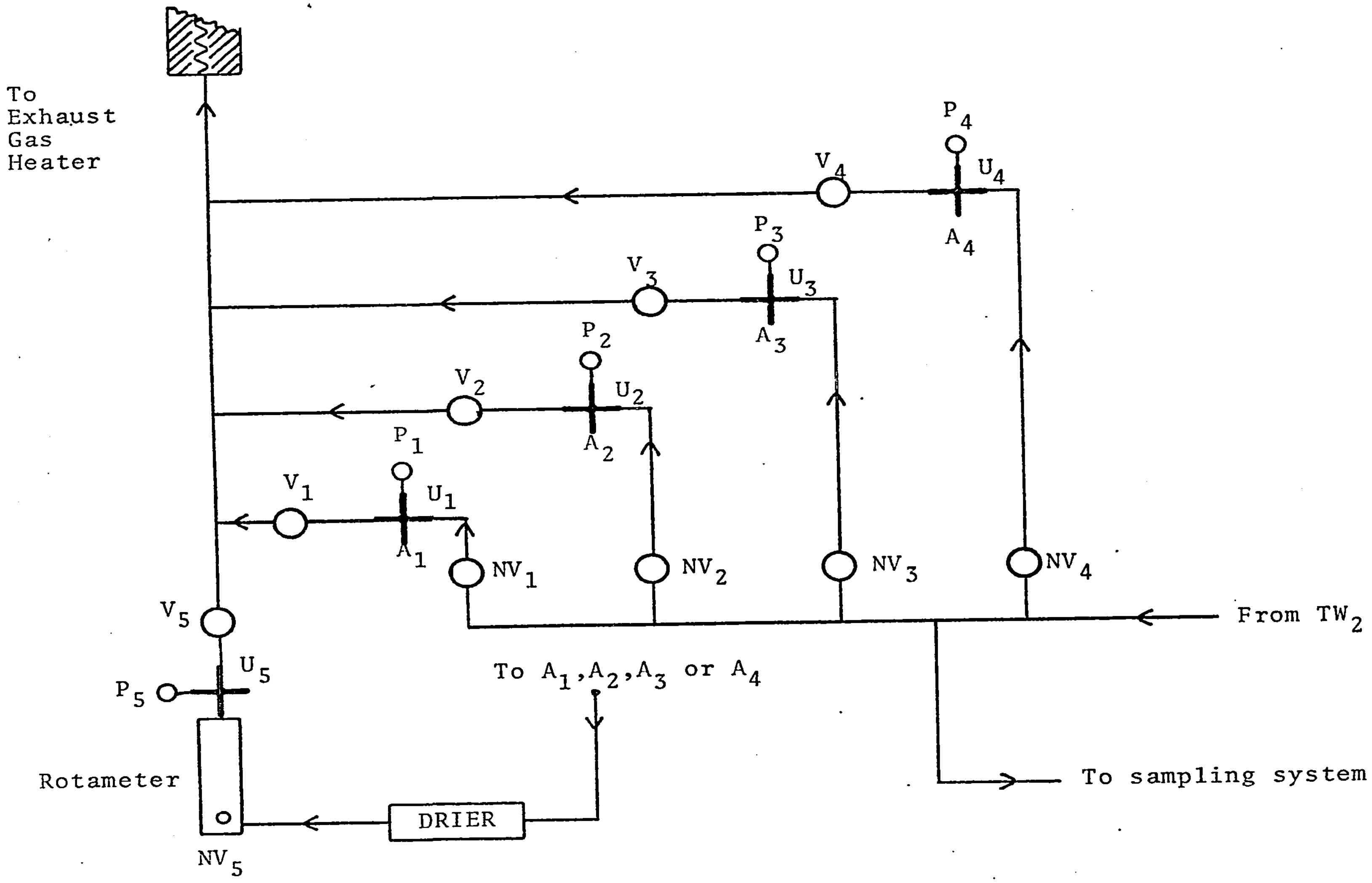

Fig. 2.5 EGR FLOW METERING SYSTEM

the first and second flow lines were equipped with a micrometer handle.

The EGR flow metering system is designed to meter a maximum exhaust gas flow of 8.0 SCFM which is about 90% of the normal air flow rate through the engine. In the present study, however, a maximum recycled gas flow of 1.5 SCFM was considered sufficient so the EGR metering system was not calibrated. Instead, a rotameter was calibrated to meter the gas flow rate.

(i) EXHAUST GAS HEATER: This comprises of a 54 feet mineral insulated heating cable which is wrapped around the pipe extending from the EGR flow metering system. For this type of heating application, the maximum recommended surface temperature of the cable is 515° F. The cable supplies 450 watts at 120 volts and 1700 watts at 240 volts*. The desired exhaust gas temperature was achieved by varying the input voltage from 0 to 140 volts.

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* It is recommended that insulation test be conducted before switching it on. Insulation should read 50 megaohms or better with no decline in reading.

(j) THERMOCOUPLE TC_1: It is a Chromel-Alumel thermocouple and has been used to measure the exhaust gas temperature immediately after the exhaust port.

(k) THERMOCOUPLE TC_2: It is an Iron-Constantan thermocouple and has been used to monitor the recycled gas temperature just before the injection into the carburetor.

In addition, a number of pressure gauges and thermometers were installed in the system to monitor pressure and temperature at various points of interest. Recycled gas temperature, exhaust gas temperature and intake air temperature were recorded on a strip chart recorder.

2.4 EXHAUST GAS ANALYSIS SYSTEM

The exhaust gas was analysed for NO_x concentration using a Chemiluminescent NO_x Analyser. Both the sampling system and the analyser are described in the following sections.

2.4.1 CONTINUOUS SAMPLING SYSTEM

Fig. 2.6 illustrates schematically the sampling system for the continuous measurement of NO_x concentration in the exhaust gas. The system consists of a sample outlet, sample lines, an exhaust gas cooler and dehumidifier, a

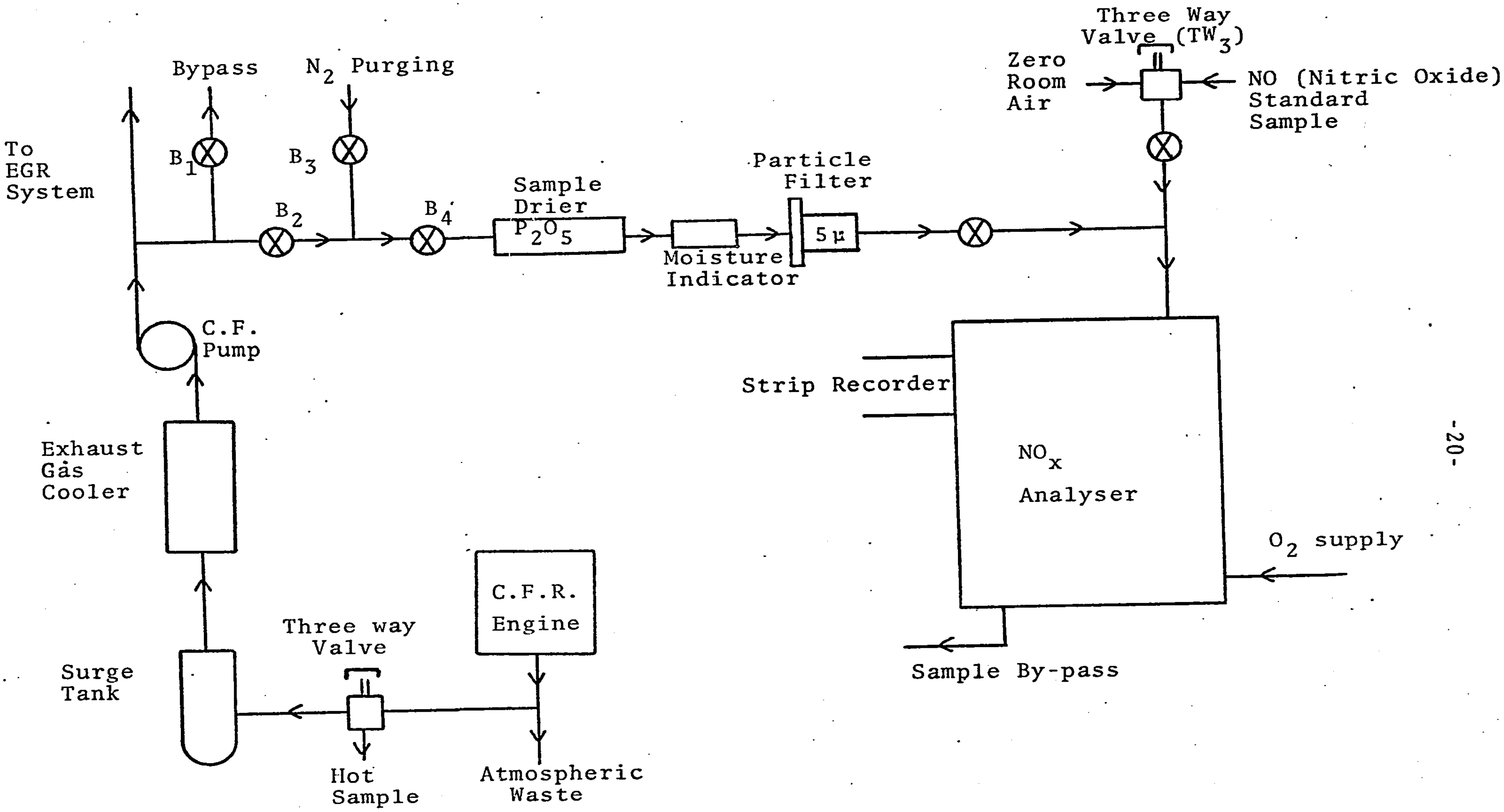

Fig. 2.6 SAMPLING SYSTEM

centrifugal pump, a by-pass line, dry nitrogen purging line, a phosphorous pentoxide sample drier, a moisture indicator, a 5 μ particle filter and flow control valves. The SAE recommended practice (30), has been adopted with respect to the instrumentation and measurement of exhaust gas emissions. This practice provides uniformity of the laboratory techniques and attempts to eliminate differences in emissions data because of different laboratory set ups.

Components prior to bypass and N_2 purging lines have been already described in section 2.3.2; other components are described below.

SAMPLE LINE: As recommended by the SAE, this line is either 0.25 inch I.D. teflon tubing or 0.25 inch O.D. stainless steel rigid tubing and the length of this line is kept as small as possible, since its length is directly related to the delay time of the entire system.

BYPASS: A centrifugal pump may continuously draw exhaust gas from the engine. A measured quantity of this gas can be recirculated to the combustion chamber and a small quantity (2 SCFH) taken by the NO_x Analyser through valves B_2 and B_4, the remaining gas being bypassed to waste.

NITROGEN PURGING: Dry N_2 gas was purged into the sampling system after each observation. This is a standard SAE recommended practice. The time lag between the exhaust port and the centrifugal pump was expected to be insignificant ✓ as the pump was drawing gas quantity comparable to the exhaust gas produced by the engine. However, there was a time lag of about 3 minutes between the pump and the NO_x analyser.

SAMPLE DRIER: It is made of a two inch diameter and eight inch long galvanized steel vessel containing about 250 gm. of anhydrous phosphorous pentoxide (P_2O_5) with a small packing of anhydrous silica gel and glass wool on both ends. The drier is capable of providing a completely dry sample for about 40 hours of sampling before a fresh charge of P_2O_5 is required. This is an essential unit as the sample before entering the NO_x analyser should be completely dry to avoid the clogging of sample capilliary of the NO_x analyser.

MOISTURE INDICATOR: To indicate moisture in the sample line, a moisture indicator was placed down stream of the sample drier. At relative humidities less than 4%, the color of dyed silica gel changed from blue to pink, indicating the need for a fresh charge of P_2O_5. The indicating effect of this indicator was regenerated by heating it to 150° C.

PARTICLE FILTER: A 5 μ micron inline removable filter with replacable sintered stainless steel element was connected downstream of the moisture indicator. The filter element was inspected occasionally and found uncontaminated.

FINE CONTROL AND THREE WAY VALVES: These were employed to provide a fine flow control of the sample through the NO_x chemiluminescent analyser. As may be seen from the schematic diagram (Fig. 2.6), the arrangement permits frequent and rapid caliberation checks. The three way valve TW_3 is necessary when the NO_x analyser is to be used in both NO and NO_x mode alternately.

The SAE recommendations presume that NDIR (Non Dispersive Infra Red) and NDUV (Non Dispersive Ultra Violet) analysers would be employed to monitor NO and NO_2 respectively. For these types of instruments gas flow and pressure in the sample cell are critical factors and therefore the SAE recommends two flowmeters, one each upstream and downstream of the analyser. However, in this study a chemiluminescent NO_x Analyser has been used in which sample flow rate and its pressure do not effect monitoring NO_x concentrations if the bypass of the sample is maintained in the vicinity of 2 SCFH. The analyser is discussed in the next section.

2.4.2 CHEMILUMINESCENT NO_x ANALYSER

A newly developed analyser, called a Chemiluminescent Gas Analyser, has been used in the present work to monitor NO_x (NO plus NO_2) concentrations in the exhaust gas. By monitoring the chemiluminescent reaction of Nitric Oxide and Ozone gases, this instrument eliminates many problems associated with the measurement of NO_x. The detector requires very small gas samples to continuously monitor NO and/or NO_x with rapid response time and negligible interference from H_2O, CO_2, CO,C_2H_4, and SO_2. In addition, the instrument has eight ranges from 2.5 ppm to 10,000 ppm, linear response, good stability, 1% full scale linearity and 1% full scale accuracy.

Fig. 2.7 shows the components of this equipment. These are:

(i) Analyser;
(ii) Control unit;
(iii) Converter;
(iv) Vacuum pump.

In addition, the following equipment are required:

1. Caliberated standard mixture of NO in N_2;
2. Pressurized cylinder of oxygen and a pressure regulator;
3. A diaphram type sample bypass pump to pull the sample through the analyser.

OPERATION:

Unlike NDIR and NDUV, operation and control of this equipment is much easier and hence requires less attention.

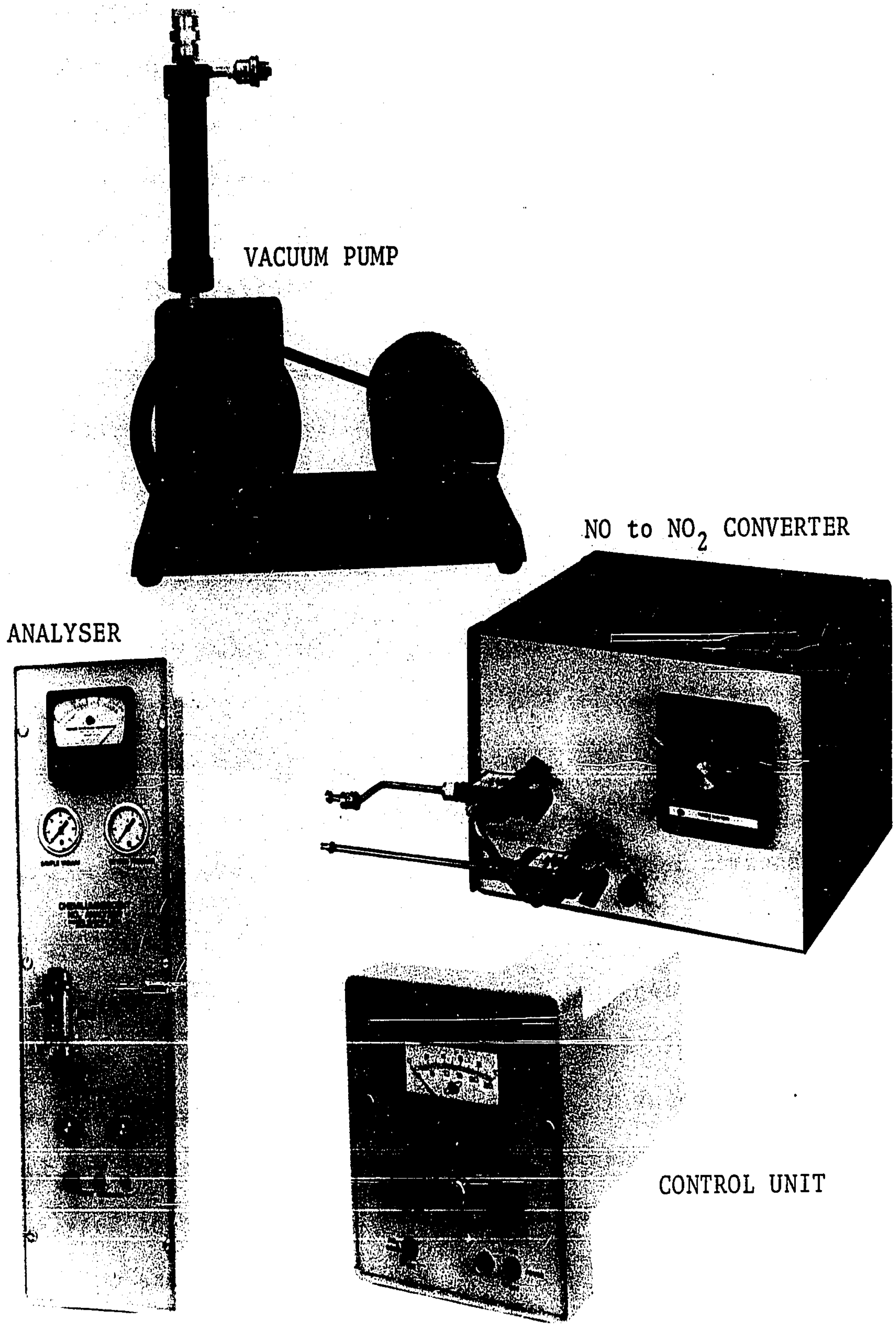

Fig. 2.7 CHEMILUMINESCENT NO_x ANALYSER

Sample pressure which must be precisely controlled for NDIR and NDUV does not effect monitoring NO_x concentration in this case. Even sample bypass of 2 SCFH which is recommended during analysis, is not a critical adjustment. This can be varied from 0.5 to 2.0 SCFH with less than 1% change in the instrument sensitivity.

Step by step calibration and detail operating procedure are described in the Instruction Manual (24) on page 8 through 13.

CALIBRATION:

The standard calibration procedure recommends that only one certified standard sample need be used to verify the calibrated equipment, however, four samples of 215, 1530, 2612 and 4297 ppm of NO were used. These samples were supplied with a certified accuracy of 2% of component by the Matheson gas company of Canada. Instrument was calibrated with 2612 ppm sample. With this calibration 4297 ppm sample was analysed to be 4420 ppm. To attain maximum accuracy 4297 ppm sample was set to read 4350 ppm and for this calibration setting 2612 ppm sample was analysed to be 2580 ppm. For this setting 215 ppm and 1530 ppm samples were analysed to be 192.5 and 1412 ppm. The 1530 ppm sample was an old sample borrowed from the

National Research Council of Canada (NRC) and was suspected to be inaccurate and hence was not used in calibration checking at the later stage.

During its calibration and occasional checking of calibration, the following interesting observations were made:

1. After the above mentioned calibration, no significant drift was observed during daily calibration checks. The final setting for three samples were as follows:

CERTIFIED SAMPLE	ANALYSED MODE	
	NO Mode	NO_x Mode
215 ppm	190 ppm	195 ppm
2612 ppm	2580 ppm	2580 ppm
4297 ppm	4350 ppm	4350 ppm

2. While the analyser was calibrated the sample vacuum gauge was set to 5 psi. Should this vacuum gauge show 4.9 psi or 5.1 psi, its setting must not be disturbed. The difference in the gauge reading is due to change in the atmospheric pressure. The sample flow regulator maintains constant flow by keeping 5 psi vacuum from the atmospheric pressure.

3. When the instrument is to be used within a few hours, power to ozone generator should be turned off and the

flow of oxygen through the ozone generator be closed off. As a result, the reaction chamber pressure drops from the operating pressure of 9.0 mm.to a minimum pressure of 0.3 mm. Hg. There is nothing to be alarmed about the pressure drop in the reaction chamber. The operating reaction chamber pressure is attained as soon as the flow of oxygen is resumed.

4. Room contamination of nitric oxide does not effect the sample detection, though the analyser takes in room air. This is because the room air is used in sample flow regulation only and does not pass through the reaction chamber.

2.5 ELECTRONIC ENGINE ANALYSER

The Engine Analyser System is an oscilloscope system used to visually observe if any major or unexpected changes occurred inside the combustion chamber as working parameters were varied. This could also help in determining whether the engine was misfiring as a result of excessive exhaust gas recirculation.

The original knockmeter pressure pickup was replaced by a Tektronix pressure sensor with a modified adapter. The Rotational Function Generator of the analyser was connected to the V groove in the engine flywheel with the friction drive adapter.

This system provides pressure versus displacement volume and pressure versus crank angle images on the oscilloscope screen. Crank angle marking also appeared on the screen but TDC mark was not aligned with the TDC of the engine. This could be done by using a magnetic transducer but was not considered necessary in the present study.

Since a suitable camera was not readily available to produce p-v diagrams from the oscilloscope, the IHP of the engine could not be evaluated during testing. However, p-v and p-θ diagrams were visually observed.

Chapter 3

EXPERIMENTAL METHODS & PROCEDURES

3.1 CALIBRATION AND MEASUREMENTS

Instrumentation and system details have already been outlined in the previous chapter. Before the intended data collection could be initiated though, the following calibrations were necessary:

1. Air Flow
2. Fuel Flow
3. Recirculated Exhaust Gas Flow.

3.1.1 AIR FLOW

A Nozzle Meter (32) was used to monitor the engine air flow. The engine air was drawn in through a precision ASME long radius flow nozzle into a pulse damping drum, and then out through a flexible hose and Intake Air Drier to the engine carbureter. By measuring the pressure difference across a 3/4 inch diameter nozzle, the air flow rate can be calculated by using the calibration and correction curves supplied with the equipment. The pressure difference across the nozzle is measured in inches of water by a manometer.

CALIBRATION: Air flow was theoretically calculated to be 9.71 CFM. Unfortunately no standard air flow meter with this flow rate was available to calibrate the nozzle meter. A PRECISION WET TEST METER (25) was acquired for a short period of time however, which had a maximum capacity of 4.75 SCFM. This provided only one point on the supplied calibration curves. Calculations showed that the nozzle meter was indicating 0.5% high flow. This was assumed to be quite accurate for practical purposes.

ASSOCIATED DIFFICULTIES:

While performing experiments, it was discovered that the engine was satisfactorily firing up to calculated air fuel ratio of 35. This is highly inconceivable. Further it may be noted that fuel flow measurement was quite accurate. Appendix C includes an estimate which revealed that air flow meter indicates very high values and also listed therein is a tentative technique used to estimate air flow rate. As a result a correction factor of 0.655 was applied to the measured air flow rate.

It may be noted that once accurate air flow rate through the engine has been measured, a different suitable correction factor may have to be applied to the computed air fuel ratios.

3.1.2 FUEL FLOW

Since the engine has been primarily designed to rate fuels, it has three small fuel bowls each with its own individual float. To provide a continuous fuel supply, fuel was drawn from a fuel container by siphon action to the fuel bowls.

CALIBRATION: In order to measure the fuel flow rate, fuel bowls were graduated by affixing scaled paper on one side of the sight glass. These graduations were clearly read from the other side of the sight glass.

'SHELL REGULAR' gasoline was used throughout the investigation. Its density was found to be 0.7255 grams per cubic centimeter (cc) on an electronic balance. For each fuel bowl eight readings were taken by adding 100 cc of fuel each time and observing the difference in the fuel level through the sight glass. From 24 readings for three bowls, 22 readings were 2.6 cm and the remaining two were 2.55 cm for each 100 cc of fuel added to the bowls. Hence 2.6 cm on bowl scale corresponds to 100 cc of fuel. If

x = Fuel Level Movement (in cm)

t = Corresponding Time (in minutes)

then,

$$\text{Fuel flow rate} = \frac{x}{2.6} \cdot \frac{0.7255 \times 100}{t} \text{ gm/min.}$$

$$= \frac{72.55}{2.6} \cdot \frac{x}{t} \cdot \frac{60}{453.6} \text{ lb/hr.}$$

$$= 3.691 \frac{x}{t} \text{ lb/hr.}$$

$$= 3.691 \frac{\text{Fuel Level Movement (cm)}}{\text{Time (minute)}} \text{ lb/hr.}$$

During testing, fuel level movement and the corresponding time (with a stop watch) were recorded, using the above relation the fuel flow rate was calculated.

3.1.3 RECIRCULATED EXHAUST GAS FLOW

The EGR flow metering system has been already described in section 2.3.2 (see fig. 2.5). To meter the exhaust gas flow rate using this system, it would be necessary to calibrate this metering system with a standard flowmeter. Instead, a rotameter with two balls (stainless steel and pyrex) was calibrated from a standard flow meter very accurately. Should a need arise, the calibrated rotameter can be used to calibrate the Metering System. The rotameter calibration is discussed in Appendix D.

The rotameter can measure up to 1.5 SCFM of exhaust gas. This volume rate can provide up to 20% recycled gas in the intake charge and was regarded sufficient for the present study. Calibration of the EGR flow metering system was thus not performed. Instead the rotameter was connected to one of the four parallel metering lines through a silica gel drier to meter dry exhaust gas for recycling into the carburetor.

PERCENT EGR

To measure the dilution of intake air, percent EGR or percent dilution was defined as follows:

$$\text{PERCENT EGR} = \frac{\text{volume of recycled exhaust gas}}{\text{volume of intake air without the EGR}} \times 100$$

It may be noted that EGR fraction or recycled gas fraction is synonymous to the percent EGR.

3.2 TESTING AND DATA COLLECTION

The total effort required for Engine modifications, instruments installation, design, experimentation and computer programming had made the project quite large, hence it was decided not to obtain very extensive data covering all the features in the system.

The purpose of the experimental part of this study has been outlined in Chapter 1. The system maintenance has been described in Appendix E. Preliminary testing and investigation was conducted to determine which variables, apart from two main variables, namely, the EGR fraction and NO_x concentration, would also be worth considering. The Standard Operating Conditions (SOC) are defined by the values of the operating parameters as shown in Table 3-1. The effect of any one variable was studied

TABLE 3-1

STANDARD OPERATING CONDITIONS (SOC)

Compression ratio	8:1
Speed, rpm	900 ± 9
Intake air temperature, °F	(75-85) ± 2
Mixture temperature, °F	180 ± 2
Spark advance	10° BTC
EGR temperature, °F	(75-87) ± 3
Oil pressure, psig	33 ± 3
Coolant temperature, °F	210 ± 1
Oil temperature, °F	130 ± 5
Intake valve opens	10° ATC
Intake valve closes	34° BTC
Exhaust valve opens	40° BBC
Exhaust valve closes	15° ATC
Valve overlap	5°
EGR pump vacuum, in.Hg.	12.5
FUEL	SHELL REGULAR

TABLE 3-2

VARIABLE OPERATING CONDITIONS (VOC)

Air fuel ratio	14.0 to 23.6
Humidity, grain/lb air	23 to 72
Mixture temperature, °F	75 to 200
EGR fraction	0 to 20%
EGR temperature, °F	80 to 475
Sampling pump vacuum, in.Hg.	0 to 20

by changing its value from that listed in the SOC. The values of the variable parameters are shown in Table 3-2. The parameters listed below were continuously monitored on a strip chart recorder:

1. Exhaust gas temperature
2. Room temperature
3. Recirculated gas temperature
4. NO_x concentration.

In addition, peak pressure in the combustion cycle was also monitored from the Engine Analyser unit described in section 2.5. Any abnormal changes in p-v and p-θ images were observed from the oscilloscope screen.

Throughout the data collection, vacuum on the suction side of the pump was maintained at 12.5 in. Hg. This was essential as the NO_x concentration in the exhaust was found to depend on the suction side vacuum of the pump. The vacuum of 12.5 in. Hg. was selected to provide a maximum of 20% exhaust gas recirculation.

As a result of preliminary investigations and predetermined aims, it was decided to acquire data along the following lines:

(i) Effect of EGR Temperature on NO_x concentration for fixed EGR fractions.

Data was acquired for four different EGR fractions and an air fuel ratio of 17.35. Recirculated exhaust temperature was varied from 80° to 475° F while other parameters were as defined by the SOC. Results for single air fuel ratio revealed that there was no need to repeat the test for different air fuel ratios.

(ii) Effect of Volume of recycled exhaust gas on NO_x concentration.

Experiments were conducted to determine the behavior for five different air fuel ratios varying from 14.0 to 23.6. Other operating conditions were as defined by the SOC. The trend observed was similar to that available in literature (22,26). These tests were carried out primarily for the following reasons:

(a) Air fuel ratio calculations were not definite because of possible error in air flow measurement as outlined in section 3.1.1. Acquiring NO_x data served as a tool to ensure that calculated air fuel ratios were not significantly incorrect.

(b) To suggest, if possible, what air fuel ratio and percent EGR are best suited from NO_x emissions view point.

(iii) Effect of intake air Humidity on NO_x concentration in conjunction with the EGR.

Data was acquired for three air fuel ratios, four sets of EGR fractions and several sets of humidity. For humidity variation, there is no mechanical provision and one has to rely upon environmental humidity. For this reason, a wide range of data could not be acquired. Other operating conditions were as defined by the SOC.

(iv) Effect of Mixture Temperature on NO_x concentration.

This trend was observed for various air fuel ratios. Exhaust temperature and combustion peak pressure were also closely observed in addition to NO_x concentration and mixture temperature.

(v) Effect of Suction Side pressure of pump in the EGR system on NO_x concentration.

It was observed that reported NO_x concentrations in the exhaust gas were largely dependent on the suction side vacuum of the EGR pump. For this reason suction side vacuum was maintained at 12.5 in. Hg. throughout data collection. The vacuum of 12.5 in.Hg. was selected to meet the maximum gas flow requirement through the EGR system.

Chapter 4

EXPERIMENTAL RESULTS

The experimental apparatus described in the previous chapters allowed the acquisition of the experimental data.

4.1 REPEATABILITY

One very important consideration of any experimental data is its repeatability. During the data acquisition, repeatability was checked several times for randomly selected points. Whenever it had been possible to attain the same operating conditions on some other day, the repeatability was checked. However this was seriously constrained by humidity variation. To overcome this difficulty, the repeatability data was acquired along the following lines:

1. While performing experiments for EGR fraction variation, NO_x concentration was initially observed with no EGR. This reading was repeated after the EGR fraction variation data was acquired. The observations were reproducible within 2.0%.

2. To check reproducibility for a sample, it was analysed twice with a nitrogen purge between each flow.

3. At other times, after recording a set of data, some intermediate reading was checked and found to be in order.

4.2 OBSERVATIONS AND COMMENTS

It has been pointed out in section 3.1.1 and Appendix C that due to certain discrepencies, air flow could not be measured accurately but a tentative attempt was made to monitor it. Fig. 4.1 shows that maximum NO_x concentration occurs at the air fuel ratio of 18.0 while the same is reported (Ref. 10, Fig. 1) to occur at 15.5. This reveals that estimated air fuel ratio is higher than the actual one. It may be noted that once the correct air flow is measured, these air fuel ratios may be simply corrected by applying an appropriate correction factor.

A method of data acquisition has been outlined in section 3.2. This relates five sets of different parameters. Each is discussed here:

(i) Effect of the EGR Temperature

As emphasized in Chapter 1, any reduction in combustion temperature effectively reduces NO_x concentration. Fig. 4.2 shows NO_x concentration versus EGR temperature. It is quite apparent from this fig. that the effectiveness

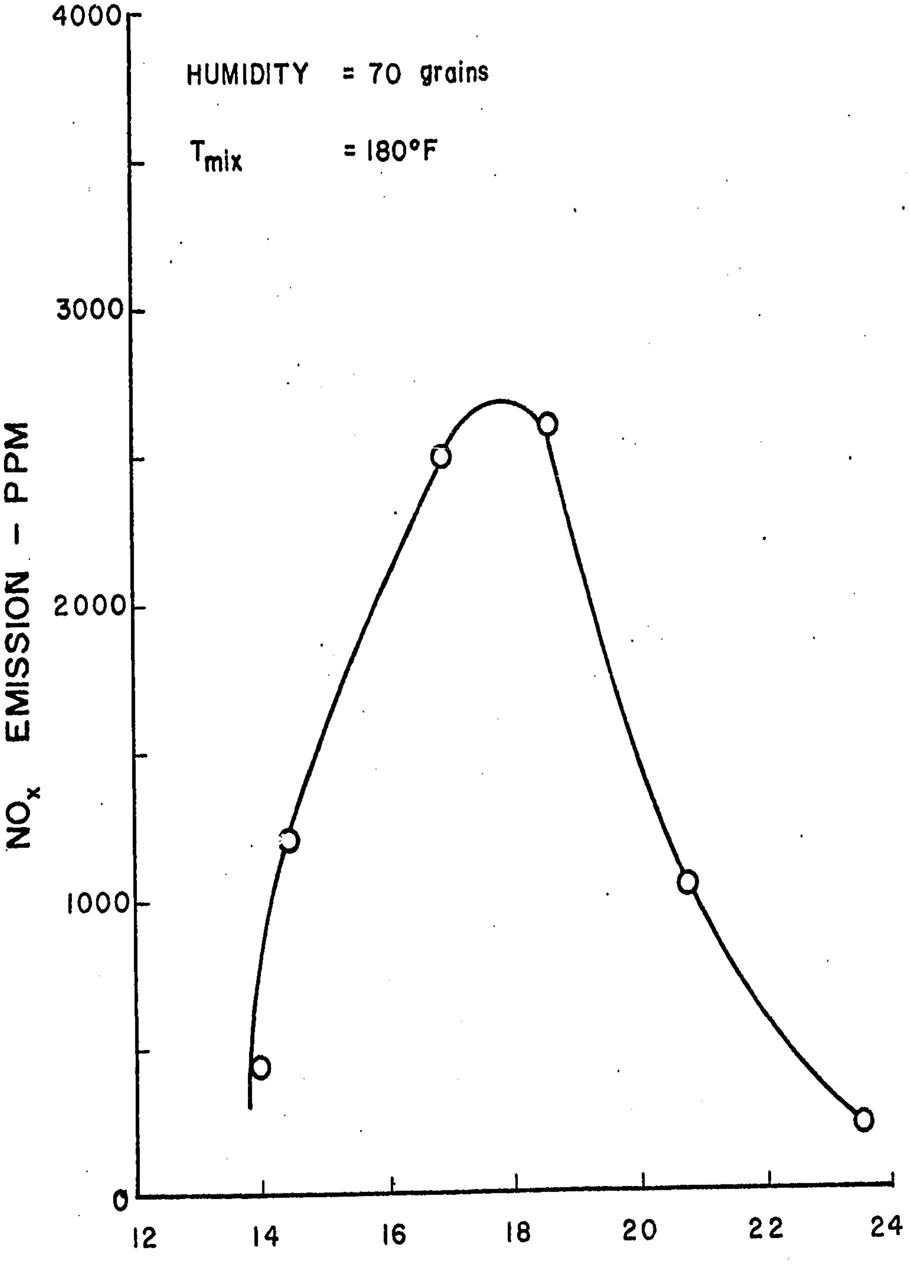
4000
3000
2000
1000
0
HUMIDITY = 70 grains
T_{mix} = 180°F
NO_x EMISSION - PPM
12
14
16
18
20
22
24
AIR-FUEL RATIO - BY WEIGHT

FIG. 4·1

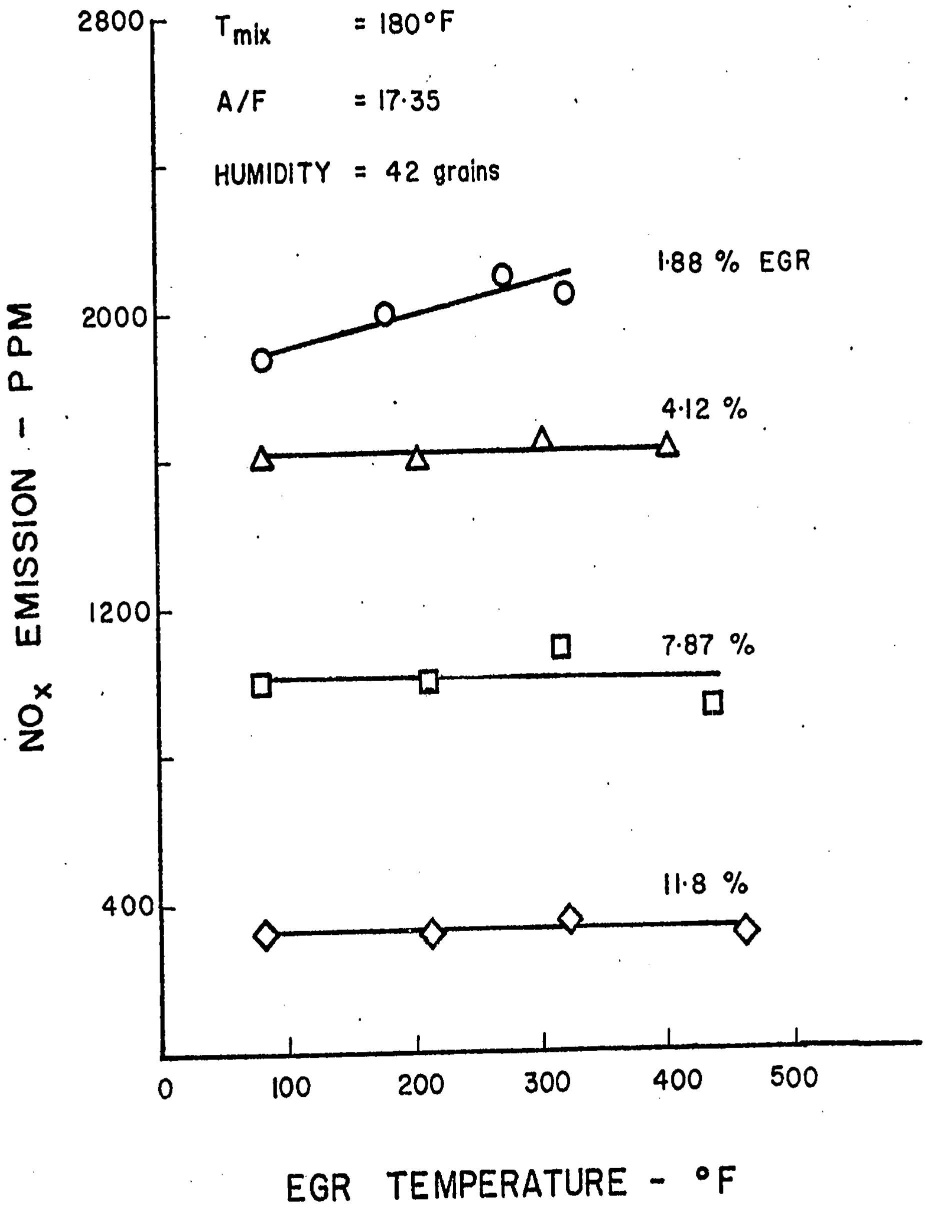
T_{mix} = 180°F
A/F = 17·35
HUMIDITY = 42 grains
1·88 % EGR
4·12 %
7·87 %
11·8 %
2800
2000
1200
400
NOx EMISSION - PPM
0
100
200
300
400
500
EGR TEMPERATURE - °F

FIG. 4·2

of the EGR is largely independent of the recirculated gas temperature. The curve for 1.88% recirculation indicates that there is a slight increase in NO_x concentration with the EGR temperature. An increase in recirculated gas temperature increases the total charge energy which would be expected to elevate the peak cycle temperature and hence NO_x concentration. It may be noted though, that such energy addition is not substantial. On the energy considerations, however, the trend depicted by 1.88% recirculation curve should have been more effective and pronounced for 4.12%, 7.37% and 11.8% recirculation. Therefore, the trend for 1.88% recirculation can be attributed to experimental error. Hence it may be concluded that NO_x concentration in the exhaust is independent of recirculated gas temperature up to 500^o F.

To the best of the author's knowledge, there is no experimental data available on this behaviour. The theoretical model of Chapter 6 (Fig. 6.3) does predict some increase in NO_x concentration as EGR temperature increases. Newhall (6) also reported from his theoretical investigations that nitric oxide reduction is dependent on the temperature of the recycled gas.

The analytical results included in Chapter 6 are based on the equilibrium combustion model and assumes that the volumetric efficiency of the engine would not decrease as the temperature of the recycled gas increased for a constant recycled gas fraction. The experimental observations however, indicated a decrease in the volumetric efficiency as the recycled gas temperature was increased. It may be commented that the observed change in the volumetric efficiency could be responsible for the difference in the analytical and experimental results.

(ii) EFFECT OF EGR VOLUME

Fig. 4.3 shows NO_x concentration on log scale against volume percent of recycled gas in the intake charge for various air fuel ratios. This demonstrates that NO_x level in the exhaust gas is largely dependent on air fuel ratio. It is further seen that curves for these air fuel ratios are almost parallel, signifying that effectiveness* of the EGR in reducing NO_x emissions is almost the same and is not largely dependent on air fuel ratio.

Absolute concentration of NO_x depends on the humidity of intake air as reported by Brown and others (26). They developed an equation for correction factor for the

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* Implies the percent reduction in NO_x for the same recycled gas fraction.

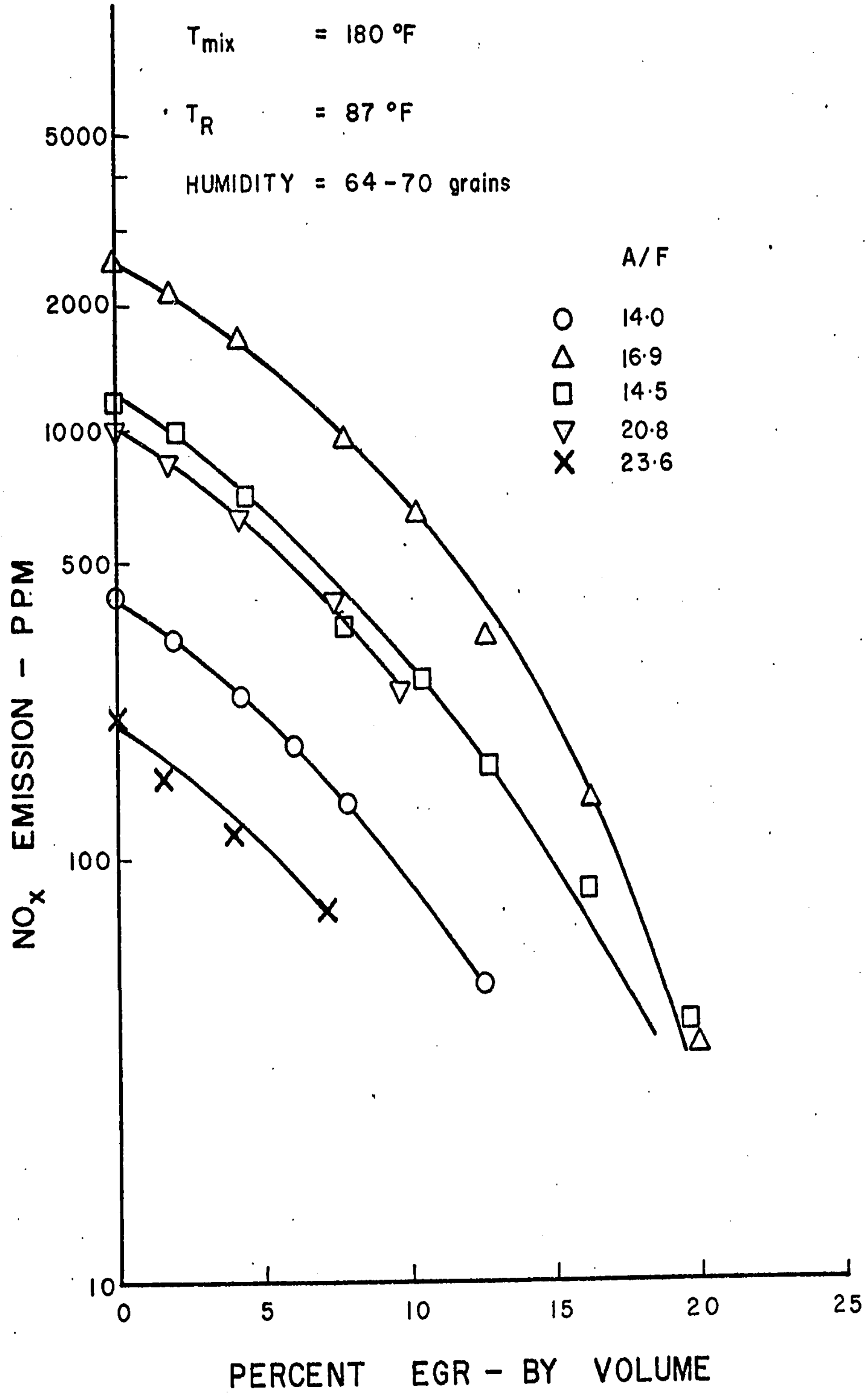

T_{mix} = 180 °F
T_R = 87 °F
HUMIDITY = 64-70 grains
A/F
○ 14·0
△ 16·9
□ 14·5
▽ 20·8
✕ 23·6
5000
2000
1000
500
100
10
0
5
10
15
20
25
NO_x EMISSION - P.P.M.
PERCENT EGR - BY VOLUME

FIG. 4·3

effect of humidity on NO_x concentration. However, if the results are plotted in terms of percent reduction of NO_x against recycled gas fraction, these become independent of humidity. This is because the correction factor drops out when NO_x concentration is converted to percent reduction in NO_x.

Fig. 4.4 shows percent reduction in NO_x level against percent recycled gas in the intake charge for six air fuel ratios. The dashed lines indicate a certain range within which NO_x reductions for a specific percent of recycled gas may be expected, irrespective of mixture air fuel ratio. The range is as wide as 20%. These points are again plotted for rich and lean mixtures as shown in Fig. 4.5 and 4.6 respectively. Both curves show that the effectiveness of the EGR is not dependent on air fuel ratio as emphasized before. (The validity of the trend is obviously of some doubt for Fig. 4.6). For rich mixtures (Fig. 4.5), it is apparent that the error incurred by drawing a single curve is within 3.0% except at two points where it is 5.0%. An error of 3.0 to 5.0% may be permissible, so an EMPIRICAL EQUATION is derived using all data points in Fig. 4.5 employing a least square fit. This equation holds up to 20% intake charge dilution.

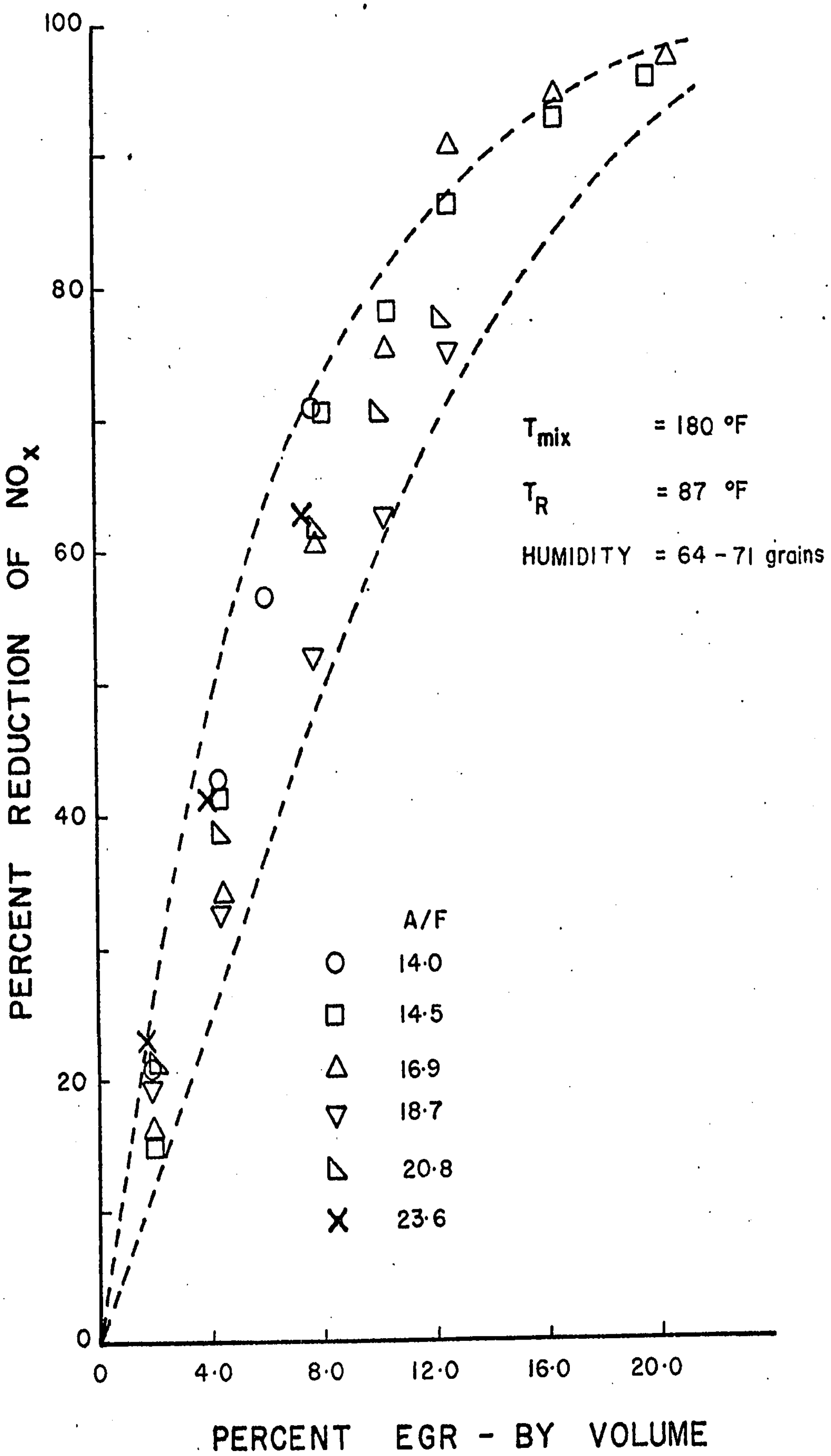

100
80
60
40
20
0
0
4·0
8·0
12·0
16·0
20·0
PERCENT REDUCTION OF NO_x
PERCENT EGR - BY VOLUME
T_{mix} = 180 °F
T_R = 87 °F
HUMIDITY = 64 - 71 grains
A/F
○ 14·0
□ 14·5
△ 16·9
▽ 18·7
◺ 20·8
X 23·6

FIG. 4·4

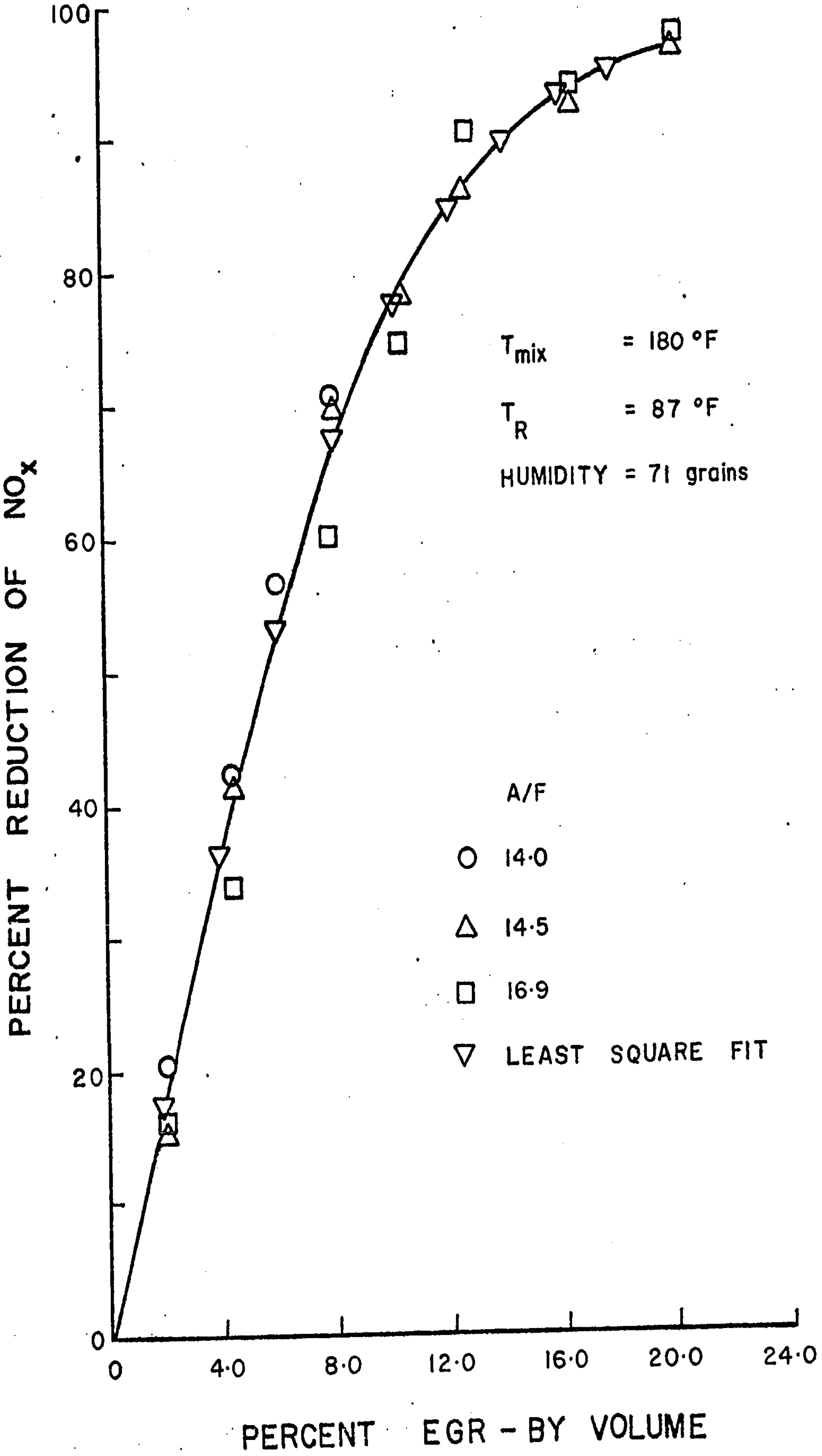

100
80
60
40
20
0
PERCENT REDUCTION OF NO_x
0
4·0
8·0
12·0
16·0
20·0
24·0
PERCENT EGR - BY VOLUME
T_{mix} = 180 °F
T_R = 87 °F
HUMIDITY = 71 grains
A/F
○ 14·0
△ 14·5
□ 16·9
▽ LEAST SQUARE FIT

FIG. 4·5

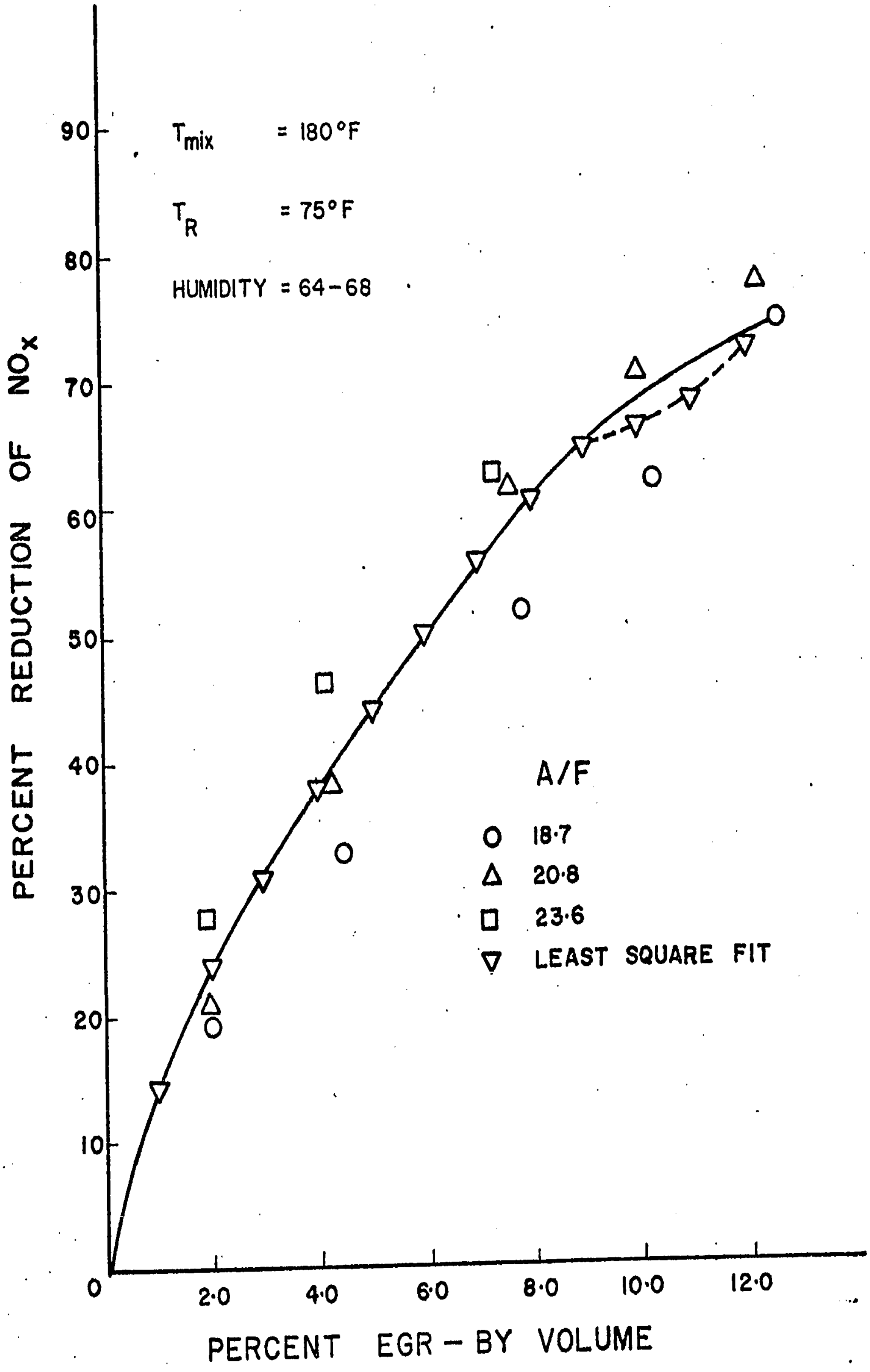

T_{mix} = 180°F
T_R = 75°F
HUMIDITY = 64–68
PERCENT REDUCTION OF NO_x
90
80
70
60
50
40
30
20
10
0
2·0
4·0
6·0
8·0
10·0
12·0
A/F
○ 18·7
△ 20·8
□ 23·6
▽ LEAST SQUARE FIT
PERCENT EGR – BY VOLUME

FIG. 4·6

The equation assumed the following form:

$$y = a_o + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5 \qquad \ldots.(1)$$

where,

y = percent reduction in NO_x concentration

x = percent EGR

a_o-----a_5 are constants

$a_o = -\ 0.1958128$

$a_1 = \ \ 0.7829502 \times 10$

$a_2 = \ \ 0.6961558$

$a_3 = -\ 0.1129190$

$a_4 = \ \ 0.5142152 \times 10^{-2}$

$a_5 = -\ 0.8021326 \times 10^{-4}$

This equation may be used as a tool by the designer to anticipate the order of reductions in NO_x concentration for a specific value of recycled gas fraction. As stated above, the equation is independent of air fuel ratio, humidity and temperature of the recycled gas. Further work in this direction may be to determine how this equation is changed as spark advance is varied. If the equation is found to be insensitive to spark advance, then the general equation will provide very worthwhile information about NO_x reduction by the EGR technique.

A similar empirical relation has been developed for lean mixtures which holds up to 13.0% intake charge dilution. The error incurred by drawing a single curve in this case is within 5.0% except at one point where it is 10%. The equation assumed the same form as eq. 1 but the constants are different as given below:

$a_0 = -\ 0.2463306$

$a_1 = 0.1974182 \times 10^2$

$a_2 = -\ 0.5661617 \times 10$

$a_3 = 0.1107294 \times 10$

$a_4 = -\ 0.9893811 \times 10^{-1}$

$a_5 = 0.3172433 \times 10^{-2}$

It may be noted that the upper part of the curve (shown by dashed line, Fig. 4.6) given by this equation is not accurate. It is recommended that more data points be acquired and incorporated in the least square fit equation for lean mixtures.

Analytical results, shown in Fig. 6.4 and 6.7, predict that the reductions in NO emission for a recycled gas fraction are within 5% of each other for lean mixtures and within 2% of each other for moderately rich mixtures ($\emptyset > 1.1$). However, the variation is significantly large for mixtures near stoichiomatic ratio ($0.95 < \emptyset < 1.1$).

(iii) EFFECT OF INTAKE AIR HUMIDITY

Effect of intake air humidity has been studied

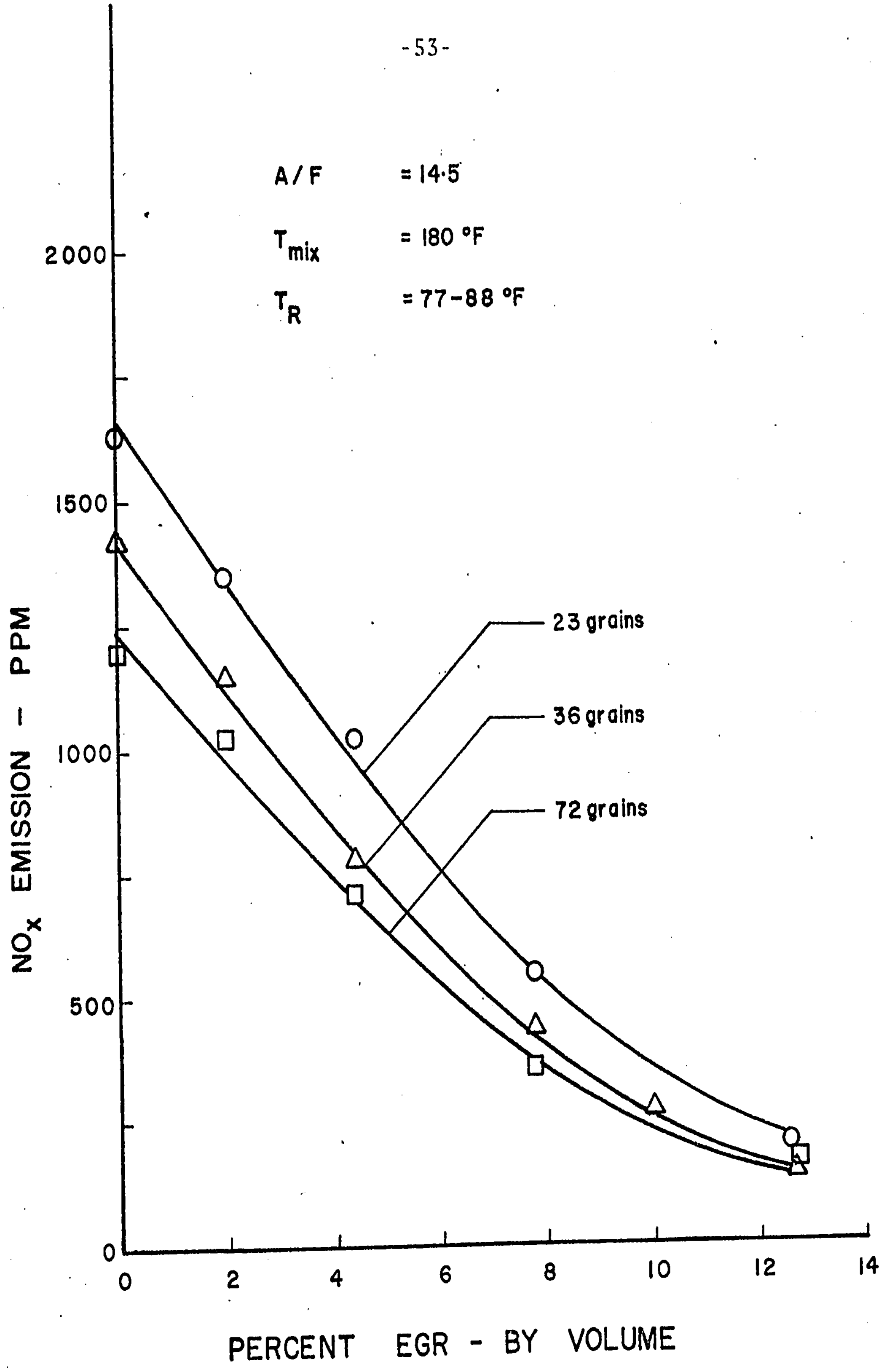

A/F = 14·5
T_{mix} = 180 °F
T_R = 77-88 °F
2000
1500
1000
500
0
NO_x EMISSION - PPM
23 grains
36 grains
72 grains
0
2
4
6
8
10
12
14
PERCENT EGR - BY VOLUME

FIG. 4·7

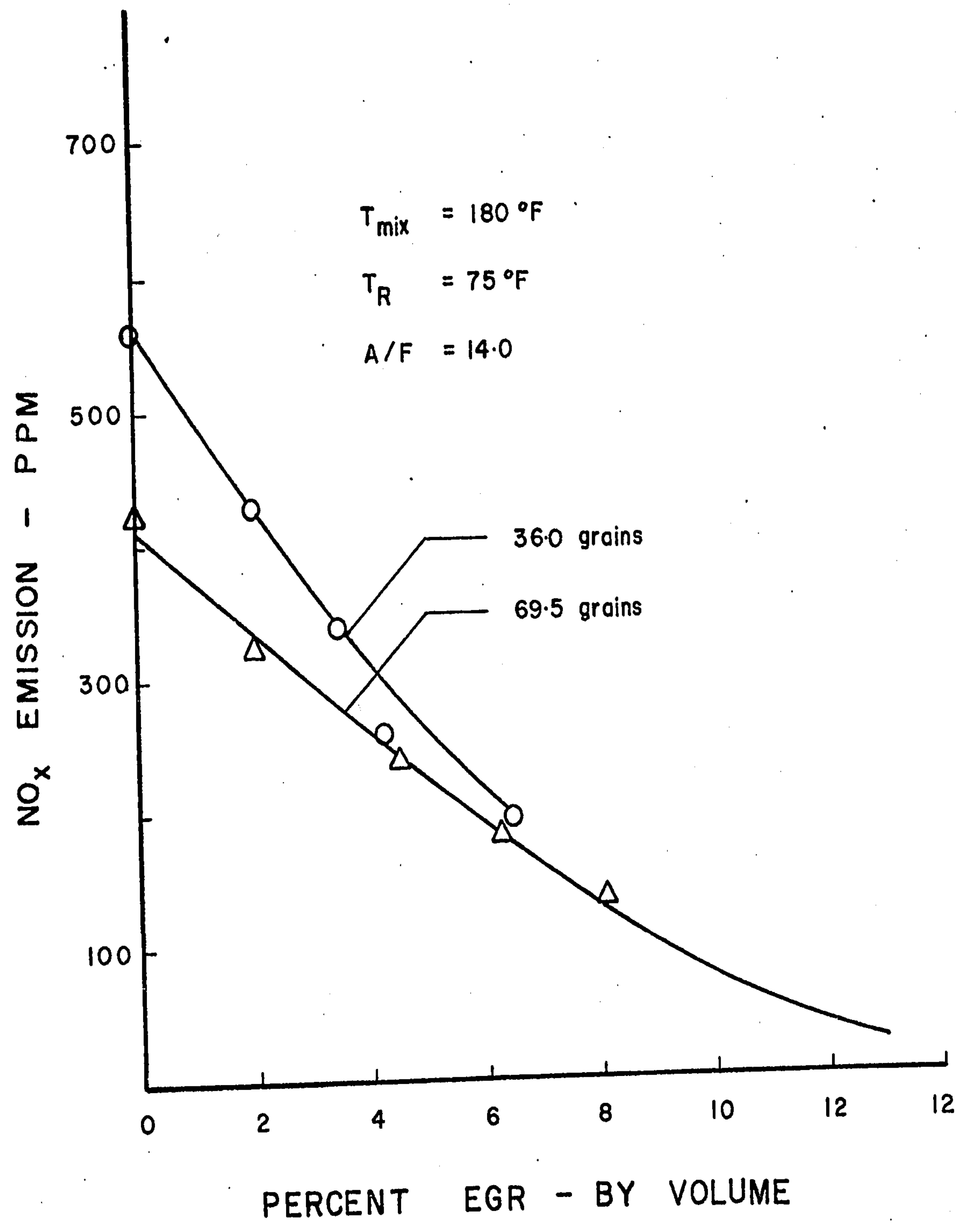

T_{mix} = 180 °F
T_R = 75 °F
A/F = 14·0
36·0 grains
69·5 grains
700
500
300
100
NO_x EMISSION - PPM
0
2
4
6
8
10
12
12
PERCENT EGR - BY VOLUME

FIG. 4·8

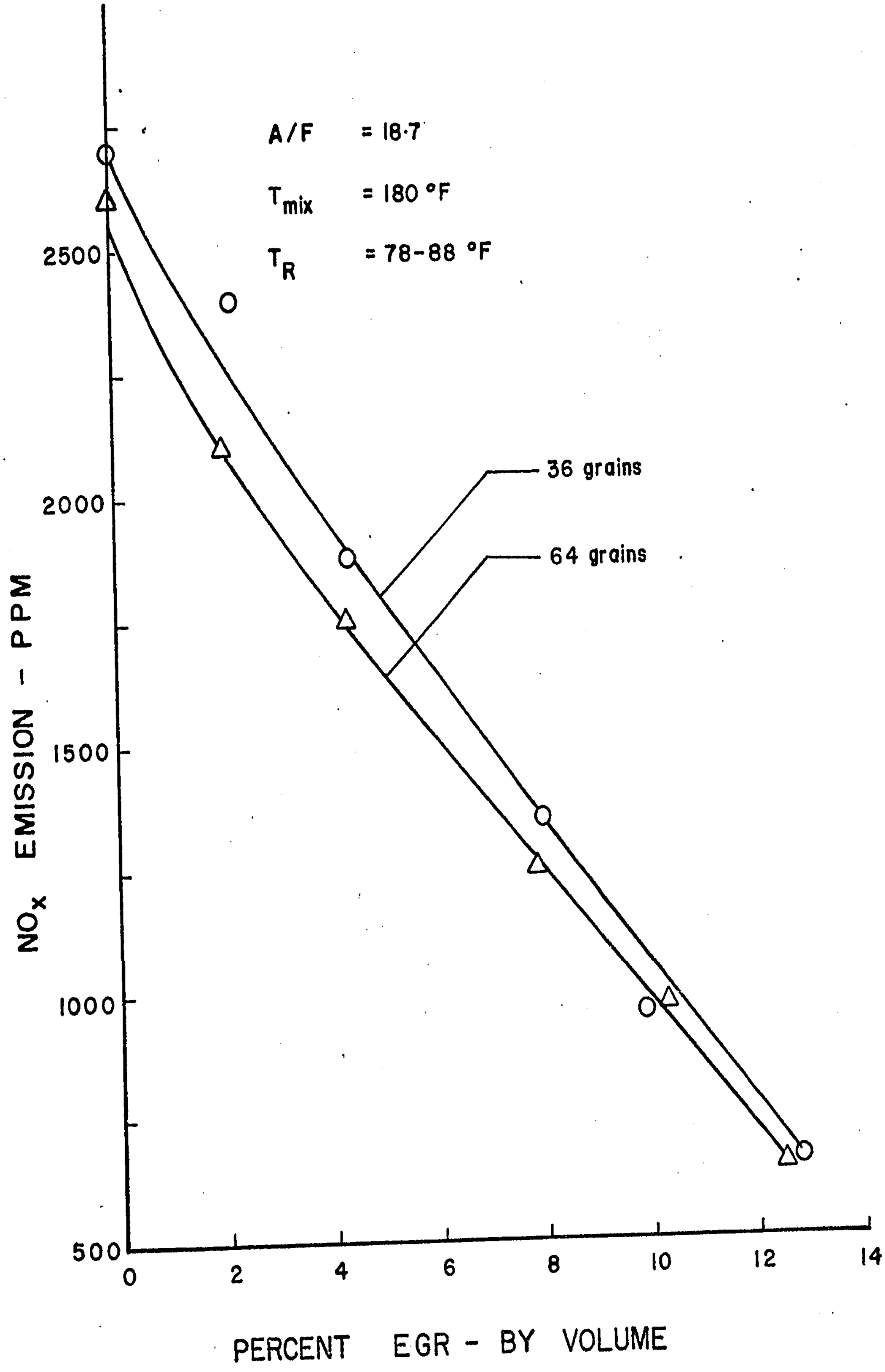

A/F = 18·7
T_{mix} = 180 °F
T_R = 78-88 °F
36 grains
64 grains
2500
2000
1500
1000
500
0
2
4
6
8
10
12
14
NO_x EMISSION - PPM
PERCENT EGR - BY VOLUME

FIG. 4·9

(26-28) but it has not been studied in conjunction with the exhaust gas recirculation, though Nicholls and others (8) studied the effect of water injection on NO_x emissions in conjunction with the EGR. As mentioned in section 3.2 no mechanical system was employed for humidity variation of intake air. Rather it depended on local weather conditions.For this reason an extensive data on this study could not be recorded.

Fig. 4.7 shows the effect of recycled gas quantity on NO_x concentration for three humidities of 23 grains, 36 grains and 72 grains (per pound of dry intake air). It is apparent from the graph that the change in the intake moisture from 23 grains to 72 grains is as effective in reducing NO_x as the recycling of 2.3% exhaust gas. This data further reveals that NO_x concentration is reduced to a smaller extent by humidity changes in the intake air as the recycled gas quantity increases. This may be explained by the fact that water moisture acts like an inert gas in the combustion chanber as does the exhaust gas. At no or small recycled gas quantity, the effect of intake moisture would be significant since moisture quantity is comparable to recycled gas quantity. However, at higher recycling rates, the moisture effect is negligible compared to the EGR effect.

To see how the effectiveness of humidity variation in the present context may change as mixture air fuel ratio is altered, the data in figures 4.7, 4.8 and 4.9 may be studied. If the effect of humidity on NO_x level is measured as the equivalent of percent recycled gas, the following could be observed for the change of intake humidity from 36 grains to approximately 70 grains.

Air-Fuel Ratio	Reduction in NO_x (In equivalent % EGR)
14.00	2.3 % EGR
14.50	1.2 % EGR
18.7	0.6 % EGR

That is, reduction in NO_x emission due to humidity depends on mixture air fuel ratio. Hence in summary:

1. The effect of intake air humidity change on NO_x emissions diminishes as the recycled gas quantity increases.

2. The intake moisture effect on NO_x emission is more promising for rich mixtures as compared to lean mixtures.

(iv) EFFECT OF MIXTURE TEMPERATURE

The effect of mixture temperature on NO_x concentration is shown in Fig. 4.10 for four air fuel ratios. As the mixture was heated from 90° F to 210° F, NO_x concentrations were observed to decrease or increase depending on whether the initial mixture is rich or lean. The change in NO_x concentration for the air fuel of 17.7 (stoichoimatic ratio being 17.5) is critical as NO_x concentration increases by 66% for the change in mixture temperature from 96° F to 200° F. For rich mixture combustion, NO_x concentration decreases as the mixture temperature increases. However, as the mixture becomes less rich (from air fuel ratio of 14.9 to 16.6), the effectiveness of mixture temperature in reducing NO_x emission decreases. But for a lean mixture (air fuel ratio 18.8), NO_x concentration increases with mixture temperature but it is not so sharp as it is with the mixture very close to the stoichoimatic ratio.

The mixture near the stoichoimatic ratio behaves very differently from rich or lean mixture. This is apparent from Fig. 4.11, which shows cycle peak pressure versus mixture temperature. These curves are drawn for four air fuel ratios. It may be mentioned that both air flow and fuel flow to the engine decreased continuously as the mixture temperature was increased, that is, the volumetric efficiency of the engine decreases as the

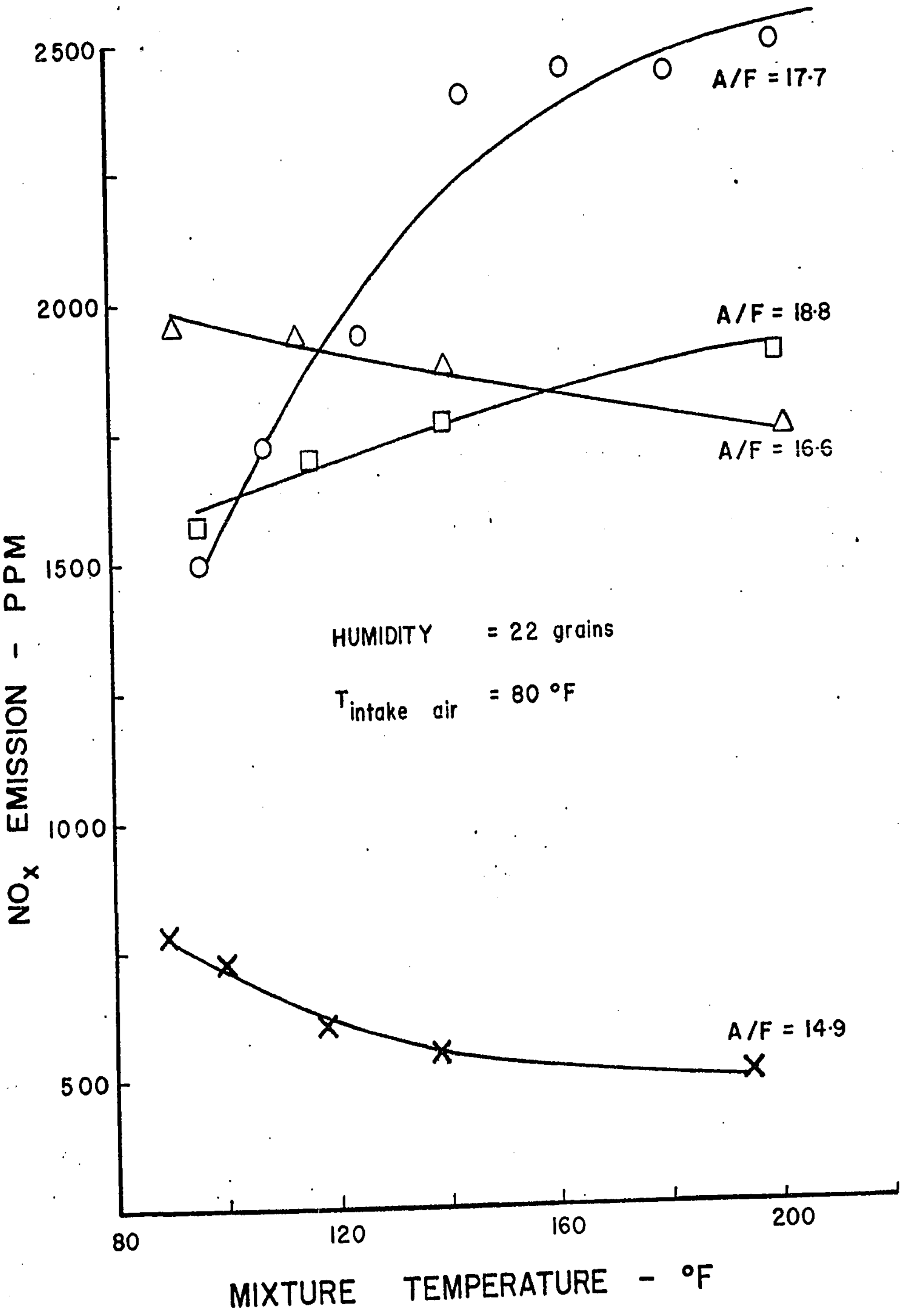

2500
2000
1500
1000
500
NO$_x$ EMISSION - PPM
80
120
160
200
MIXTURE TEMPERATURE - °F
A/F = 17·7
A/F = 18·8
A/F = 16·6
A/F = 14·9
HUMIDITY = 22 grains
T$_{intake\ air}$ = 80 °F

FIG. 4·10

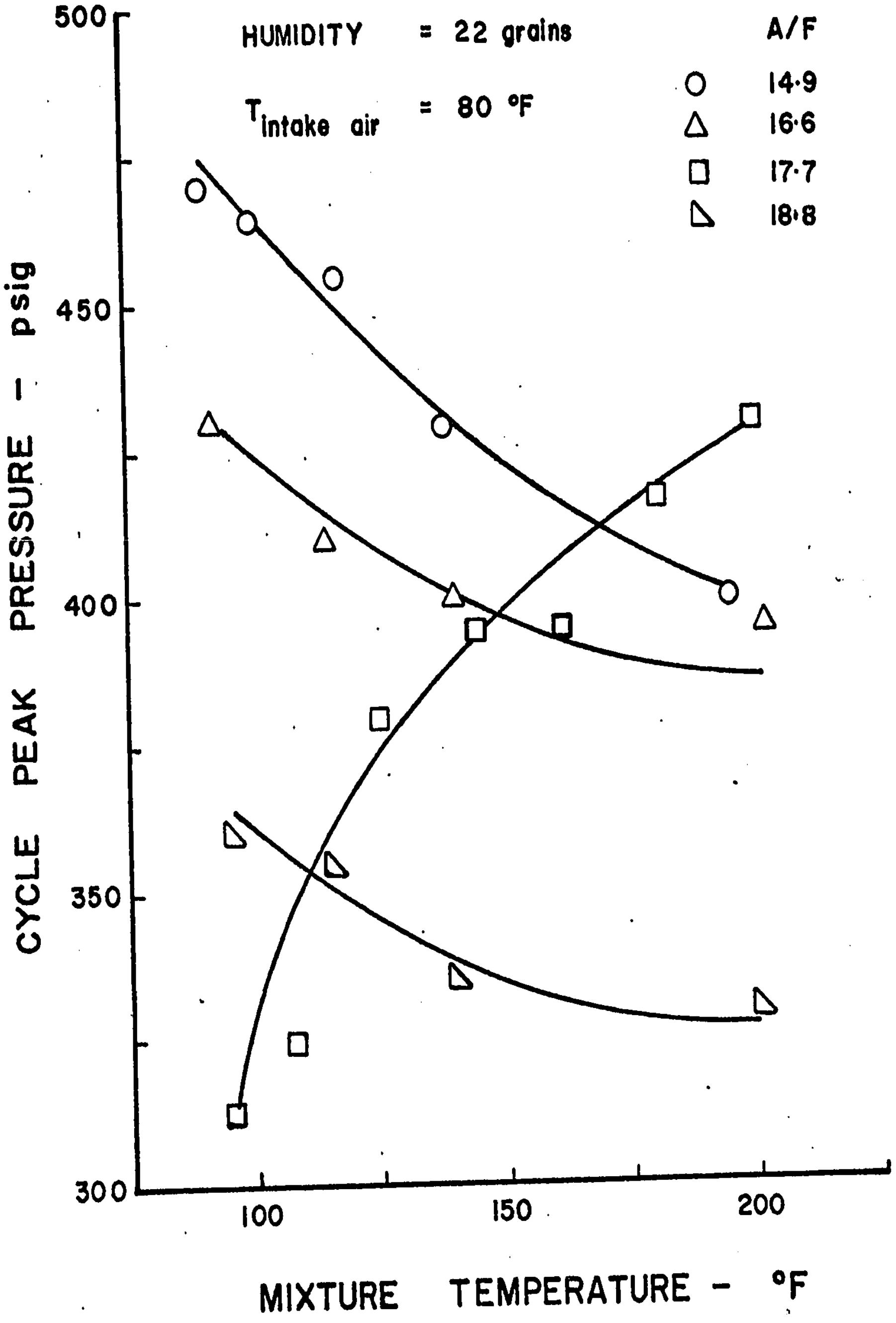

HUMIDITY = 22 grains
T intake air = 80 °F
A/F
○ 14·9
△ 16·6
□ 17·7
◺ 18·8
CYCLE PEAK PRESSURE - psig
500
450
400
350
300
100
150
200
MIXTURE TEMPERATURE - °F

FIG. 4.11

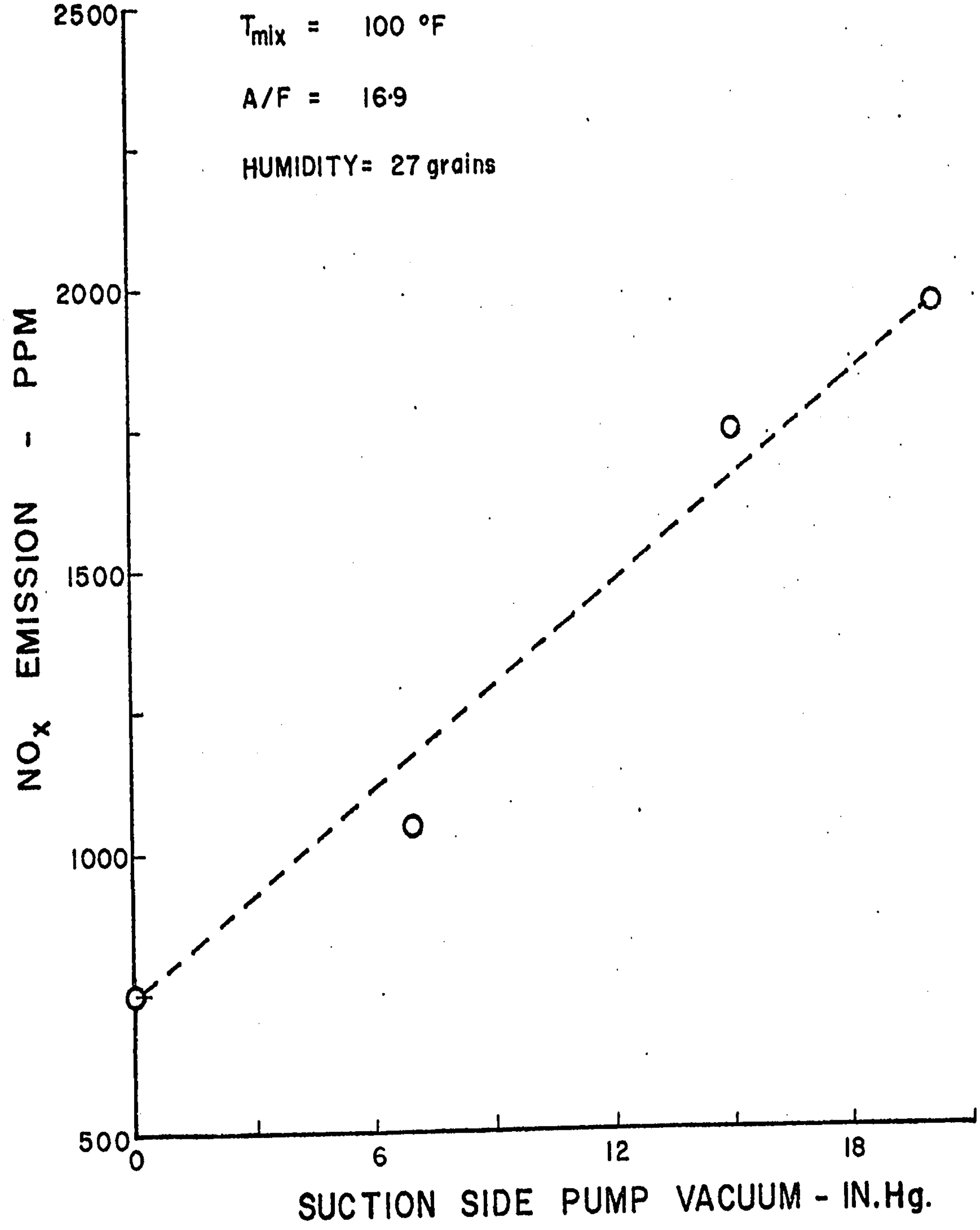
mixture is heated.

It may be tentatively concluded that near the stoichoimatic mixture conditions nitric oxide concentration depends heavily on the mixture temperature. Otherwise, for lean mixtures NO_x concentration increases while for rich mixture it decreases as the mixture is heated. Fleming (17) reported that the effect of mixture temperature on exhaust emissions is insignificant from 160^o - 280^o F. This may be confirmed for the temperature range 160^o - 200^o F from Fig. 4.11 as well. At lower temperature however, this is not apparently so.

Analytical results, shown in Fig.6.10, (Chapter 6), depict that nitric oxide concentration in the exhaust gas increases with mixture temperature. Fig.6.10 shows the variation for four air fuel ratios: lean (ϕ = 0.8, 0.9), stoichoimatic (ϕ = 1.0) and rich (ϕ = 1.1). During testing, as pointed out above, the volumetric efficiency decreases as the mixture is heated. On the contrary, the analytical model assumes constant volumetric efficiency. This may explain the difference in the experimental and the analytical results.

(v) EFFECT OF SUCTION SIDE PRESSURE OF PUMP IN THE EGR SYSTEM

Fig. 4.12 shows the effect of suction side pump



T_{mix} = 100 °F
A/F = 16·9
HUMIDITY= 27 grains
2500
2000
1500
1000
500
NO_x EMISSION - PPM
0
6
12
18
SUCTION SIDE PUMP VACUUM - IN.Hg.

FIG. 4·12

vacuum on NO_x concentration. The exact shape of the curve may be questionable. It is certain though, that NO_x concentration changes very sharply. The trend was checked three times and found to be the same as reported. The intention is to show the potential of valve overlap in the reduction of NO_x emissions. Benson and Stebar (21) reported the effect of 16° and 66° valve overlaps on NO_x emissions. However, in the present study the effect of valve overlap on NO_x emissions was indirectly studied by changing the pressure at the exhaust port. The trend observed is more promising even though the valve overlap is only 5°. The intake valve opens at 10° ATC and the exhaust valve closes at 15° ATC.

The observed behaviour can be explained by the fact that valve overlap results in the charge dilution, that is, a small quantity of exhaust gas enters the combustion chamber through valve overlap during intake stroke of the engine. As the exhaust port pressure is decreased by creating vacuum in the suction side of the EGR system, the charge dilution by the valve overlap reduces. As a result, NO_x concentration increases.

To draw any specific conclusions, the following is recommended for further study:

(1) Vacuum near the exhaust port be monitored.

(2) Manifold Vacuum be monitored.

(3) As suggested in section 3.1.1, an accurate air flow measurement device be used to observe the changes in the amount of fresh charge taken in.

(4) The engine power output be measured using the p-v diagram photograph taken from the engine analyser oscilloscope.

(5) The effect of spark advance and retard be also studied in this context.

(6) The effect of increasing exhaust port pressure (by some other artificial means) on NO_x emissions may also be studied.

4.3 SUMMARY OF RESULTS

The experimental results are presented in previous sections of this chapter. The repeatability of the reported data is quite good. The effects of changes in several variables on the NO_x emissions are presented. These variables are: EGR volume, EGR temperature, intake air humidity, mixture temperature and vacuum at the exhaust port.

4.4 CONCLUSIONS

The following conclusions are based on the work presented:

(1) NO_x emissions are not effected by variation of recycled gas temperature from 80 - 500° F.

(2) Effectiveness of EGR in reducing NO_x emissions is almost independent of air fuel ratio. The level of NO_x emissions itself is, of course, largely dependent on air fuel ratio. Two empirical equations have been developed, one each for rich and lean mixture, to relate NO_x reduction to percent EGR.

(3) Increasing moisture content of the intake-air tends to reduce NO_x concentration in the exhaust gas. The effectiveness of humidity increase in NO_x tends to decrease as the amount of recycled gas in the intake charge increases. Intake-air moisture effect on NO_x concentration is more promising for rich mixtures as compared to lean mixtures.

(4) As the air fuel mixture is heated from 90° through 200° F, NO_x concentration in the exhaust gas is seen to increase or decrease according to initial lean or rich mixture. Near stoichoimatic ratio, however, NO_x emissions increase very sharply with mixture temperature.

(5) It is evident that valve overlap results in charge dilution which substantially reduces NO_x concentration in the exhaust gas. Recommendations for further study have been listed in the discussion (page 63).

Chapter 5

FURTHER UTILITY OF THE SYSTEM

Experimental set-up has been described in Chapter 2. The system was designed to cover as many test variables as possible with the flexibility for future modifications.

5.1 PARAMETERS

Following are the parameters with the specified range that can be varied for experimental purposes:

Compression ratio	: 4.46 - 16.00
Intake air temperature	: 40° - 160° F
Spark	: 40° BTC - 40° ATC
Mixture temperature	: 75° - 300° F
Air fuel ratio	: 12 - 24
Percent EGR	: 0 - 90
EGR temperature	: 75° - 500° F
EGR humidity	: Dry to maximum in the exhaust
EGR pump vacuum	: 0 - 25 inch, Hg.
Exhaust port pressure	: 0.25 - 5.0 psig
Intake air humidity	: 10° F dewpoint to atmos.humidity

5.2 FURTHER STUDY

In the previous section parameters that can be varied are listed. Any number of listed parameters can be varied or kept unaltered. Five useful combinations of these parameters were undertaken in this study. Besides these combinations, other possible interesting set for further investigations may be:

(i) SPARK: In the present study, all tests were conducted for a fixed spark setting of 10^{o} BTC. This spark setting may be changed from 40^{o} BTC to 40^{o} ATC to acquire data on exhaust emissions.

(ii) COMPRESSION RATIO: One of the methods to reduce NO_x concentration in the engine exhaust is to decrease compression ratio. It can be varied from 4.46 to 16.00.

(iii) POWER: The engine is coupled with a synchronous motor capable of keeping the engine speed constant at 900 rpm. If the power measurement is desirable, I.H.P. can be measured by photographing p-v image from the engine analyser oscilloscope.

(iv) EXHAUST PRESSURE: It has been indicated in this study that valve overlap results in substantial reductions of NO_x emissions. The charge dilution thus provided by the valve overlap may be further studied by increasing pressure at the exhaust port.

To do this, the globe valve leading to atmospheric exhaust may be set to appropriate position. Another desirable parameter in this reference may be the measurement of the exhaust port pressure.

(v) LARGE QUANTITY OF EGR: In the present study a maximum of 20% exhaust gas was recycled. For this flow measurement, a calibrated rotameter was used. For higher flow rate up to as much as 90% EGR, flow metering system described in 2.2.2 may be used. The metering system may be calibrated using the rotameter.

(vi) EGR & MIXTURE TEMPERATURE: The effect of mixture temperature on NO_x emissions has already been discussed. Depending upon whether or not the mixture is rich or lean, NO_x concentration decreases or increases when the mixture is heated. A further extension of this problem would be to observe the effect of mixture temperature on NO_x emissions as the exhaust gas is recycled and to compare the effectiveness of the EGR for different mixture temperatures.

(vii) OTHER GASES: Apart from exhaust gas recycling, CO_2, N_2, A, He, etc., may be injected into the combustion chamber. The effect of recycling these gases has been studied (22) but this may be used for further investigations.

(viii) EXHAUST GAS HUMIDITY: Humidity of the recycled exhaust gas may be varied from dry to the amount of moisture available in the engine exhaust. In this work, only dry exhaust gas was recycled. The moisture in the exhaust is not expected to behave any differently than the moisture in the intake air, however, this experimental set-up provides this facility.

(ix) VARIOUS FUEL: 'Shell Regular' was the fuel used in this study. Other fuels like Indolene, Octane, heptane or lead free fuel may be used to study emissions.

(x) SAMPLE VACUUM: As the vacuum is created near the exhaust port, NO_x concentration tends to increase because less charge dilution takes place at the exhaust port. Here this fact has been merely reported. Its effect with other parameters, including exhaust gas recirculation, may be the subject for further investigation.

5.3 GENERAL RECOMMENDATIONS

To have an efficient utility of the system, a few modifications may be necessary:

1. AIR FLOW MEASUREMENT: It has been pointed out in section 3.1.1 that air flow measurement was not accurate and an alternative technique was employed to measure the air flow tentatively. For accurate flow measurement, one of the following three methods may be used:

(i) CRITICAL FLOW NOZZLE: It is a nozzle with Sonic flow conditions at the throat. Measuring pressure upstream and downstream of the throat and using gas tables, air flow rate can be measured very accurately.

(ii) EXHAUST ANALYSIS: This is an indirect procedure to determine air fuel ratio. In this method exhaust gas is analysed for CO_2, CO, and O_2 using Gas Partitioner or Orsat apparatus. For a known carbon to hydrogen ratio in the fuel, air fuel ratio can be directly read from D'Alleva tables (29) for the analysed exhaust components.

(iii) MERRIAM LAMINAR FLOW METER: It is a laminar flow orifice meter with pressure damping chamber. This has been used in reference (8).

2. VARIABLE COMPRESSION: Engine cylinder head is movable to adjust the desired compression ratio. This may cause severe straining of the exhaust port flange whose movement is restricted by surge tank support and globe valve bracket. These supports may be suitably modified to permit this movement.

3. FUEL SUPPLY: In the existing arrangements, fuel is carried to fuel bowl by siphon action. However, if due attention is not paid to the fuel flow rate, it may overflow the fuel bowl and spill over the floor. A suitable arrangement may be designed for continuous fuel supply to the engine.

4. EXHAUST OUT FAN: Engine exhausts into the yellow exhaust pipe provided in the test cell. There is no exhaust fan in the long pipe leading to atmosphere, it causes significant back pressure build up. This may alter the engine performance. An exhaust fan, therefore, must be installed in the exhaust line.

5. CARBON DEPOSIT: To avoid sooting in the exhaust gas cooler, it is recommended that a particle filter be installed upstream of the cooler.

Chapter 6

ANALYTICAL INVESTIGATIONS

6.1 ANALYSIS

The study of chemical kinetics of the Internal Combustion Engine has been undertaken to evaluate the concentration of various exhaust gas components by a digital computer simulation of the engine cycle. Fifteen reaction products at chemical equilibrium resulting from the combustion process of hydrocarbon fuel in air have been computed. The thermodynamic cycle employed is basically the Otto cycle. The fuel air mixture with and without recycled exhaust gas is compressed polytropically. Compression is followed by constant pressure combustion, giving rise to a chemical equilibrium distribution of species. It is well established that nitric oxide concentration in the engine exhaust corresponds approximately to chemical equilibrium concentration calculated for the peak combustion temperature (6,15,19,33-35). The concentration level is, however, several orders of magnitude greater at this temperature than at the final exhaust temperature. Throughout the analysis, nitric oxide concentration has been evaluated at the adiabatic flame temperature which is assumed to be the peak cycle temperature. All computations have been carried out for one mole of fuel.

6.2 BASIC PROCEDURE

As a result of fuel air combustion in the engine, the following fifteen species are assumed to constitute the exhaust gas:

Major Constituents: CO_2, H_2O, N_2, O_2 or CO

Minor Constituents: H_2, H, OH, O, N, NO, C, C_2H_2, NH_3 and CH_4.

One of the major species in the exhaust gas is O_2 or CO depending on whether the initial fuel air mixture is lean or rich. If the fuel is represented by C_xH_y, the number of moles of each specie in the combustion products by $n_{(SPECIE)}$ (e.g., n_{CO_2}, n_{O_2}, etc.), number of moles of oxygen in the intake mixture by n_{RO_2}; the standard carburetion (combustion) equation can be written as follows: (for each mole of fuel)

$$\begin{aligned} C_xH_y + n_{RO_2}(O_2 + 3.76\, N_2) \longrightarrow\ & n_{CO_2}CO_2 + n_{H_2O}H_2O + n_{O_2}O_2 \\ & + n_{N_2}N_2 + n_{H_2}H_2 + n_{CO}CO + n_H H \\ & + n_O O + n_N N + n_{NO}NO + n_C C \\ & + n_{C_2H_2}C_2H_2 + n_{NH_3}NH_3 \\ & + n_{CH_4}CH_4 + n_{OH}OH \quad .....(1) \end{aligned}$$

In air, N_2 to O_2 ratio(by volume) of 3.76 is standard. In general, equation (1) can be abbreviated as:

$$\sum_{i=1}^{3} n_i A_i \longrightarrow \sum_{j=1}^{15} n_j B_j \qquad \ldots\ldots(2)$$

Where A_i and B_j are the reactants and products in the combustion process and n_i and n_j are the molar concentrations of reactants and products respectively. For a specific fuel and an assumed intake mixture condition, all three n_i's would be known in the reactants. To compute 16 unknowns namely, adiabatic flame temperature (T) and 15 molar concentrations (n_j's) in the combustion products, 16 independent equations must be employed. These are:

(a) Four equations of conservation of atoms C,H,O and N.

(b) One energy conservation equation.

(c) Eleven independent equilibrium equations.

(a) Conservation of Atoms

Carbon: $$x = n_{CO_2} + n_{CO} + n_C + 2n_{C_2H_2} + n_{CH_4} \qquad \ldots\ldots(3)$$

Hydrogen: $$y = 2n_{H_2O} + 2n_{H_2} + n_H + n_{OH} + 2n_{C_2H_2} + 3n_{NH_3} + 4n_{CH_4} \qquad \ldots\ldots(4)$$

Oxygen: $n_{CO_2} = 2\ n_{CO_2} + n_{H_2O} + 2\ n_{O_2} + n_{CO} + n_{OH}$

$+ n_O + n_{NO}$ .....(5)

Nitrogen: $3.76 \times n_{CO_2} = 2\ n_{N_2} + n_N + n_{NO} + n_{NH_3}$ .....(6)

(b) Energy Conservation Equation

$$\sum_{i=1}^{3} n_i H_i(T_{in}) = \sum_{j=1}^{15} n_j H_j(T) \qquad .....(7)$$

where T_{in} = Intake air temperature

T = Adiabatic flame temperature

H = Enthalpy of species i or j at T_{in} or T.

(c) The following 11 independent chemical equilibrium equations are employed for the combustion equation (1).

1. $CO_2 \xrightarrow{K_{p_1}(T)} CO + \frac{1}{2}\ O_2$

2. $CO_2 + H_2 \xrightarrow{K_{p_2}(T)} CO + H_2O$

3. $CO_2 + C \xrightarrow{K_{p_3}(T)} 2\ CO$

4. $2\ C + H_2 \xrightarrow{K_{p_4}(T)} C_2H_2$

5. $CO + 3\ H_2 \xrightarrow{K_{p_5}(T)} CH_4 + H_2O$

6. $H_2O \xrightarrow{K_{p_6}(T)} \frac{1}{2}H_2 + OH$

7. $\frac{1}{2} O_2 \xrightarrow{K_{p_7}(T)} O$

8. $\frac{1}{2} H_2 \xrightarrow{K_{p_8}(T)} H$

9. $\frac{1}{2} N_2 \xrightarrow{K_{p_9}(T)} N$

10. $\frac{1}{2} O_2 + \frac{1}{2} N_2 \xrightarrow{K_{p_{10}}(T)} NO$

11. $\frac{1}{2}N_2 + 3/2H_2 \xrightarrow{K_{p_{11}}(T)} NH_3$

where $K_{p_1}(T)$---$K_{p_{11}}(T)$ are chemical equilibrium constants.

Let two important quantities be defined:

1. EQUIVALENCE RATIO Ø

The equivalence ratio is a normalized non-dimensional quantity and is defined as

$$\emptyset = \frac{\left(\frac{\text{fuel}}{\text{oxidizer}}\right)}{\left(\frac{\text{fuel}}{\text{oxidizer}}\right)\text{ stoichiometric}} \qquad .....(8)$$

An equivalence ratio of less than one is fuel lean; greater than one, fuel rich and equal to one stoichiometric.

2. STOICHIOMETRIC MIXTURE RATIO

The stoichiometric mixture ratio corresponds to complete combustion reaction. For systems with C, H, O and N atoms only, the stoichiometric reactants composition is the one which could produce only CO_2, H_2O and N_2 on the basis of atom conservation.

Heptane C_7H_{16} has been used as the fuel for the analytical study. The stoichiometric equation for heptane is written as:

$$C_7H_{16} + 11.0\ (O_2 + 3.76\ N_2) \longrightarrow 7\ CO_2 + 8\ CO_2 + 3.76 \times 11.0\ N_2 \quad .....(9)$$

In order to write equation (1) with the variable initial mixture conditions, it is essential to include equivalence ratio ϕ.

$$\phi = \frac{1/n_{RO_2}}{1/11.0} \quad \text{(As defined in equation 8)}$$

$$\therefore\ n_{RO_2} = \frac{11}{\phi}$$

Hence equation (1) for heptane becomes:

$$C_7H_{16}. + \frac{11}{\phi}\ (O_2 + 3.76\ N_2) \longrightarrow \text{PRODUCTS OF COMBUSTION} \quad .....(10)$$

Since these 16 equations cannot be solved simultaneously an iterative procedure shown in Fig. 6.1 has been adopted. All eleven equilibrium equations and the energy equations depend upon the adiabatic flame temperature which is

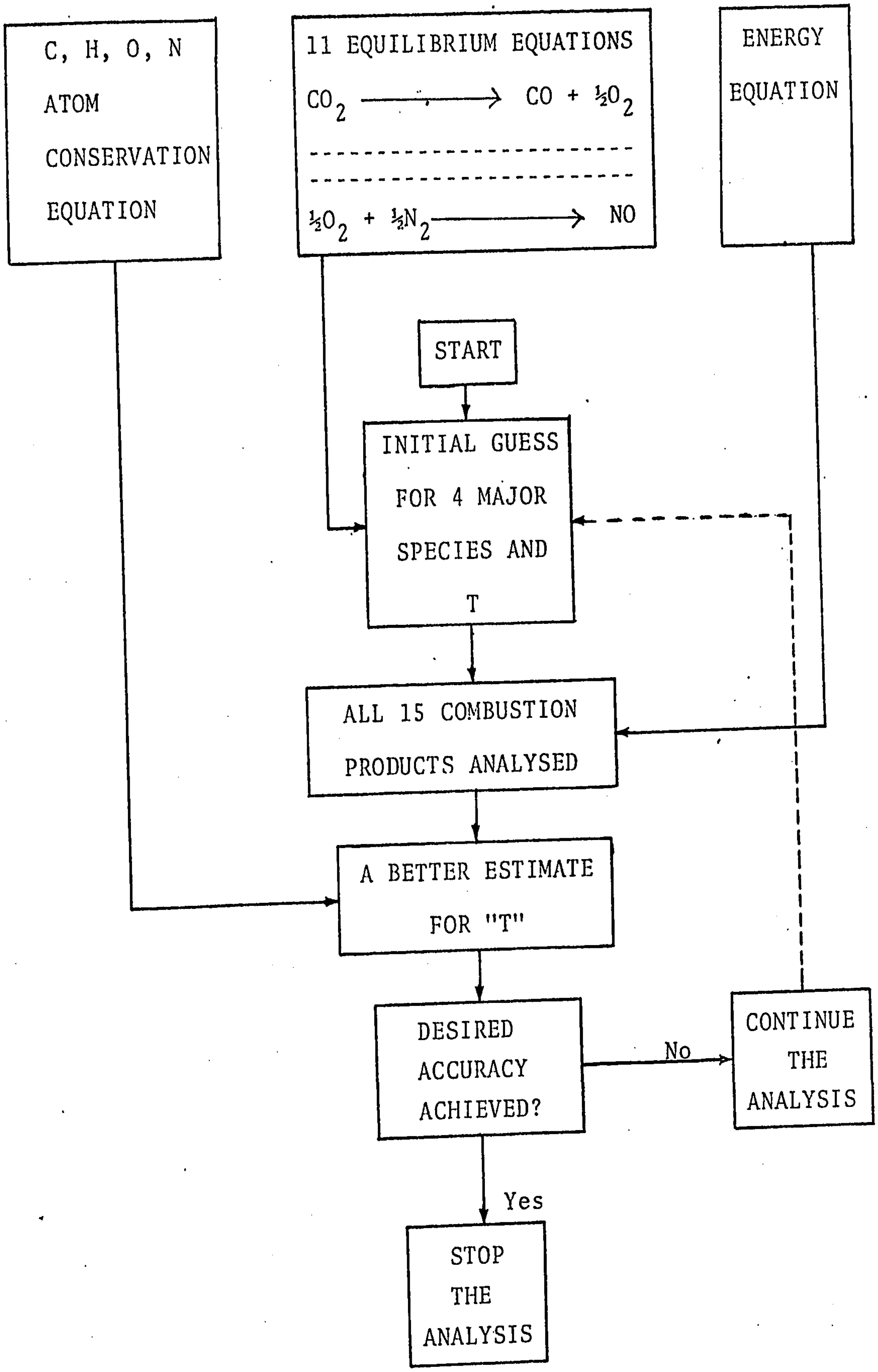


Fig. 6.1 BASIC PROCEDURE FOR THE EXHAUST ANALYSIS

chosen suitably but arbitrarily. Data for equilibrium constants and enthalpy of formation are available in the reference (36-37). Only 12 equations have yet been mentioned for the iterative procedure, hence to solve for 16 unknowns, remaining four atom conservation equations must be used to provide an initial guess for the major species. These major components are then used in the equilibrium equation to estimate the concentration of remaining 11 species in the exhaust gas. With all specie concentrations known, the energy equation is employed to predict a better value of the assumed adiabatic temperature. A better estimate of four major species for the next iteration is calculated using four atom conservation equations and 11 species estimated in the previous iteration. With the newly calculated adiabatic flame temperature and four major species concentration, the procedure is repeated to estimate adiabatic temperature and 11 species. This procedure is continuously repeated until the exhaust gas is analysed to the desired accuracy. The procedure has been illustrated in Fig. 6.1.

The technique used in estimating the major species and species themselves is slightly different for $\phi < 1.0$ and $\phi \geq 1.0$.

INITIAL GUESS FOR MAJOR SPECIES

$\phi < 1.0$: $\phi < 1.0$ implies that the available air is in excess of that needed for complete combustion, so the concentration of O_2, CO_2, N_2 and H_2O can be roughly estimated for the first iteration by assuming a complete combustion of the fuel and neglecting the quantity of other specie.

$\phi > 1.0$: In case of $\phi < 1.0$ it is apparent that besides N_2, CO_2 and H_2O, O_2 is one of four major components in the product gas. However, in this case, it is not so. $\phi \geq 1.0$ implies that the available O_2 for the combustion is just sufficient or scarce so it can't be a major specie. It is obvious that as air fuel mixture becomes richer, CO concentration would tend to increase because of incomplete combustion, hence CO has been assumed to be a major specie besides CO_2, H_2O and N_2. For the above mentioned reason complete combustion of the fuel can't be assumed even for rough estimation of the major species. So H_2O and CO are first suitably guessed and hence CO_2 and N_2. This is necessary only for the first iteration.Once initiated for $\phi = 1.0$, a rough estimate of the four major specie for the subsequent equivalence ratios may be taken from the results of the specie concentrations for the preceding equivalence ratios. A number of arbitrary rough estimates for major species were tried for $\phi = 1.0$. The iteration for the specie converged for a specific set of major species. This set was used to initiate the iteration process.

STANDARD CARBURETION (SC) AND EXHAUST GAS RECIRCULATION (EGR)

Standard Carburetion is the term which shall be used frequently to indicate that only air and fuel were admitted into the engine cylinder for combustion. The term Exhaust Gas Recirculation would indicate that a definite fraction of the total charge admitted into the engine was exhaust gas in addition to the appropriate fuel and air quantities.

The procedure for exhaust gas analysis outlined so far considers the standard carburetion only. Additional steps for the EGR analysis are described hereafter.

EXHAUST GAS RECIRCULATION (EGR)

Once the exhaust gas had been analysed for the standard carburetion, a specific fraction of the exhaust gas was recycled along with the fresh air fuel charge. The fresh air fuel charge was assumed to decrease in proportion to the quantity of recycled exhaust gas to maintain the total quantity of the charge admitted into the engine unchanged. Thus the changes in the total energy of the reactants as well as the changes in the quantity of major species were accounted for proportionately and the above iteration procedure was followed. Having found new concentration of exhaust components and adiabatic flame temperature, again the same quantity of exhaust gas was recycled with the fresh charge and exhaust species analysed. The whole procedure was continuously repeated until the exhaust gas analysis was the same for both exhaust gas going into the engine and coming out of the engine. In other words, a steady state was reached. The recycled gas fraction or EGR fraction FIN is defined as follows:

$$\text{FIN} = \frac{\text{Number of moles of exhaust gas recycled}}{\text{Total number of moles of fresh charge without the EGR}} \quad .....(11)$$

It is quite evident from equation (9) that number of moles of reactants are different from the number of moles of exhaust gas. Hence, another term is required which can relate FIN, total number of moles of exhaust gas and number of moles of recycled gas. The term is designated as F and is defined as follows:

$$\text{F} = \frac{\text{Number of recycled gas moles}}{\text{Total no. of moles in the exhaust with the EGR}} \quad .....(12)$$

Dividing equation (11) by (12)

$$\frac{\text{FIN}}{\text{F}} = \frac{\text{Total no. of moles in the exhaust with the EGR}}{\text{Total no. of moles of fresh charge without the EGR}} \quad .....(13)$$

Hence the equation with the EGR is

$$(1\text{-FIN}) \left\{ C_7H_{16} + \frac{11}{\phi} (O_2 + 3.76\ N_2) \right| + F \ \{ XN\ (K+1) \}$$

$$\longrightarrow \text{PRODUCTS} \quad XN\ (K+1) \qquad .....(14)$$

where x N (K+1) = Total no. of moles in the exhaust gas (A Computer Program Notation)

While the equation for the standard carburetion may be written as:

$$C_7H_{16} + \frac{11}{\phi} (O_2 + 3.76\ N_2) \longrightarrow XN\ (K+1) \qquad .....(15)$$

Equation (13) reduces to

$$\frac{FIN}{F} = \frac{XN\ (K+1)}{1 + \frac{11}{\phi}(1 + 3.76)}$$

$$\simeq \frac{x\ N\ (K+1)}{4.76 (\frac{11}{\phi})} \qquad \text{as } 1 << \frac{11}{\phi} (4.76)$$

or

$$FIN = \frac{F\ .\ XN\ (K+1)}{4.76\ (\frac{11}{\phi})} \qquad .....(16)$$

Detailed calculation procedure shall be described in section 6.4.

6.3 LIMITATION OF ANALYTICAL MODEL

The analysis and the simulation of the engine cycle is based on the assumptions summarized as follows:

1. Nitric oxide in the exhaust gas is assumed to exist at its adiabatic flame temperature (chemical equilibrium) concentration.

2. Combustion is assumed to occur spontaneously and at constant pressure.

3. Fuel is assumed to be composed of carbon and hydrogen atoms only. There are no other impurities like sulphur or lead.

4. Charge dilution by the cylinder residuals and because of valve overlap is assumed to be small and hence neglected.

5. As a result of the EGR, reductions in the intake air and fuel quantity are assumed to be in the same proportion.

6. Total number of moles of fresh air fuel charge as well as moles of recycled gas admitted into the engine are assumed to be unchanged for various initial mixture temperature and recycled gas temperature.

7. The effect of the temperature gradients in the combustion chamber is neglected.

While examining the validity of these assumptions in the light of actual engine performance, it should be kept in mind that the analysis is intended only to demonstrate behavioral trends.

The assumed instantaneous combustion process implies essentially an extremely high rate of flame propogation resulting in a high peak combustion temperature. In this event the predicted concentration of nitric oxide would be greater than the actual one.

Recycling the exhaust gas would be expected to retard the rate of flame propogation. This influence of exhaust recycle on flame speed would produce an additional temperature reduction over and above that produced by the dilution effect considered. In this case, the reduction of nitric oxide by exhaust recycle would be expected to be greater than that given by the present analysis. It may be emphasized that the effect of any reduction in the flame speed produced by exhaust recycling would result in some penalties on engine performance. However, the reduction in the flame speed may be compensated to some extent by advancing the ignition timing.

It was observed in the actual engine testing that the reductions in the fuel flow are faster than the reductions in the intake air flow as the recycled gas quantity is increased. In the analysis, however, it was assumed that the reductions in the fuel flow and air flow are in the same proportions. Assumption no. 6 implies that total mass flow admitted into the engine is assumed to be unchanged. While the total volume of the intake charge would change as the air fuel mixture temperature and/or recycled gas temperature is altered.

6.4 COMPUTER PROGRAMMING

To implement the computational procedures outlined in section 6.2 for the exhaust gas analysis, a computer program has been developed. The computer program was divided into two parts as follows:

(i) Main program;

(ii) Subprograms.

The main program carried out the iterations for the exhaust gas analysis while 24 subprograms provided data for 11 equilibrium constants and 13 species* enthalpy as a function of temperature. These subprograms were called

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* Enthalpy data for the remaining two species namely C_2H_2 and CH_4 were not included as the small quantities ($10^{-25}\%$) of these traces present in the exhaust gas does not contribute to the energy equation.

in the main program at the appropriate step. To include equilibrium constants (K_p) and specie enthalpy (H) data as a function of temperature, six degree polynomials were prepared. Each subprogram employed one polynomial to compute the value of K_p or H for a specific temperature in the main program.

6.4.1 NOMENCLATURE FOR PROGRAMMING

Some of the symbolic names for FORTRAN language are listed in Table 6-1. The remaining auxiliary names are explained in the programs by comment cards.

TABLE 6-1

SYMBOLIC NAMES FOR FORTRAN LANGUAGE

AA	difference in PROENT & REAENT
A_1	no. of carbon atoms in one mole of fuel (x)
A_2	no. of hydrogen atoms in one mole of fuel (y)
A_3	total no. of oxygen atoms in the intake air
A_4	total no. of nitrogen atoms in the intake air
CP	specific heat of the exhaust gas
CP_1---CP_4	specific heat of CO_2, H_2O, O_2 and N_2
CR	compression ratio
ER ( )	arrays for the difference in the species compositions in subsequent iterations with EGR
F	recycled exhaust gas fraction (exhaust side)
FIN	recycled exhaust gas fraction (intake side)
H(1)---H(7)	polynomial constants
K	no. of iterations performed for exhaust gas concentration
L	no. of iterations performed for a flame temperature
P	peak pressure of combustion
P_1---P_{12}	specie enthalpy of CO_2---C_7H_{16}
$PHCO_2$---PHC7H	subprograms for CO_2---C_7H_{16}

PHI	equivalence ratio
PROENT	total enthalpy of product gas per mole of fuel
R_1	reactant enthalpy of fuel C_7H_{16}
R_2	enthalpy of intake O_2
R_3	enthalpy of intake N_2
REAENT	total intake reactant enthalpy
RHC7H	subprogram for fuel C_7H_{16} enthalpy
T	adiabatic flame temperature
TIN	intake air temperature
TR	recycled exhaust gas temperature
W( )	array to store exhaust analysis for the preceded iteration
X( )	array to store mole fraction of the exhaust gas analysis (SG)
XNCH	no. of moles of C_2H_2
$XNCO_2$	no. of moles of CO_2 in exhaust
XK(1)---XK(11)	equilibrium constants K_{p_1}---$K_{p_{11}}$
XKP(1)---XKP(11)	subprograms for K_{p_1}---$K_{p_{11}}$
XN(K+1)	total no. of moles of exhaust gas after Kth iteration
XNN_2, XNO_2---$XNNH_3$	no. of moles of N_2, O_2---NH_3 in exhaust
XX	no. of atoms of carbon in fuel formula
Y( )	array to store mole fractions of the exhaust analysis (EGR)
YY	no. of atoms of hydrogen in fuel formula
YYY	half of YY
ZZ	stoichiomatic no. of moles of O_2.

6.4.2 POLYNOMIALS

As previously stated, 24 polynomials were prepared for equilibrium constants and enthalpy of species data as a function of temperature. Polynomials for the equilibrium constants and enthalpy of species were represented by XKP1, XKP2---XKP11 and $XNCO_2$, XNO_2---XNC7H respectively. The polynomials assumed the following form:

$$XKP(1) = H(1) + H(2)T + H(3)T^2 + H(4)T^3 + H(5)T^4 + H(6)T^5 + H(7)T^6$$

$$XNCO_2 = H(1) + H(2)T + H(3)T^2 + H(4)T^3 + H(5)T^4 + H(6)T^5 + H(7)T^6$$

where H(1)---H(T) are constants obtained for the specific data for each polynomial.

In the early stages of programming four, six and eight degree polynomials were prepared for the data and the order of error incurred in the original data was found to be 2.0%, 0.1% and 0.09% respectively. Hence six degree polynomials were prepared for the data. Temperature range and other details of the data used in the polynomial making are listed below. It should be emphasized that variation in the parameters in the actual computer program should not exceed these limits, otherwise the computations may be absurd because of inaccurate data supplied to the main program by the polynomials.

(A) EQUILIBRIUM CONSTANTS (K_p)

(a) Range of temperature : 1000^0 - 3000^0 K

(b) Temperature for which the data has been used in the polynomial making : 1000, 1300, 1600, 2000, 2300, 2600 and 3000^0 K

(c) Maximum error : 0.025%

(d) Source of the data : reference no. 37

(B) ΔH(T) FOR 13 SPECIES

$$\Delta H(T) = \text{Total energy in the specie}$$

$$= H(T) - H(298) + \Delta H_f^0\,(298)\ \text{cal/gm.mole}$$

where

$H(T)$ = Enthalpy of specie at temp. T

$\Delta H_f^0(298)$ = Enthalpy of formation of the specie at 298^0 K (cal/gm.mole)

(a) Range of Temperature

(i) Fuel C_7H_{16} : 300^0–500^0 K

(ii) 12 species (other than fuel) : 298 – 4750^0 K

(b) Temperature for which the data has been in the making

(i) Fuel C_7H_{16} : 300, 310, 320, 330, 350, 400 and 450^0 K

(ii) Other species : 298, 1000, 1800, 2500, 3250, 4000 and 4750^0 K

(c) Maximum error

(i) Fuel : 1% (300 - 350^0 K)
: 0.025% (350 - 450^0 K)

(ii) Other species : 0.01%

(d) Source of data : Reference no. 36,37

(e) The 12 species were : CO_2, H_2O, O_2, N_2 CO, H_2, OH, O, H, N, NO and C

6.4.3 ITERATIONS

As mentioned earlier, the major species of $\phi \geq 1.0$ and $\phi < 1.0$ were different and the iterative procedure was slightly different for both cases. Also the computer programs were separately written for standard carburetion and exhaust gas recirculation. Thus in all four computer programs were developed which are attached in Appendix G. Listed in table 6-2 are the major species and the initial guess for the adiabatic temperature for $\phi < 1.0$ and $\phi \geq 1.0$. These figures were selected after preliminary computations.

TABLE 6-2

	ADIABATIC FLAME TEMPERATURE	MAJOR SPECIES FOR C_7H_{16}
$\phi<1.0$	$T = 1500^{\circ}$ K $\phi \leq 0.6$ $T = 1200^{\circ}$ K $0.6< \phi < 1.0$	$CO_2 = 7.0$ $H_2O = 8.0$ $O_2 = {}^{n}RO_2 - 11.0$ $N_2 = 3.76 \cdot {}^{n}CO_2$
$\phi\geq1.0$	$T = 2500 - 200 \cdot \phi$	$CO_2 = 6.3$ $H_2O = 7.5$ $CO = 7.0 - {}^{n}CO_2 = 0.7$ $N_2 = 3.76 \cdot {}^{n}CO_2$

Table 6-3 shows the summary of the limits and accuracies where the iteration process was terminated.

TABLE 6-3

	STANDARD CARBURETION		EXHAUST GAS RECIRCULATION	
	$\phi < 1.0$	$\phi \geq 1.0$	$\phi < 1.0$	$\phi \geq 1.0$
AA	50	50	25.0	50.0
ΔT	1.0	1.0	1.0	1.0
C_1	0.1%	--	0.1%	--
C_2	--	1.0%	--	0.5%
CC	--	1.0%	--	0.5%
ER	--	--	T -- 0.1% CO -- 0.1% NO -- 0.1% XN(K+1)-0.1%	T -- 0.5% CO -- 0.5% NO -- 0.1% XN(K+1)-0.5%
K	5	5	5	5
Program Number see (App.G)	I	II	III	IV

where,

AA = Maximum difference in reactant & products enthalpy for the final adiabatic flame temperature (calories/gm.mole)

ΔT = Maximum difference in two consecutive flame temperature for which products species are analysed (^{o}K)

C_1 = Maximum difference in the concentration of NO in two consecutive iterations (moles per mole of fuel)

C_2 = Maximum difference in the concentration of H_2 in two consecutive iterations (moles per mole of fuel)

CC = Maximum difference in the concentration of CO in two consecutive iterations (moles per mole of fuel).

K = Minimum no. of iterations for products species for every value of adiabatic flame temperature

6.4.4 FEATURES OF THE COMPUTER PROGRAMS

The computer programs developed are capable of analysing any hydrocarbon fuel C_xH_y for fifteen exhaust products at adiabatic flame temperature. If the expansion stroke of the engine cycle is also included in the analysis, the programs can analyse exhaust gas at the exhaust temperature.

To analyse any fuel C_xH_y, the following two steps should be taken:

1. Write down the stoichiomatic equation of combustion for the fuel. Thus calculate ZZ and change three cards for XX, YY and ZZ in the program.
2. Prepare a polynomial for the fuel enthalpy and replace the data cards of heptane fuel by these data cards in the end of the program.

The computer programs provide the exhaust gas analysis (15 species) and adiabatic flame temperature in tabular form for the range of variation shown in Table 6-4. These parameters are:

TABLE 6-4

PARAMETERS	RANGE					
	SC			EGR		
	$\phi < 1.0$	$\phi \geq 1.0$	DO LOOP #	$\phi < 1.0$	$\phi \geq 1.0$	DO LOOP #
TIN, °K	300-500	300-500	44	300-500	300-500	45
CR	†	†	43	†	†	46
TR, °K	-	-	n/a*	300-1000	300-1000	47
FIN	-	-	n/a.	0.0-0.5	0.0-0.4	48
ϕ	0.50-0.98	1.0-1.4	49	0.50-0.98	1.0-1.3	49
COMPUTER PROGRAM # (APP.G)	I	II		III	IV	

† Any suitable range

* Not applicable

(1)	Intake-air temperature (TIN)	(SC & EGR)
(2)	Compression ratio (CR)	(SC & EGR)
(3)	Recycled gas temperature (TR)	(EGR only)
(4)	Percent recycling (FIN)	(EGR only)
(5)	Equivalence ratio (Ø)	(SC & EGR)

The interval of variation of these parameters can be as small as desired within the specified range of variation. Table 6-4 shows DO LOOP # in which some cards need be changed for this purpose. As an illustrative example of the procedure, consider program I and TIN variation. The corresponding DO LOOP # is 44. The program reads (App.G).

```
        ------------
        ------------
1.      TIN = 200.0
2.      DO 44 IB = 1,3
3.      TIN = TIN + 100.0
        -----------------
        -----------------
        -----------------
4.   44 CONTINUE
```

Card 3 specifies the interval of variation in TIN is 100° K, while the initial value is 200 + 100 = 300° K. Card 2 specifies that the loop would be executed three times. That is, TIN would assume three different values, 300, 400 and 500° K. These cards should be changed according to the requirement. If a fixed value of TIN is desired for the variation of other parameters, specify the fixed value of TIN in card 1 and delete the remaining cards. Similar procedure is to be followed with other parameters.

Since the assumed combustion occurs at constant pressure, the developed computer program is also adaptable to DIESEL and GAS TURBINES exhaust analysis. In these cases, the expansion stroke of the combustion cycle is to be simulated and incorporated into the program suitably.

The programs could also be easily modified to study the effects of water injection in the combustion chamber and effects of intake air humidity on the exhaust gas concentrations.

6.4.5 ERROR ANALYSIS

Data for the species enthalpy (ΔH) and the equilibrium constants (K_p) have been used in the computation. The magnitude of error incurred in the original data for the polynomial formation is listed in section 6.4.3, Table 6-3. It must be realised that the error thus incurred is over and above the error in the data itself. To analyse the effect of inaccurate data on the exhaust gas analysis, three computer programs were executed for $\phi < 1.0$, standard carburetion. In each case, error introduced in the data was up to 15%.

(i) Effect of error in K_p's

The effect of error thus incurred on NO concentration was up to 12% (i.e., about 80% of the error introduced in K_p's).

(ii) Effect of error in $\Delta H(T)$'s

The effect of error thus incurred on NO concentration was up to 1.5% (i.e., about 10% of the error introduced in $H(T)$'s).

(iii) Effect of equal error in K_p's and $\Delta H(T)$'s

The order of error in NO is about the same as the magnitude of error thus incurred.

6.5 RESULTS

Four computer programs have been developed:

I $\phi < 1.0$, Standard Carburetion (S.C.)
II $\phi \geq 1.0$, S.C.
III $\phi < 1.0$, Exhaust Gas Recirculation (E.G.R.)
IV $\phi \geq 1.0$, E.G.R.

The text of these programs is listed in Appendix G.

The programs are capable of providing exhaust emission data for various operating variables listed in Table 6-4. Some of the representative curves prepared from the computer data are shown in Figures 6.2 to 6.10. A large number of

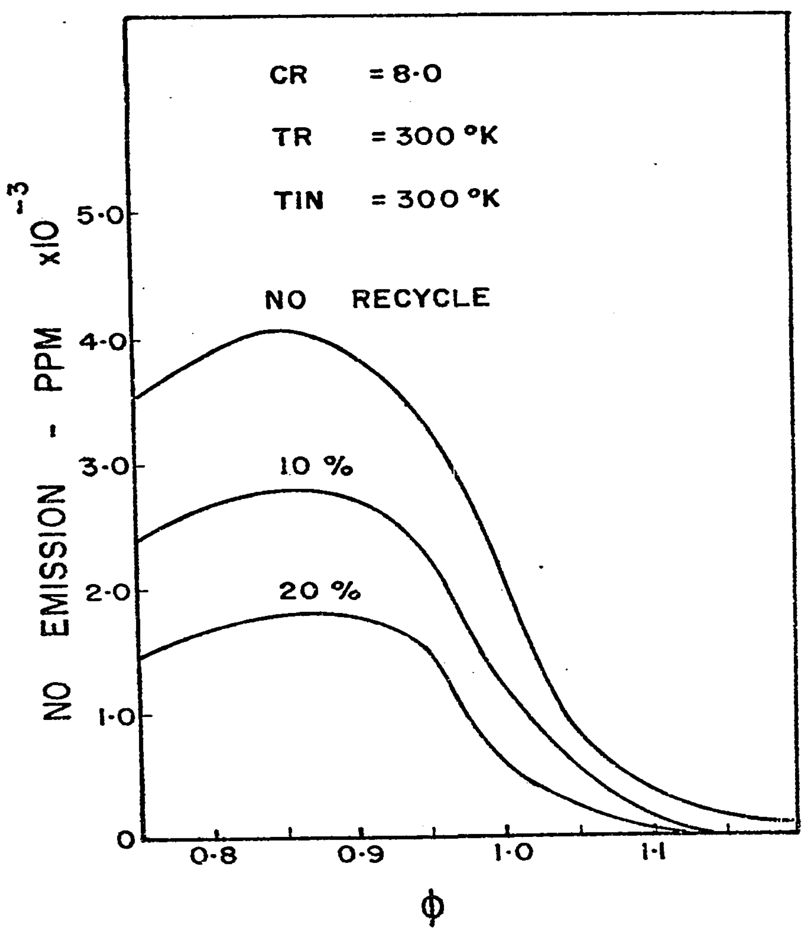
CR = 8·0
TR = 300 °K
TIN = 300 °K
NO RECYCLE
10 %
20 %
NO EMISSION - PPM x10^{-3}
5·0
4·0
3·0
2·0
1·0
0
0·8
0·9
1·0
1·1
ϕ

FIG. 6·2

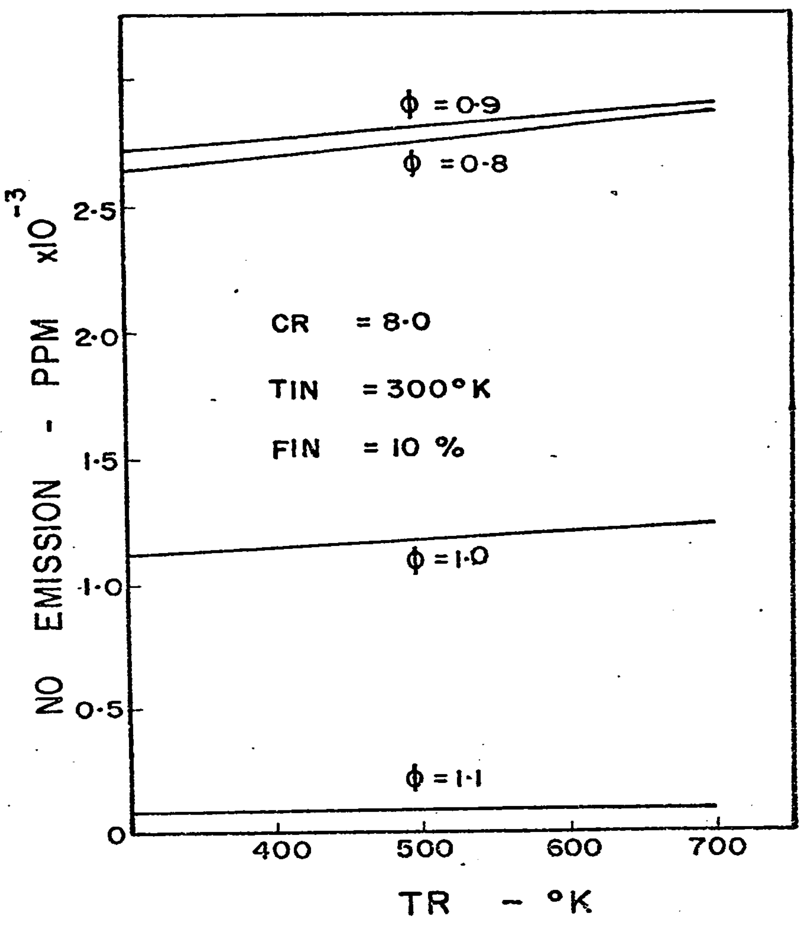
ϕ = 0·9
ϕ = 0·8
CR = 8·0
TIN = 300°K
FIN = 10 %
ϕ = 1·0
ϕ = 1·1
NO EMISSION - PPM x10^{-3}
2·5
2·0
1·5
1·0
0·5
0
400
500
600
700
TR – °K

FIG. 6·3

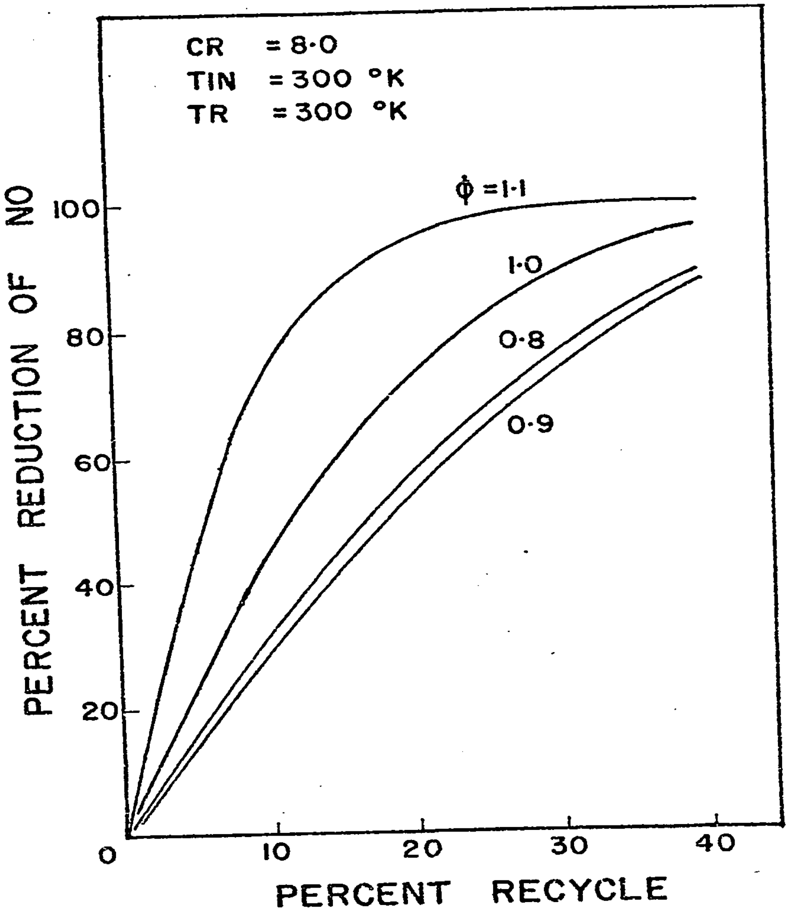
CR = 8·0
TIN = 300 °K
TR = 300 °K
ϕ = 1·1
1·0
0·8
0·9
PERCENT REDUCTION OF NO
100
80
60
40
20
0
10
20
30
40
PERCENT RECYCLE

FIG. 6·4

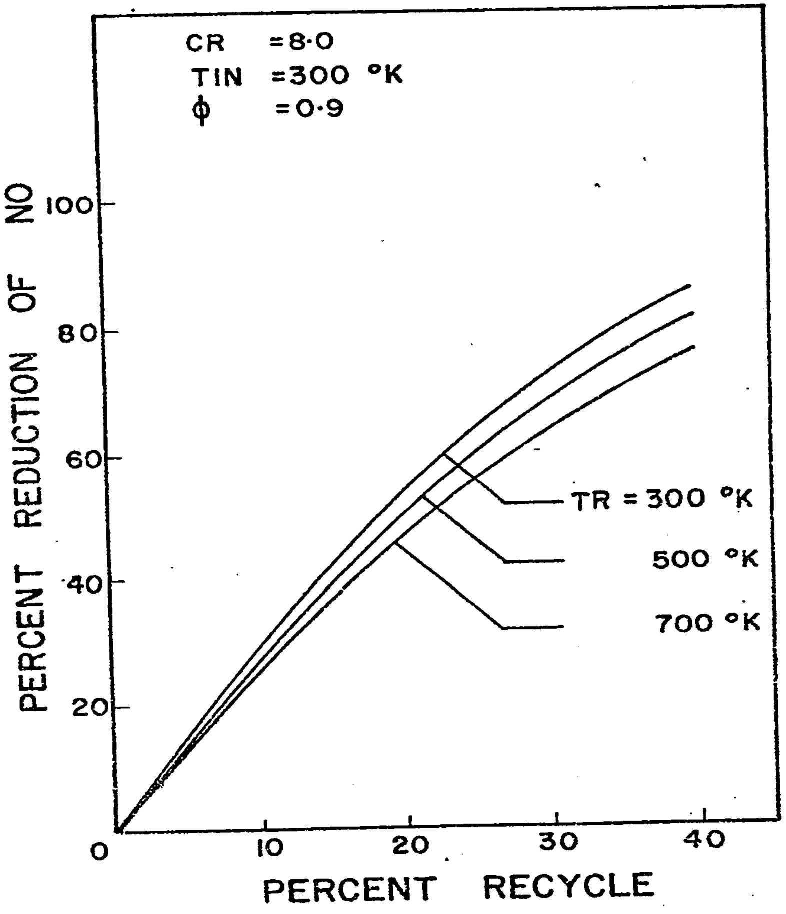
CR = 8·0
TIN = 300 °K
ϕ = 0·9
TR = 300 °K
500 °K
700 °K
PERCENT REDUCTION OF NO
100
80
60
40
20
0
10
20
30
40
PERCENT RECYCLE

FIG. 6·5

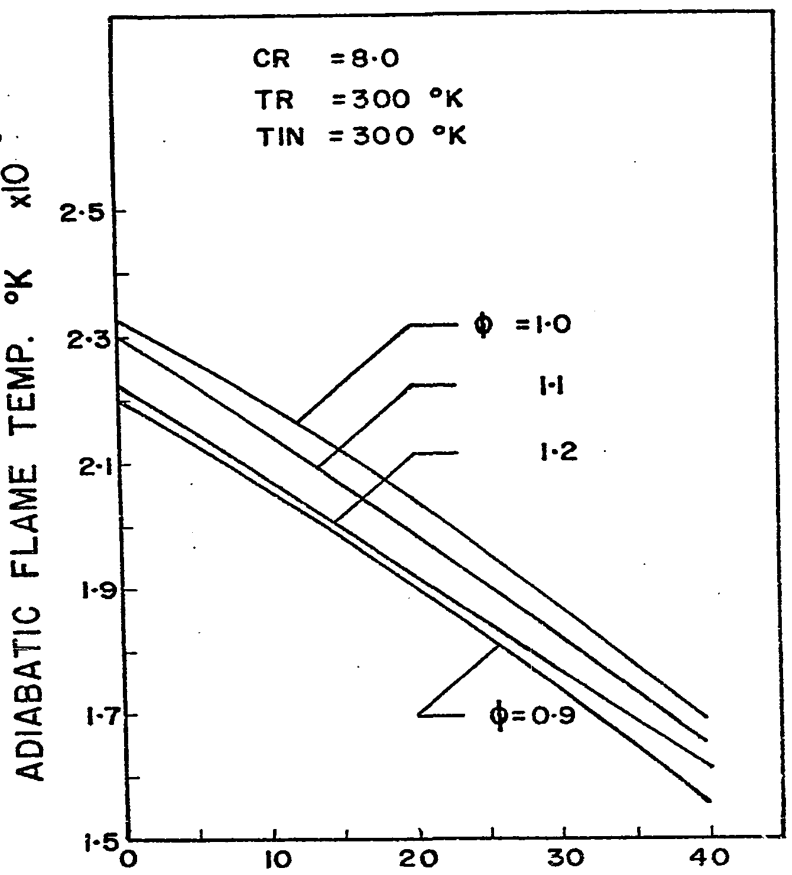
CR =8·0
TR =300 °K
TIN =300 °K
ADIABATIC FLAME TEMP. °K x10^{-3}
2·5
2·3
2·1
1·9
1·7
1·5
0
10
20
30
40
PERCENT RECYCLE
ϕ =1·0
1·1
1·2
ϕ=0·9

FIG. 6·6

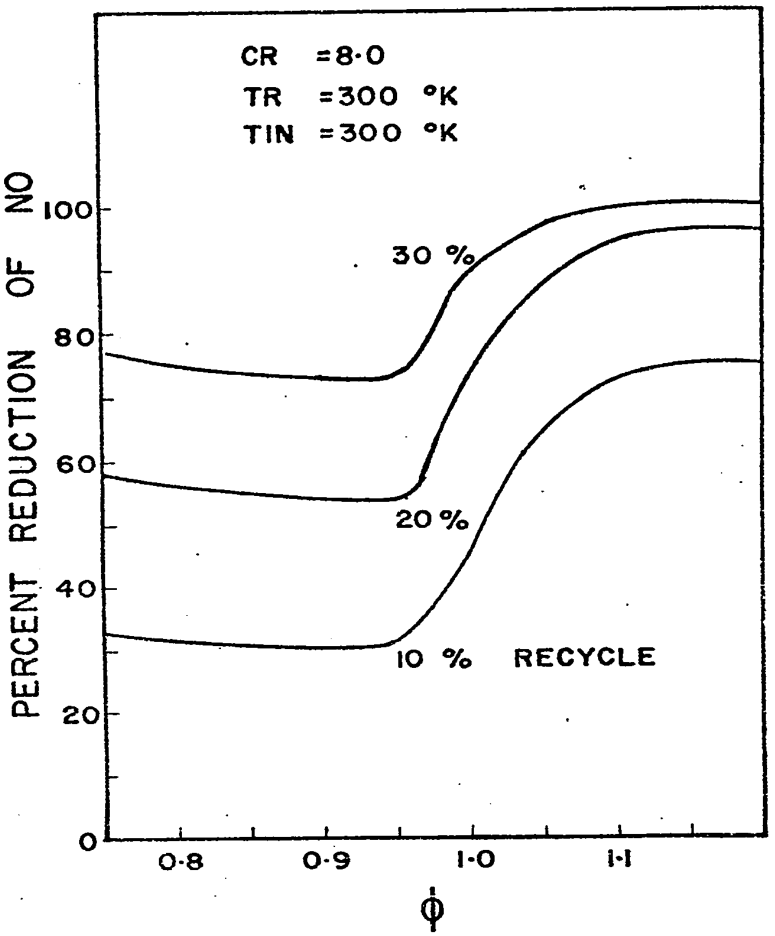
CR =8·0
TR =300 °K
TIN =300 °K
PERCENT REDUCTION OF NO
100
80
60
40
20
0
0·8
0·9
1·0
1·1
ϕ
30 %
20 %
10 % RECYCLE

FIG. 6·7

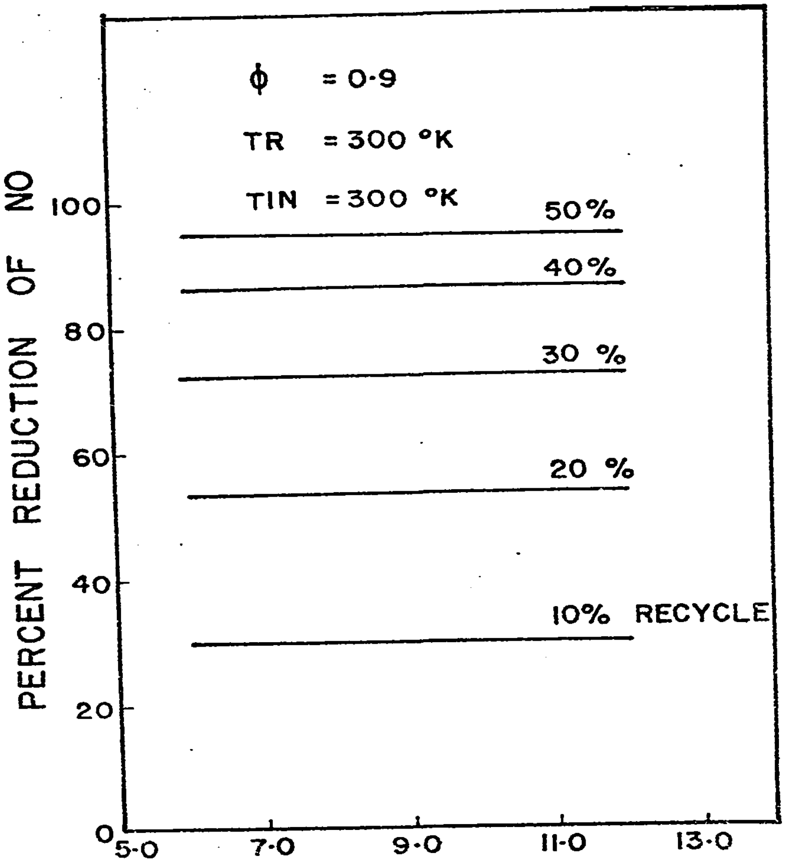
ϕ = 0·9
TR = 300 °K
TIN = 300 °K
50%
40%
30 %
20 %
10% RECYCLE
PERCENT REDUCTION OF NO
100
80
60
40
20
0
5·0
7·0
9·0
11·0
13·0
COMPRESSION RATIO

FIG. 6·8

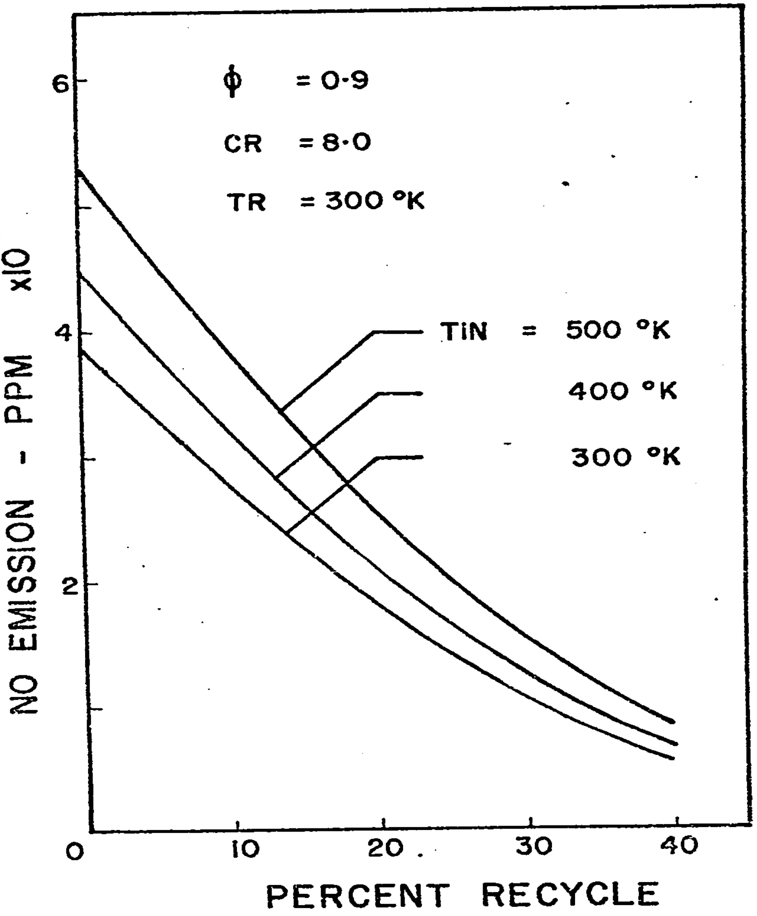
ϕ = 0·9
CR = 8·0
TR = 300 °K
TIN = 500 °K
400 °K
300 °K
NO EMISSION - PPM x10⁻³
6
4
2
0
10
20
30
40
PERCENT RECYCLE

FIG. 6·9

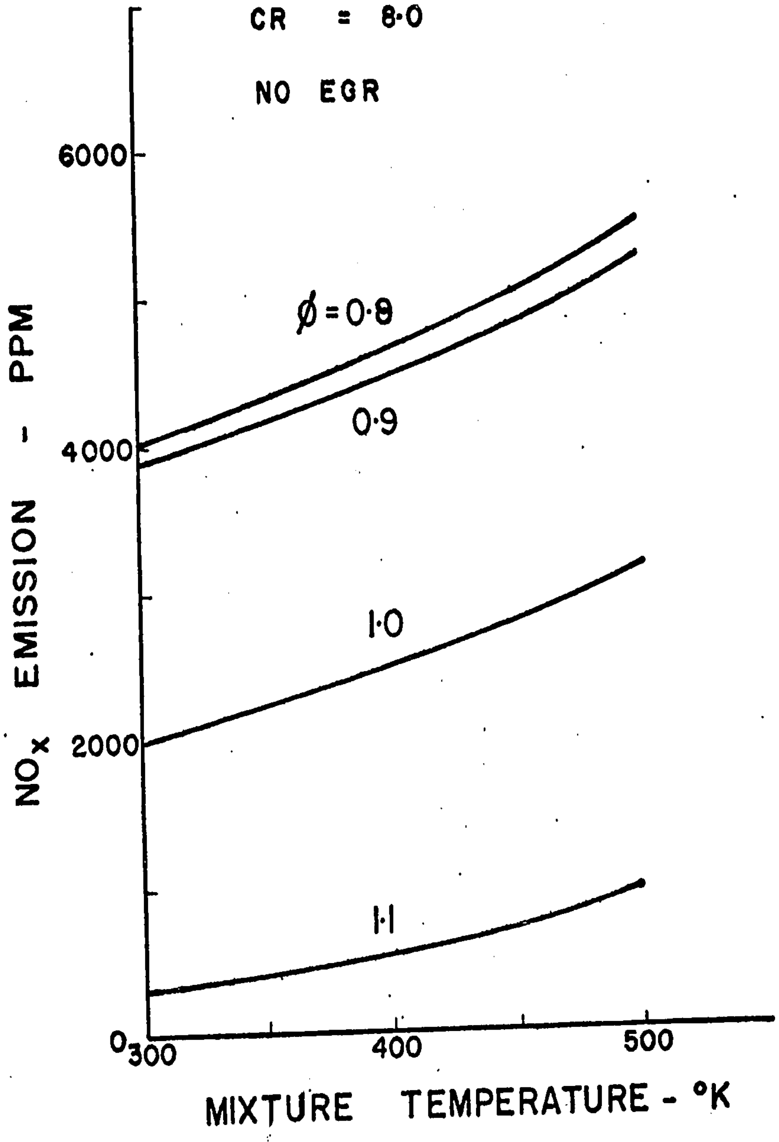
CR = 8·0
NO EGR
6000
4000
2000
0
NOx EMISSION - PPM
ϕ = 0·8
0·9
1·0
1·1
300
400
500
MIXTURE TEMPERATURE - °K

FIG. 6·10

such curves can be plotted and the results be critically analysed.

It may be noted that the EGR work presented here completely agrees in trend with the work of Newhall (6). Also the Standard Carburetion results agree in trend and magnitude with the work presented at the Combustion Generated Air Pollution Seminar (38). It is interesting to observe the similarities in the results of the above mentioned three studies, since the author was unaware of Newhall's work until the present Programs had been developed. It may be mentioned that Newhall's paper does not describe the technique used in the analysis and the assumptions employed in the present work differ from the paper to some extent. (Newhall's study assumed constant volume combustion). The paper does not include the following information:

1. How the recycled gas fraction was computed?
2. Which fuel was employed for the study?

The representative results presented here have already been commented upon and compared (where possible) with the experimental results in section 4.2. The writer is purposely avoiding the analysis and the interpretation of these results, since it would be merely a repetition of the analysis available in references (6,38).

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APPENDIX A

U.S. EXHAUST EMISSION STANDARDS

YEAR	EMISSIONS gm/mile					
	CALIFORNIA			FEDERAL		
	HC	CO	NO_x	HC	CO	NO_x
Pre-1966	11.0	80.0	4-6	11.0	80.0	4-6
1966	3.5	36.0	NR*	11.0	80.0	4-6
1968	3.5	36.0	NR	3.5	36.0	NR
1970	2.2	23.0	NR	2.2	23.0	NR
1971	2.2	23.0	4.0	2.2	23.0	NR
1972	1.5	23.0	3.0	3.4	39.0	NR
1973	1.5	23.0	3.0	3.4	39.0	3.0
1974	1.5	23.0	1.3	3.4	39.0	3.0

	NATIONAL			
	HC	CO	NO_x	PARTICULATES
1975	0.41	3.4	3.0	0.10
1976	0.41	3.40	0.40	0.03

---

* NO requirement.

APPENDIX B

CFR LOW SPEED ENGINE SPECIFICATIONS

Compression ratio	4.46 to 16.00
Standard bore, in.	3.25
Stroke, in.	4.50
Displacement, cu.in.	37.33
Spark plug size, mm	18
Intake valve opens, ATC	10°
Exhaust valve closes, ATC	15°
R.P.M.	900 ± 9

APPENDIX C

AIR FLOW CORRECTION FACTOR

The theoretical air flow rate was calculated and compared with the observed air flow rate as follows:

THEORETICAL AIR FLOW:

DATA,

Air temperature = 75° F

Air flow meter reading = 0.87", H_2O

Displacement volume = 37.33 inch^3

R.P.M. = 900

For 100% volumetric efficiency

Air flow rate $= 37.33 \times \frac{900}{2}$ cu.in/min.

$= \frac{37.33 \times 450}{12 \times 12 \times 12}$ CFM

= 9.71 CFM

Density of air at 75° F = 0.0742 lb/ft^3

$\therefore$ Air flow rate = 9.71 x 0.0742 lb/min.

= 43.2 lb/hr

MEASURED AIR FLOW (from supplied calibration charts*)

Air flow rate = 49.0 x 0.986 lb/hr

= 48.4 lb/hr

---

* Reference 32

For a compression ratio of 8 and an assumed B.H.P. of 1.2, volumetric efficiency is calculated to be 90% when engine is being motored. This would be expected to be even smaller when engine is firing.

Therefore,

Theoretical air flow = 0.90 x 43.2 lb/hr
= 38.88 lb/hr
but, Measured air flow = 48.4 lb/hr

In the actual case, the measured air flow should be smaller than the theoretical flow rate because of higher gaseous temperature in the combustion chamber. Hence, the error in the measured air flow, which is calculated to be 24.5%, would be still higher.

The air flow rate was estimated by using information published in (15), which is given below:

Air flow rate = 1.1×10^{-2} lb/sec
Mixture temperature = 180° F
Engine R.P.M. = 1200
Compression ratio = 7

The engine size, type and other specifications are similar to the engine used in this study except the engine speed is 900 rpm in the present system.

At 900 rpm, air flow rate would be = $\frac{900}{1200}$ x 39.6 lb/hr

= 29.7 lb/hr

With the engine, under similar operative conditions as mentioned above, the following data was acquired.

Air flow meter reading = 0.77", H_2O

Intake air temperature = 74° F

Therefore,

Measured air flow = chart reading x temperature factor

= 46.0 x 0.986 lb/hr

= 45.4 lb/hr

Hence,

CORRECTION FACTOR = $\frac{29.7}{45.4}$

= 0.655

This correction factor has been used to correct the air flow rate given by nozzle meter.

Using this correction factor, the plot of NO_x emission versus air fuel ratio appears as shown in Fig.4-1. If this curve is compared with the results published in Reference (10, Fig. 1), it is revealed that the calculated air fuel ratio is higher by about 2.5 and stoichiometric ratio is in the neighbourhood of 17.5.

DRY AIR: Air flow rate thus obtained was divided by $(1.0 + W_m)$ where W_m is the moisture in lb per lb of dry air. In results only dry air fuel ratio is specified.

APPENDIX D

ROTAMETER CALIBRATION

A rotameter with 1.5 SCFM capacity was used to meter dry exhaust gas flow. It was calibrated with both floats (pyrex and stainless steel) simultaneously, using a precision standard flowmeter, called WET TEST METER (25). The exhaust gas after being cooled in the exhaust gas cooler was recycled to the engine carbureter through a silica gel drier, the rotameter and the standard flowmeter. This calibration arrangement ensured identical operating conditions during calibration and metering. The temperature of the exhaust gas through the rotameter was maintained at 84^0 F throughout the calibration. Fig. A shows the calibration curve thus acquired for the exhaust gas. Some important features to be kept in mind are:

1. To ensure that dry exhaust gas was passing through the rotameter, silica gel was replaced in the drier well before it became saturated.

2. Pressure drop across the standard flow meter was measured with a mercury manometer and was used in calculating the flow rate.

3. For a fixed reading of the rotameter, the flow rate was almost independent of upstream pressure.

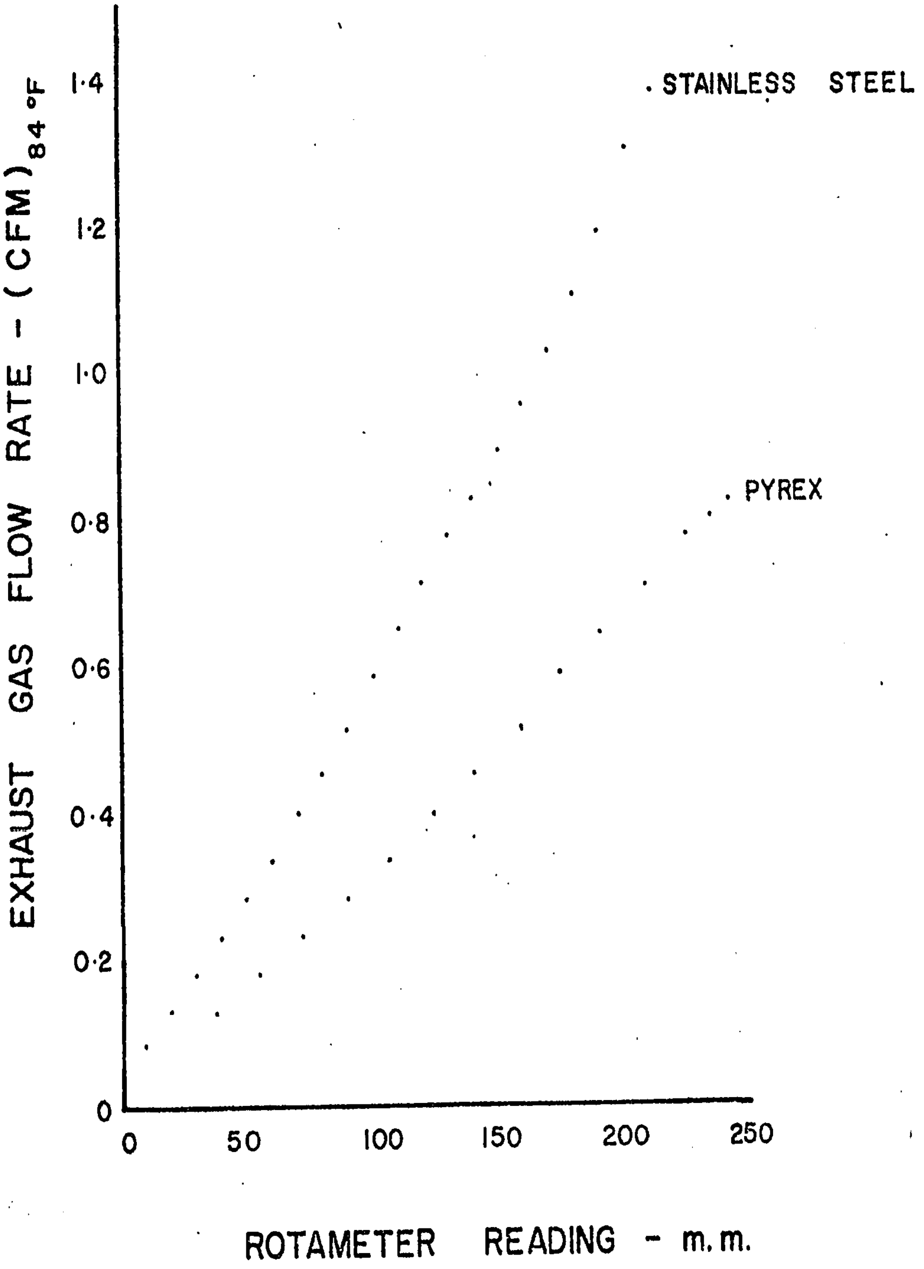
EXHAUST GAS FLOW RATE - (CFM)$_{84}$ °F
1·4
1·2
1·0
0·8
0·6
0·4
0·2
0
STAINLESS STEEL
PYREX
0
50
100
150
200
250
ROTAMETER READING - m.m.

FIG. A

4. The calibration was repeatable within an experimental error of 1.0%.

5. While metering the exhaust gas flow at temperatures other than 84° F, a temperature correction factor was applied to the flow rate read off the calibration curve.

APPENDIX E

SYSTEM MAINTENANCE

A complete and detailed procedure is given in Ref. (31). However, some important features to be kept in mind are:

ENGINE:

1. Prior to starting the engine, make sure that exhaust globe valve is completely open.
2. 550 volt power supply to the synchronous A.C. motor be connected according to the colour code. Failure to observe this may result in opposite direction of rotation of the engine and thus the exhaust port would become the suction port and vice versa.
3. When the engine has reached the operating temperature water level in the cylinder condenser must be at the "operating level" mark.

EGR SYSTEM:

1. During system operation, check hourly for water condensation at surge tank, exhaust gas cooler, particle filter and pump filter drains.

2. Clean the carbon deposit from the sheath of the exhaust temperature thermocouple, otherwise, it is liable to give meaningless information.

3. Before switching on the EGR gas heater, check the resistance between ground and one of the power terminal of the heater. This resistance should be at least 50 mega ohms.

4. If the pump shows excessive suction side vacuum, for completely open EGR globe valve, it indicates that the particle filter element has been clogged up and requires replacement or cleaning with methanol. Excessive vacuum on suction side may damage the pump.

5. Lubricant level of the EGR pump may be periodically checked.

APPENDIX F

SAMPLE CALCULATIONS

To illustrate the calculation procedure, one representative set of data is presented as follows:

DATA:

General,

Mixture temperature = 180° F

NO_x concentration = 2100 ppm

Humidity, W_m = 64 grains/lb of air

= 0.00915 lb/lb of air

Cycle peak pressure = 320 psig.

Suction side vacuum at EGR pump = 12.5 inHg.

Air flow,

Nozzle meter reading = 0.75 in. H_2O

Intake air temperature, T_1 = 75° F

Air density at T_1 = 0.07418 lb/ft^3

Air temp. correction factor*, CF_1 = 0.986

Air flow correction factor†, CF_2 = 0.655

---

* Reference 32

† Appendix C

Fuel flow,

Fuel scale movement, x = 4.0 cm

Time (corresponding to x), t = 9.48 minutes

EGR flow,

Rotameter reading (st. steel float) = 20 mm

EGR temperature, T_2 = 78^{0} F

EGR temp. correction factor, CF_3 = $\frac{460 + t_2}{460 + 84}$

Exhaust gas density at T_2 = 0.07368 lb/ft^3

CALCULATIONS:

Air flow,

Nozzle meter air flow rate, W_1 = 45.4 lb/hr
(from calibration curve, ref. 32)

Actual air flow rate = W_1 x CF_1 x CF_2

= 45.4 x 0.986 x 0.655 lb/hr

= 29.320 lb/hr

therefore, Dry air flow rate = 29.320/(1 + W_m)

= $\frac{29.320}{(1.0 + 0.00915)}$ lb/hr

= 29.046 lb/hr

also, Volume air flow rate $= \frac{29.046}{(\text{density})\ 75^{\circ}\ F}$

$= \frac{29.046}{60 \times 0.07418}$ CFM

$= \underline{6.526\ \text{CFM}}$

Fuel flow,

Fuel flow rate (see section 3.1.3) $= 3.691 \frac{x}{t}$ lb/hr

$= 3.691 \frac{4.0}{9.48}$ lb/hr

$= \underline{1.556\ \text{lb/hr}}$

EGR flow,

EGR flow rate (see Fig.A) at T_2 $= 0.1334 \left(\frac{460 + 78}{460 + 84}\right)$ CFM

$= \underline{0.132\ \text{CFM}}$

Therefore, by definition

Air fuel ratio (by weight) $= \frac{29.046}{1.556}$

$= \underline{18.7}$

and Percent EGR $= \frac{0.132}{6.526} \times 100$

$= \underline{2.02\ \%}$

APPENDIX G

COMPUTER PROGRAM I

1. Standard Carburetion
2. $\phi < 1.0$

```
C     AGARWAL V.K. (DEPT. OF MECH. ENG. UNIVERSITY OF OTTAWA)
C
C     STANDARD CARBURETICN
C
C     ANALYSIS FOR HEPTANE AS FUEL FOR VARIOUS VALUES OF PHI
C
C     COMPOSITION OF AIR BY VOLUME ASSUMED N2IS TO O2 = 3.76 IS TO 1
C
C     PRODUCT COMPOSITION ANALYSIS
C
C     COMPOSITION OF TRACES ASSUMED ZERO AND MAJOR CONSTITUENTS FOUND
C
C     COMPUTING TRACES CCMPOSITION
C
C     PHI IS LESS THAN ONE
C
C     **********************************************************
C     DESCRIPTION OF NOMANCLATURE USED IN THE PROGRAM
C     **********************************************************
C
C     PREFIX  X  IS USED TO CONVERT FLOATING PT. VARIABLE INTO AN INTEGER
C
C     K AFTER  X  -- EQUILIBRIUM CCNSTANT
C
C     N AFTER  X  -- NUMBER CF MOLES
C
C    EXAMPLES
C     XK(N)...... EQUILIBRIUM CONSTANT
C
C     XNKP....... EQUILIBRIUM
C
C     XNCO2...... NO. CF MCLES OF CO2
C
C     XNNO....... NO. OF MOLES CF NO
C
C     XN(K+1).... TOTAL # MCLES
C
C     REAENT..... REACTANT ENTHALPY CF FRESH CHARGE
C
C     PROENT..... PRODUCT ENTHALPY OF EXHAUST GAS
C
C     PENTLO..... LCW PRODUCT ENTHALPY (EGR FRACTION ENTHAPY )
C
```

```
C   GENERAL
C
C          TIN :-  INTAKE AIR TEMPERATURE
C
C          J  :-  TAKING CARE OF CATA CARD READING
C
C          P  :-  PRESSURE
C
C          MA :-  CONTRCLLING  INITIAL GUESS OF XNCO
C
C          MB :-  SUBSEQUENT FLAME TEMP. CONVERGENCE
C
C          MM :-  DATA CARD READING
C
C          L  :-  COUNT FCR # OF ITERATIONS FOR FLAME TEMPERATURE
C
C          K  :-  COUNT FOR # OF ITERATIONS FOR COMPOSITIONS CF PRODUCTS
C
C      **********************
C      FIRST ITERATION
C      ***********************
C
      DIMENSION Y(19,7),XK(11),XN(29)
      J=1
      CR=4.0
      DO 43 IA=1,4
      CR=CR+2.0
      P=CR**1.3
      TIN=200.0
      DO 44 IB=1,3
      TIN=TIN+100.0
      M=0
      PHI=0.45
C
C     FUEL SYMBOL IS CXXHYY
C
C     C7H16 (HEPTANE) IS THE FUEL IN THIS PROGRAM
C
C     THEREFORE   XX=7.0   YY=16.0
C
C     ZZ= STOICHIOMATIC # OF MOLE OF CXYGEN
C
C     STOICHIOMATIC EQ'N IS C7H16+11(02+3.76 N2) = 7CO2+8H2O+11*3.76**N2
C
```

```
C      THEREFORE     ZZ=11.0
C
       XX=7.0
       YY=16.0
       YYY=YY/2.0
       ZZ=11.0
       DO 49  M=1,5
       L=0
       PHI=PHI+0.1
C
C      INITIAL FLAME TEMPERATURE HAS BEEN ASSIGNED ARBITRARILY
C
       IF(PHI.LE.0.6) T=1500.0
       IF(PHI.GT.0.6.AND.PHI.LE.1.0) T=2200.0
C
C      LOOP 19 CALCULATES FINAL FLAME TEMPERATURE & EXHAUST COMPONENTS
C
 19    RO2=ZZ/PHI
       XNO2=RO2-ZZ
       XNCO2=XX
       XNH2O=YYY
       XNN2=3.76*RO2
  6    A1 = XNCO2
       A2 = XNH2O*2.0
       A3=RO2*2.0
       A4=XNN2*2.0
C
C      CALCULATING VALUES OF EQUILIBRIUM CONSTANTS
C
       XN(1)=XNCO2+XNH2O+XNO2+XNN2
       XK(1)=XKP1(T,J)
       XK(2)=XKP2(T,J)
       XK(3)=XKP3(T,J)
       XK(4)=XKP4(T,J)
       XK(5)=XKP5(T,J)
       XK(6)=XKP6(T,J)
       XK(7)=XKP7(T,J)
       XK(8)=XKP8(T,J)
       XK(9)=XKP9(T,J)
       XK(10)=XKP10(T,J)
       XK(11)=XKP11(T,J)
       K=0
       C=0.0
C
```

```
C     LOOP 40 ITERATES EXHAUST COMPOSITION FOR A GIVEN FLAME TEMP.
C
 40   K=K+1
      B=P/XN(K)
      XNCO=XNCO2*XK(1)*(B*XNO2)**(-0.5)
      XNH2=(XNCO*XNH2O)/(XNCO2*XK(2))
      XNC=(XNCO**2.0)/(XNCO2*XK(3))
      XNCH=XNH2*XK(4)*(XNC*B)**2
      XNCH4=(XNCO*XNH2*XK(5)/XNH2O)*(B*XNH2)**2
      XNOH=XNH2O*XK(6)*((B*XNH2)**(-0.5))
      XNO=XK(7)*((B/XNO2)**(-0.5))
      XNH=XK(8)*((B/XNH2)**(-0.5))
      XNN=XK(9)*((B/XNN2)**(-0.5))
      XNNO=XK(10)*(XNO2*XNN2)**(0.5)
      XNNH3=XK(11)*B*XNH2*(XNN2*XNH2)**(0.5)
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     ITERATION IS STOPPED IF ERROR IN SUBSEQUENT *NO* CONCENTRATION
C                (TEST) IS LESS THAN  0.1 %
C
      TEST=(XNNO-C)/XNNO
      D=ABS(TEST)
      C=XNNO
      IF(D.LT.0.001.AND.K.GE.5) GO TO 50
C
C     ***********************
C     SUBSEQUENT ITERATIONS
C     ***********************
C
       XNCO2=A1-XNCO-XNC-2.0*XNCH-XNCH4
        XNH2O=(A2-2.0*XNH2-XNH-XNOH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
        XNO2=(A3-2.0*XNCO2-XNH2O-XNCO-XNOH-XNO-XNNO)/2.0
         XNN2=(A4-XNN-XNNO-XNNH3)/2.0
      IF(XNO2.LE.0.0) XNO2=0.2
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     XN(TOTAL) IS THE  # OF TOTAL MOLES USED FOR THE SUBSEQUENT ITERATION
C
      GO TO 40
C
C     ***********************************
C     ITERATIONS FOR ADIABATIC TEMPERATURE
```

```
C     LCCP 40 ITERATES EXHAUST COMPOSITION FOR A GIVEN FLAME TEMP.
```

```
C     ************************************
C
 50   L=L+1
      IF(L.GT.15) GO TO 55
C
C     CCMPUTING PRODLCT GAS ENTHALPY
C
      P1=PHCO2(T,J)
      P2=PHH2O(T,J)
      P3=PHO2(T,J)
      P4=PHN2(T,J)
      P5=PHCO(T,J)
      P6=PHH2(T,J)
      P7=PHOH(T,J)
      P8=PHO(T,J)
      P9=PHH(T,J)
      P10=PHN(T,J)
      P11=PHNO(T,J)
      P12=PHC(T,J)
      PROENT=XNCO2*P1+XNH2O*P2+XNO2*P3+XNN2*P4+XNCO*P5+XNH2*P6+XNC*P12+X
     1NOH*P7+XNO*P8+XNH*P9+XNN*P10+XNNO*P11
C
C     REACTANT ENTHALPY =H(C7H16)+RO2*H(O2)+3.76*RO2*H(N2)
C
      R1=RHC7H(TIN,J)
      R2=PHO2(TIN,J)
      R3=PHN2(TIN,J)
      REAENT=R1+RO2*R2+3.76*RO2*R3
C
C     APPROXIMATE SP. HEAT ASSUMED 500  CAL/GM MOLE OF FUEL
C
      AA=PRCENT-REAENT
      AB=ABS(AA)
      T1=T-(AA/500.0)
      P11=PHCO2(T1,J)
      P22=PHH2O(T1,J)
      P33=PHO2(T1,J)
      P44=PHN2(T1,J)
      CP1=(P1-P11)
      CP2=(P2-P22)
      CP3=(P3-P33)
      CP4=(P4-P44)
      CP=(XNCO2*CP1+XNH2O*CP2+XNO2*CP3+XNN2*CP4)/(T-T1)
      CP=ABS(CP)
```

```
      TNEW=T-(AA/CP)
      DIFF=TNEW-T
      BB=ABS(DIFF)
C
C     ITERATION FOR THE FLAME TEMPERATURE IS STOPPED WHEN THE
C     CIFFERENCE IN PRODUCT & REACTANT ENTHALPIES IS < 50.0 AND  ERROR
C        IN THE FLAME TEMPERATURE IS < 1.0 KELVIN
C
      IF(AB.LT.50.0.ANC.BB.LT.1.0) GO TO 55
      T=TNEW
      J=J+1
      GO TO 19
   55 Y(1,M)=T
      Y(2,M)=PHI
      Y(3,M)=XNCO2/XN(K+1)
      Y(4,M)=XNH2O/XN(K+1)
      Y(5,M)=XNO2/XN(K+1)
      Y(6,M)=XNN2/XN(K+1)
      Y(7,M)=XNCO/XN(K+1)
      Y(8,M)=XNH2/XN(K+1)
      Y(9,M)=XNC/XN(K+1)
      Y(10,M)=XNCH/XN(K+1)
      Y(11,M)=XNCH4/XN(K+1)
      Y(12,M)=XNOH/XN(K+1)
      Y(13,M)=XNO/XN(K+1)
      Y(14,M)=XNH/XN(K+1)
      Y(15,M)=XNN/XN(K+1)
      Y(16,M)=XNNO/XN(K+1)
      Y(17,M)=XNNH3/XN(K+1)
      Y(18,M)=L
      Y(19,M)=K
      BB=10.0
   49 CONTINUE
      WRITE(6,501)P,TIN,CR
  501 FCRMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC COMBUSTION CF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MCLE FRACTIONS FCR VARYING',//,5X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MOLE FRACTICN.',/,10X,'CR=',F5.2)
      WRITE(6,500)((Y(I,M),M=1,5),I=1,19)
  500 FCRMAT(///,10X,'T',5(1X,F14.3),//,8X,'PHI',5(1X,F14.3),//,8X,'CO2'
     1,5(1X,E14.7),//,8X,'H2O',5(1X,E14.7),//,9X,' O2',5(1X,E14.7),//,9X,
     2'N2',5(1X,E14.7),//,7X,'  CO',5(1X,E14.7),//,8X,' H2',5(1X,E14.7),
     3//,9X,'C ',5(1X,E14.7),//, 7X,'C2H2',5(1X,E14.7),//, 8X,'CH4',5(1X
```

```
     4,E14.7),//,9X,'CH',5(1X,E14.7),//,9X,'O',5(1X,E14.7),//,9X,'H',5(1
     5X,E14.7),//,10X,'N',5(1X,E14.7),//,9X,'NO',5(1X,E14.7),//,8X,'NH3'
     6,5(1X,E14.7),//,10X,'L',5(9X,F6.1),//,10X,'K',5(9X,F6.1))
44    CONTINUE
43    CONTINUE
1000  RETURN
      END
      FUNCTION XKP1(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP1=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP2=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP3(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP3=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP4(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP4=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP5(T,J)
```

```
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP5=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP6(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP6=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP7(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP7=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP8(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP8=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP9(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP9=10.0**CONSTT
      RETURN
      END
```

```
      FUNCTION XKP10(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP10=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP11(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP11=10.0**CONSTT
      RETURN
      END
      FUNCTION PHCO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
       PHCO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-94052.0-2238.1
      RETURN
      END
      FUNCTION PHH2O(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
       PHH2O=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-57798.0-2367.7
      RETURN
      END
      FUNCTION PHO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2069.8
      RETURN
      END
      FUNCTION PHN2(T,J)
      DIMENSION H(7)
```

```
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHN2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2072.3
      RETURN
      END
      FUNCTION PHCO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHCO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-26415.7-2072.6
      RETURN
      END
      FUNCTION PHH2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHH2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2023.8
      RETURN
      END
      FUNCTION PHOH(T,J)
      CIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHOH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+10060.0-2106.2
      RETURN
      END
      FUNCTION PHO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+59159.0-1607.4
      RETURN
      END
      FUNCTION PHH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+52089.0-1481.2
```

```
      RETURN
      END
      FUNCTION PHN(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
 151  FORMAT(5E14.7)
         PHN=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+112750.0-1481.0
      RETURN
      END
      FUNCTION PHNO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
 151  FORMAT(5E14.7)
        PHNO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+21600.0-2194.2
      RETURN
      END
      FUNCTION PHC(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
 151  FORMAT(5E14.7)
         PHC=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+171698.0-1558.9
      RETURN
      END
      FUNCTION RHC7H(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
 151  FORMAT(5E14.7)
       RHC7H=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-44885.0
      RETURN
      END
```

APPENDIX G

COMPUTER PROGRAM II

1. Standard Carburetion
2. $\phi \geq 1.0$

```
C      AGARWAL V.K. (DEPT. OF MECH. ENG. UNIVERSITY OF OTTAWA)
C
C      STANDARD CARBURETION
C
C      FOR NEXT PHI,APPROXIMATION OF MAJOR CONSTITUENTS HAS BEEN TAKEN
C      FROM PREVIOUS VALUE OF PHI,SO PHI=1.0 IS TO BE RUN FIRST
C
C      ANALYSIS FOR HEPTANE AS FUEL FOR VARIOUS VALUES OF PRESSURES
C
C      COMPOSITION OF AIR BY VOLUME ASSUMED N2IS TO O2 = 3.76 IS TO 1
C
C      PRODUCT COMPOSITION ANALYSIS
C
C      COMPOSITION OF TRACES ASSUMED ZERO AND MAJOR CONSTITUENTS FOUND
C
C      COMPUTING TRACES COMPOSITION
C
C      PHI IS EQUAL TO OR GREATER THAN ONE
C
C      ***********************************************************
C      DESCRIPTION OF NOMANCLATURE USED IN THE PROGRAM
C      ***********************************************************
C
C      PREFIX  X  IS USED TO CONVERT FLOATING PT. VARIABLE INTO AN INTEGE
C
C      K AFTER  X  -- EQUILIBRIUM CONSTANT
C
C      N AFTER  X  -- NUMBER OF MOLES
C
C     EXAMPLES
C       XK(N)...... EQUILIBRIUM CONSTANT
C
C       XNKP....... EQUILIBRIUM
C
C       XNCO2...... NO. OF MOLES OF CO2
C
C       XNNO....... NO. OF MOLES OF NO
C
C       XN(K+1).... TOTAL # MOLES
C
C       REAENT..... REACTANT ENTHALPY OF FRESH CHARGE
C
C       PROENT..... PRODUCT ENTHALPY OF EXHAUST GAS
C
```

```
C     PENTLO..... LOW PRODUCT ENTHALPY (EGR FRACTION ENTHAPY )
C
C
C  GENERAL
C
C        TIN:-  INTAKE AIR TEMPERATURE
C
C        J  :-  TAKING CARE OF DATA CARD READING
C
C        P  :-  PRESSURE
C
C        MA :-  CONTROLLING  INITIAL GUESS OF XNCO
C
C        MB :-  SUBSEQUENT FLAME TEMP. CCNVERGENCE
C
C        MM :-  CATA CARD READING
C
C        L  :-  COUNT FOR # CF ITERATIONS FOR FLAME TEMPERATURE
C
C        K  :-  COUNT FCR # OF ITERATIONS FOR COMPOSITIONS OF PRODUCTS
C
C        MP :-  MP=0  FOR STANDARD CARBURETION
C               MP> &=1 FOR ***EGR***
C
C      NP :-  PRINTS STANDARD CARBURETION RESULTS ONLY WHEN
C             TIN OR CR IS ALTERED
C
C
C      **********************
C      FIRST ITERATION
C      **********************
C
       DIMENSION Y(20,5),XK(11),XN(30),A(17)
       YMC=0.0
       MM=1
       J=1
       A(1)=0.7
       CR=4.0
       DO 47 JA=1,8
       CR=CR+1.0
       P=CR**1.3
       TIN=200.0
       DO 48 JB=1,3
       TIN=TIN+100.0
```

```
C
C     FUEL SYMBOL IS CXXHYY
C
C     C7H16 (HEPTANE) IS THE FUEL IN THIS PROGRAM
C
C     THEREFORE   XX=7.0   YY=16.0
C
C     ZZ= STOICHIOMATIC # OF MOLE OF OXYGEN
C
C     STOICHIOMATIC EQ'N IS C7H16+11(O2+3.76 N2) = 7CO2+8H2O+11*3.76**N2
C
C     THEREFORE    ZZ=11.0
C
      XX=7.0
      YY=16.0
      YYY=YY/2.0
      ZZ=11.0
      PHI=0.9
      DO 49 M=1,5
      MB=0
      MA=1
      PHI=PHI+0.1
      L=0
C
C     INITIAL FLAME TEMPERATURE HAS BEEN ASSIGNED ARBITRARILY
C
      T=2500.0-PHI*200.0
 19   RO2=ZZ/PHI
      XNCO=A(MA)
      XNN2=3.76*RO2
      XNCO2=XX-XNCO
      XNH2O=7.5
      GO TO 6
C
C     CHECK WHETHER LOOP  22  IS USEFUL
C
 22   MA=MA+1
      YMC=YMC+1.0
      S=YMC/2.0
      IA=S
      WRITE(6,183)YMC,S,IA,MA,XNCO
183   FORMAT(/,10X,'YMC,S,IA,MA ARE AS FOLLOWS',/,10X,2(F15.5),/,10X,2(I
     115),5X,'XNCO=',E14.7)
      IF(S-IA) 181,181,182
```

```
C
C      [illegible]
C
C      [illegible]
C
181    A(MA)=A(MA-1)+C.1*YMC
       GC TO 24
182    A(MA)=A(MA-1)-0.1*YMC
 24    XNCO=A(MA)
C
C      XNCC IN LCOP 7  CCMES FROM THE ITERATION FOR WHICH TEMP. ITERATION
C         HAS BEEN DONE
C
C      IF MA CHANGES EVEN THEN XNH2O IS BEING TAKEN FROM PREVIOUS ITERATI
C
C      SINCE FUEL IS C7H16  SO  A1=7.0  A2=16.0
C
         XNH2O=(A2-2.0*XNH2-XNH-XNCH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
         XNCO2=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
          XNN2=(A4-XNN-XNNO-XNNH3)/2.0
       WRITE(6,184)XNCO2,XNH2O,XNCC,XNN2
184    FORMAT(5X,'XNCO2=',F10.4,5X,'XNH2O=',F10.4,5X,'XNCO=',F10.4,5X,
      1'XNH2=',F10.4)
  6    A1=XX
       A2=YY
       A3=RO2*2.0
       A4=XNN2*2.0
C
C      CALCULATING VALUES OF EQUILIBRIUM CONSTANTS
C
  7    XN(1)=XNCO2+XNH2C+XNCC+XNN2
       XK(1)=XKP1(T,J)
       XK(2)=XKP2(T,J)
       XK(3)=XKP3(T,J)
       XK(4)=XKP4(T,J)
       XK(5)=XKP5(T,J)
       XK(6)=XKP6(T,J)
       XK(7)=XKP7(T,J)
       XK(8)=XKP8(T,J)
       XK(9)=XKP9(T,J)
       XK(10)=XKP10(T,J)
       XK(11)=XKP11(T,J)
       K=0
       C=0.0
       CC=0.0
C
C      LOOP 40 ITERATES EXHAUST COMPOSITION FOR A GIVEN FLAME TEMP.
C
 40    K=K+1
```

```
      IF(K.GT.25) J=J+1
      IF(K.GT.25) GO TC 22
      B=P/XN(K)
      XNO2=((XK(1)*XNCO2/XNCO)**2.0)/B
      XNH2=(XNCO*XNH2O)/(XNCO2*XK(2))
      XNC=(XNCO**2.0)/(XNCO2*XK(3))
      XNCH=XNH2*XK(4)*(XNC*B)**2
      XNCH4=(XNCO*XNH2*XK(5)/XNH2O)*(B*XNH2)**2
      XNOH=XNH2O*XK(6)*((B*XNH2)**(-0.5))
      XNO=XK(7)*((B/XNC2)**(-0.5))
      XNH=XK(8)*((B/XNH2)**(-0.5))
      XNN=XK(9)*((B/XNN2)**(-0.5))
      XNNO=XK(10)*(XNO2*XNN2)**(0.5)
      XNNH3=XK(11)*B*XNH2*(XNN2*XNH2)**(0.5)
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     ITERATION IS STOPPED IF ERROR IN SUBSEQUENT H2 & CO CONCENTRATION
C     IS LESS THAN  1 %
C
      TEST=(XNH2-C)/XNH2
      TEST1=(XNCO-CC)/XNCO
      D=ABS(TEST)
      E=ABS(TEST1)
      C=XNH2
      CC=XNCO
      IF(MB.EQ.1) GC TC 33
      IF(D.LE.0.050.AND.E.LE.0.050.AND.K.GE.5) GO TO 51
      GO TO 34
   33 IF(D.LE.0.010.AND.E.LE.0.010.AND.K.GE.5) GO TO 50
C
C     ************************
C     SUBSEQUENT ITERATIONS
C     ************************
C
   34   XNCC=A1-XNCO2-XNC-2.0*XNCH-XNCH4
         XNH2O=(A2-2.0*XNH2-XNH-XNOH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
         XNCO2=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
           XNN2=(A4-XNN-XNNO-XNNH3)/2.0
      XNCO1=A1-XNCO2-XNC-2.0*XNCH-XNCH4
       XNCO21=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
      XNCO=(XNCO+XNCC1)/2.0
      XNCO2=(XNCO2+XNCO21)/2.0
       XNCC=A1-XNCO2-XNC-2.0*XNCH-XNCH4
```

```
      IF(XNCO.LE.0.0) XNCO=0.5
      XN(K+1)=XNCO2+XNH2O+XNN2+XNC2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     XN(TOTAL) IS THE  # OF TOTAL MOLES USED FOR THE SUBSEQUENT ITERATI
C
      GO TO 40
C
C     ***********************************
C     ITERATIONS FOR ADIABATIC TEMPERATURE
C     ***********************************
C
50    IF(D.GT.0.001.OR.E.GT.0.001) GO TO 34
51    L=L+1
      IF(MM.EQ.1) J=1
      IF(L.GT.10) GO TO 55
      P1=PHCO2(T,J)
      P2=PHH2O(T,J)
      P3=PHO2(T,J)
      P4=PHN2(T,J)
      P5=PHCO(T,J)
      P6=PHH2(T,J)
      P7=PHOH(T,J)
      P8=PHO(T,J)
      P9=PHH(T,J)
      P10=PHN(T,J)
      P11=PHNO(T,J)
      P12=PHC(T,J)
      PROENT=XNCO2*P1+XNH2O*P2+XNC2*P3+XNN2*P4+XNCO*P5+XNH2*P6+XNC*P12+X
     1NCH*P7+XNO*P8+XNH*P9+XNN*P10+XNNO*P11
C
C     REACTANT ENTHALPY =H(C7H16)+RO2*H(O2)+3.76*RO2*H(N2)
C
      R1=RHC7H(TIN,J)
      R2=PHO2(TIN,J)
      R3=PHN2(TIN,J)
      REAENT=R1+RO2*R2+3.76*RO2*R3
C
C     APPROXIMATE SP. HEAT ASSUMED 500  CAL/GM MOLE OF FUEL
C
      AA=PROENT-REAENT
      AB=ABS(AA)
      T1=T-(AA/500.0)
      P11=PHCO2(T1,J)
```

```
      P22=PHH2O(T1,J)
      F33=PHO2(T1,J)
      P44=PHN2(T1,J)
      CP1=(P1-P11)
      CF2=(P2-P22)
      CP3=(P3-P33)
      CP4=(P4-P44)
      CP=(XNCO2*CP1+XNH2O*CP2+XNO2*CP3+XNN2*CP4)/(T-T1)
      CP=ABS(CP)
      TNEW=T-(AA/CP)
      DIFF=TNEW-T
      BB=ABS(DIFF)
C
C     CP CALAULATIONS CO NOT INCLUDE  CO H2 AND OTHER SPICIES
C
C     NORMALIZATION T2=(T+TNEW)/2 HAS BEEN DONE TO ACHIEVE RAPID CONVERGENCE
C     IF DIFFERENCE EETWEEN T AND TNEW IS LARGE ENOUGH
C
      T2=(T+TNEW)/2.0
C
C     ITERATION FOR THE FLAME TEMPERATURE IS STOPPED WHEN THE
C     CIFFERENCE IN PRODUCT & REACTANT ENTHALPIES IS < 50.0 AND  ERROR
C        IN THE FLAME TEMPERATURE IS < 1.0 KELVIN
C
      IF(AB.LT.50.0.AND.BB.LT.1.0) GO TO 55
      MM=MM+1
      J=J+1
      MB=1
      IF(ABS(T-TNEW).LE.10.0) GO TO 53
      T=T2
      GO TO 7
   53 T=TNEW
      GO TO 7
   55 Y(1,M)=T
      Y(2,M)=PHI
      Y(3,M)=XNCC2/XN(K+1)
      Y(4,M)=XNH2O/XN(K+1)
      Y(5,M)=XNO2/XN(K+1)
      Y(6,M)=XNN2/XN(K+1)
      Y(7,M)=XNCO/XN(K+1)
      Y(8,M)=XNH2/XN(K+1)
      Y(9,M)=XNC/XN(K+1)
      Y(10,M)=XNCH/XN(K+1)
      Y(11,M)=XNCH4/XN(K+1)
```

```
      Y(12,M)=XNOH/XN(K+1)
      Y(13,M)=XNO/XN(K+1)
      Y(14,M)=XNH/XN(K+1)
      Y(15,M)=XNN/XN(K+1)
      Y(16,M)=XNNO/XN(K+1)
      Y(17,M)=XNNH3/XN(K+1)
      Y(18,M)=L
      Y(19,M)=K
      Y(20,M)=MA
      BB=10.0
      A(1)=XNCO
49    CONTINUE
      WRITE(6,501)P,TIN,CR
501   FORMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC CCMBUSTION CF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MOLE FRACTIONS FOR VARYING',//,5X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MOLE FRACTICN.',/,10X,'CR=',F5.2)
      WRITE(6,500)((Y(I,M),M=1,5),I=1,20)
500   FORMAT(///,10X,'T',5(1X,F14.3),//,8X,'PHI ',5(1X,F14.3),//,8X,'CO2'
     1,5(1X,E14.7),//,8X,'H2O',5(1X,E14.7),//,9X,'O2',5(1X,E14.7),//,9X,
     2'N2',5(1X,E14.7),//,7X,'  CO',5(1X,E14.7),//,8X,' H2',5(1X,E14.7),
     3//,9X,'C ',5(1X,E14.7),//, 7X,'C2H2',5(1X,E14.7),//, 8X,'CH4',5(1X
     4,E14.7),//,9X,'CH',5(1X,E14.7),//,9X,'O',5(1X,E14.7),//,9X,'H',5(1
     5X,E14.7),//,10X,'N',5(1X,E14.7),//,9X,'NO',5(1X,E14.7),//,8X,'NH3'
     6,5(1X,E14.7),//,10X,'L',5(9X,F6.1),//,10X,'K',5(9X,F6.1),//,9X,'MA
     7',5(9X,F6.1))
48    CONTINUE
47    CONTINUE
      RETURN
      END
      FUNCTION XKP1(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP1=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
```

```
[illegible]
[illegible]
[illegible]
[illegible]
X(1S*K)=XMOH\XV(K+I)
```

```
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP2=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP3(T,J)
      DIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP3=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP4(T,J)
      DIMENSICN H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP4=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP5(T,J)
      DIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP5=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP6(T,J)
      CIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP6=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP7(T,J)
      CIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
```

```
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP7=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP8(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FCRMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP8=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP9(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FCRMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP9=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP10(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FCRMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP10=10.0**CCNSTT
      RETURN
      END
      FUNCTION XKP11(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FCRMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP11=10.0**CCNSTT
      RETURN
      END
      FUNCTION PHCO2(T,J)
      DIMENSION H(7)
```

```
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHCO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-94052.0-2238.1
      RETURN
      END
      FUNCTION PHH2O(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHH2O=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-57798.0-2367.7
      RETURN
      END
      FUNCTION PHO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2069.8
      RETURN
      END
      FUNCTION PHN2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHN2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2072.3
      RETURN
      END
      FUNCTION PHCO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHCO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-26415.7-2072.6
      RETURN
      END
      FUNCTION PHH2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHH2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2023.8
```

```
      RETURN
      END
      FUNCTION PHOH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHOH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+10060.0-2106.2
      RETURN
      END
      FUNCTION PHO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+59159.0-1607.4
      RETURN
      END
      FUNCTION PHH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+52089.0-1481.2
      RETURN
      END
      FUNCTION PHN(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHN=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+112750.0-1481.0
      RETURN
      END
      FUNCTION PHNO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHNO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+21600.0-2194.2
      RETURN
      END
      FUNCTION PHC(T,J)
      DIMENSION H(7)
```

```
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHC=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+171698.0-1558.9
      RETURN
      END
      FUNCTION RHC7H(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
       RHC7H=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-44885.0
      RETURN
      END
```

APPENDIX G

COMPUTER PROGRAM III

1. Exhaust Gas Recirculation
2. $\phi < 1.0$

```
C     AGARWAL V.K. (DEPT. OF MECH. ENG. UNIVERSITY OF OTTAWA)
C
C     EXHAUST GAS RECIRCULATION
C
C     ANALYSIS FOR HEPTANE AS FUEL FOR VARIOUS VALUES OF PHI
C
C     COMPOSITION OF AIR BY VOLUME ASSUMED N2IS TO O2 = 3.76 IS TO 1
C
C      PRODUCT COMPOSITION ANALYSIS
C
C      COMPOSITION OF TRACES ASSUMED ZERO AND MAJOR CONSTITUENTS FOUND
C
C      COMPUTING TRACES COMPOSITION
C
C      PHI IS LESS THAN ONE
C
C      ***********************************************************
C      DESCRIPTION OF NOMANCLATURE USED IN THE PROGRAM
C      ***********************************************************
C
C      PREFIX  X   IS USED TO CONVERT FLOATING PT. VARIABLE INTO AN INTEGE
C
C      K AFTER   X   -- EQUILIBRIUM CONSTANT
C
C      N AFTER   X   -- NUMBER OF MOLES
C
C     EXAMPLES
C       XK(N)...... EQUILIBRIUM CONSTANT
C
C       XNKP....... EQUILIBRIUM
C
C       XNCO2...... NO. OF MOLES OF CO2
C
C       XNNO....... NO. OF MOLES OF NO
C
C       XN(K+1).... TOTAL # MOLES
C
C       REAENT..... REACTANT ENTHALPY OF FRESH CHARGE
C
C       PROENT..... PRODUCT ENTHALPY OF EXHAUST GAS
C
C       PENTLO..... LOW PRODUCT ENTHALPY (EGR FRACTION ENTHAPY )
C
C
```

```
C   GENERAL
C
C         TIN :-  INTAKE AIR TEMPERATURE
C
C         J  :-  TAKING CARE OF DATA CARD READING
C
C         P  :-  PRESSURE
C
C         MA :-  CONTROLLING  INITIAL GUESS OF XNCO
C
C         MB :-  SUBSEQUENT FLAME TEMP. CCNVERGENCE
C
C         MM :-  CATA CARD READING
C
C         L  :-  COUNT FOR # OF ITERATIONS FOR FLAME TEMPERATURE
C
C         K  :-  COUNT FCR # OF ITERATIONS FOR COMPOSITIONS OF PRODUCTS
C
C         MP :-  MP=0  FOR STANDARD CARBURETION
C                MP> &=1 FOR ***EGR***
C
C       **********************
C       FIRST ITERATION
C       **********************
C
        CIMENSION Y(19,5),XK(11),XN(25),X(19,5),PR(12),W(19,5),Z(19,5),
       1E(20)
C
C       TIN IS THE TEMPERATURE OF TFE CHARGE AT INLET MANIFOLD
C
        J=1
        TIN=200.0
        DO 45 ID=1,3
        TIN=TIN+100.0
        CR=4.0
        DO 46 IC=1,4
        CR=CR+2.0
        P=CR**1.3
        NP=0
        TR=100.0
        DO 47 IB=1,4
        TR=TR+200.0
        FIN=0.0
        DO 48 IA=1,5
```

```
      FIN=FIN+0.10
      PHI=0.70
      BB=10.0
C
C     FUEL SYMBOL IS CXXHYY
C
C     C7H16 (HEPTANE) IS THE FUEL IN THIS PROGRAM
C
C     THEREFORE   XX=7.0   YY=16.0
C
C     ZZ= STOICHIOMATIC # OF MOLE OF OXYGEN
C
C     STOICHIOMATIC EQ'N IS C7H16+11(O2+3.76 N2) = 7CO2+8H2O+11*3.76**N2
C
C     THEREFORE    ZZ=11.0
C
      XX=7.0
      YY=16.0
      YYY=YY/2.0
      ZZ=11.0
 2    DO 49  M=1,5
      MP=0
      L=0
      PHI=PHI+0.05
C
C     INITIAL FLAME TEMPERATURE HAS BEEN ASSIGNED ARBITRARILY
C
      IF(PHI.LE.0.6) T=1500.0
      IF(PHI.GT.0.6.AND.PHI.LE.1.0) T=2200.0
C
C     LOOP 19 (SKIPPING LOOP 889 VIA 7 ) CALCULATES FINAL FLAME
C     TEMPERATURE & EXHAUST COMPCNENTS FOR STANDARD CARBURETION
C
 19   RO2=ZZ/PHI
      XNO2=RO2-ZZ
      XNCO2=XX
      XNH2O=YYY
      XNN2=3.76*RO2
 6    A1=XX
      A2=YY
      A3=RO2*2.0
      A4=XNN2*2.0
C
C     WHEN GAS IS RECICULATED,INITIAL REACTANTS ARE --------------
```

```
C
C     [illegible]
C
      [illegible]
      [illegible]
      FIN=FIN+0.10
```

```
C
C      (1-FIN)C7H16+(1-FIN)RO2(O2+3.76N2)+F(PRODUCTS WITH RECIRCULATION)
C
      GO TO 7
C
C     LOOP 8 CALCULATES FINAL FLAME TEMPERATURE & EXHAUST COMPONENTS
C              FOR ***EGR***
C
8     XNCO2=XX*(1.0-FIN)+XNCO2*F
      XNH2O=YYY*(1.0-FIN)+XNH2O*F
      XNO2=(RO2- ZZ )*(1.0-FIN)+XNO2*F
      XNN2=3.76*RO2*(1.0-FIN)+XNN2*F
      XNCO=XNCO*F
      XNH2=XNH2*F
      XNC=XNC*F
      XNCH=XNCH*F
      XNCH4=XNCH4*F
      XNOH=XNOH*F
      XNO=XNO*F
      XNH=XNH*F
      XNN=XNN*F
      XNNO=XNNO*F
      XNNH3=XNNH3*F
      A1=XNCO2+XNCO+XNC+XNCH*2.0+XNCH4
      A2=XNH2O*2.0+XNH2*2.0+XNCH*2.0+XNCH4*4.0+XNOH+XNH+XNNH3*3.0
      A3=XNO2*2.0+XNCO2*2.0+XNH2O+XNCO+XNOH+XNO+XNNO
      A4=XNN2*2.0+XNN+XNNO+XNNH3
      B1=XNCO2
      B2=XNH2O
      B3=XNO2
      B4=XNN2
      D1=(1.0-FIN)*(R1+FO2*R2+3.76*RO2*R3)
      D2=PENTLO
C
C     FOR A GIVEN FIN CALCULATIONS ARE DONE REPEATEDLY BETWEEN @ 8&9
C
9     REAENT=D1+F*D2
      XNCO2=B1
      XNH2O=B2
      XNO2=B3
      XNN2=B4
C
C     CALCULATING VALUES OF EQUILIBRIUM CONSTANTS
C
```

```
    7 XN(1)=XNCO2+XNH2O+XNO2+XNN2
      XK(1)=XKP1(T,J)
      XK(2)=XKP2(T,J)
      XK(3)=XKP3(T,J)
      XK(4)=XKP4(T,J)
      XK(5)=XKP5(T,J)
      XK(6)=XKP6(T,J)
      XK(7)=XKP7(T,J)
      XK(8)=XKP8(T,J)
      XK(9)=XKP9(T,J)
      XK(10)=XKP10(T,J)
      XK(11)=XKP11(T,J)
      K=0
      C=0.0
C
C     LOOP 40 ITERATES EXHAUST COMPOSITION FOR A GIVEN FLAME TEMP.
C
   40 K=K+1
      B=P/XN(K)
      XNCO=XNCO2*XK(1)*(B*XNO2)**(-0.5)
      XNH2=(XNCO*XNH2O)/(XNCO2*XK(2))
      IF(F.GE.0.5.ANC.MP.GE.1) GO TO 471
      XNC=(XNCO**2.0)/(XNCO2*XK(3))
      XNCH=XNH2*XK(4)*(XNC*B)**2
      XNCH4=(XNCO*XNH2*XK(5)/XNH2O)*(B*XNH2)**2
      GO TO 42
  471 XNCH=0.0
      XNCH4=0.0
      XNC=0.0
   42 XNOH=XNH2O*XK(6)*((B*XNH2)**(-0.5))
      XNO=XK(7)*((B/XNO2)**(-0.5))
      XNH=XK(8)*((B/XNH2)**(-0.5))
      XNN=XK(9)*((B/XNN2)**(-0.5))
      XNNO=XK(10)*(XNO2*XNN2)**(0.5)
      XNNH3=XK(11)*B*XNH2*(XNN2*XNH2)**(0.5)
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     ITERATION IS STOPPED IF ERROR IN SUBSEQUENT *NO* CONCENTRATION
C                (TEST) IS LESS THAN  0.1 %
C
      TEST=(XNNO-C)/XNNO
      D=ABS(TEST)
      C=XNNO
```

```
      IF(D.LT.0.001.AND.K.GE.5) GO TO 50
C
C     ***********************
C     SUBSEQUENT ITERATIONS
C     ***********************
C
       XNCO2=A1-XNCO-XNC-2.0*XNCH-XNCH4
        XNH2O=(A2-2.C*XNH2- XNH-XNOH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
        XNO2=(A3-2.0*XNCO2-XNH2O-XNCO-XNOH-XNO-XNNO)/2.0
         XNN2=(A4-XNN-XNNO-XNNH3)/2.0
      IF(XNO2.LE.0.0) XNO2=0.2
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
C
C     XN(TOTAL) IS THE  # OF TOTAL MOLES USED FOR THE SUBSEQUENT ITERATI
C
      GO TO 40
C
C     ************************************
C     ITERATIONS FOR ADIABATIC TEMPERATURE
C     ************************************
C
 50   L=L+1
      IF(L.GT.10.AND.MP.GE.1) GO TO 56
      IF(L.GT.10.AND.MP.EQ.0) GO TO 55
      GO TO 140
 130  TS=T
      T=TR
C
C     COMPUTING PRODUCT GAS ENTHALPY
C
 140  P1=PHCO2(T,J)
      P2=PHH2O(T,J)
      P3=PHO2(T,J)
      P4=PHN2(T,J)
      P5=PHCO(T,J)
      P6=PHH2(T,J)
      P7=PHCH(T,J)
      P8=PHO(T,J)
      P9=PHH(T,J)
      P10=PHN(T,J)
      P11=PHNO(T,J)
      P12=PHC(T,J)
      PROENT=XNCO2*P1+XNH2O*P2+XNO2*P3+XNN2*P4+XNCO*P5+XNH2*P6+XNC*P12+X
```

```
     1NOH*P7+XNO*P8+XNH*P9+XNN*P10+XNNO*P11
      IF(ABS(T-TR    ).LE.0.01) PENTLO=PROENT
      IF(ABS(T-TR    ).LE.0.01) GO TO 52
      IF(MP.GE.1) GC TC 106
C
C     REACTANT ENTHALPY =H(C7H16)+RO2*H(O2)+3.76*RO2*H(N2)
C
      R1=RHC7H(TIN,J)
      R2=PHO2(TIN,J)
      R3=PHN2(TIN,J)
      REAENT=R1+RO2*R2+3.76*RO2*R3
C
C     APPROXIMATE SP. HEAT ASSUMED 500  CAL/GM MOLE OF FUEL
C
106   AA=PROENT-REAENT
      AB=ABS(AA)
      T1=T-(AA/500.0)
      P11=PHCO2(T1,J)
      P22=PHH2O(T1,J)
      P33=PHO2(T1,J)
      P44=PHN2(T1,J)
      CP1=(P1-P11)
      CP2=(P2-P22)
      CP3=(P3-P33)
      CP4=(P4-P44)
      IF(ABS(T-T1).LE.0.001) GO TC 159
      CP=(XNCO2*CP1+XNH2O*CP2+XNO2*CP3+XNN2*CP4)/(T-T1)
      CP=ABS(CP)
      TNEW=T-(AA/CP)
      DIFF=TNEW-T
      BB=ABS(DIFF)
      GO TO 161
159   BB=0.0
C
C     ITERATION FOR THE FLAME TEMPERATURE IS STOPPED WHEN THE
C     DIFFERENCE IN PRODUCT & REACTANT ENTHALPIES IS < 50.0 AND  ERROR
C        IN THE FLAME TEMPERATURE IS < 1.0 KELVIN
C
161   IF(AB.LT.25.0.AND.BB.LT.1.0.AND.MP.GE.1) GO TO 56
      IF(AB.LT.25.0.AND.BB.LT.1.0.AND.MP.EQ.0) GO TO 55
      T=TNEW
      J=J+1
      IF(MP.GE.1) GO TC 9
      GC TO 19
```

```
55    X(1,M)=T
      X(2,M)=PHI
      X(3,M)=XNCO2/XN(K+1)
      X(4,M)=XNH2O/XN(K+1)
      X(5,M)=XNO2/XN(K+1)
      X(6,M)=XNN2/XN(K+1)
      X(7,M)=XNCO/XN(K+1)
      X(8,M)=XNH2/XN(K+1)
      X(9,M)=XNC/XN(K+1)
      X(10,M)=XNCH/XN(K+1)
      X(11,M)=XNCH4/XN(K+1)
      X(12,M)=XNOH/XN(K+1)
      X(13,M)=XNO/XN(K+1)
      X(14,M)=XNH/XN(K+1)
      X(15,M)=XNN/XN(K+1)
      X(16,M)=XNNO/XN(K+1)
      X(17,M)=XNNH3/XN(K+1)
      X(18,M)=L
      X(19,M)=K
      NP=NP+1
      GO TO 130
52    MP=MP+1
      T=TS
      F=(FIN*4.76*RO2)/(XN(K+1))
      IF(MP.EQ.1)    L=0
      GO TO 8
56    IF(MP.GT.1) GO TO 700
      W(1,M)=T
      PHINEW=(1.0-FIN)*PHI
      W(2,M)=PHINEW
      W(3,M)=XNCO2
      W(4,M)=XNH2O
      W(5,M)=XNO2
      W(6,M)=XNN2
      W(7,M)=XNCO
      W(8,M)=XNH2
      W(9,M)=XNC
      W(10,M)=XNCH
      W(11,M)=XNCH4
      W(12,M)=XNOH
      W(13,M)=XNO
      W(14,M)=XNH
      W(15,M)=XNN
      W(16,M)=XNNO
```

```
      W(17,M)=XNNH3
      W(18,M)=FIN
      W(19,M)=XN(K+1)
      L=0
      GO TO 130
 70C  Z(1,M)=T
      PHINEW=(1.0-FIN)*PHI
      Z(2,M)=PHINEW
      Z(3,M)=XNCO2
      Z(4,M)=XNH2O
      Z(5,M)=XNO2
      Z(6,M)=XNN2
      Z(7,M)=XNCO
      Z(8,M)=XNH2
      Z(9,M)=XNC
      Z(10,M)=XNCH
      Z(11,M)=XNCH4
      Z(12,M)=XNOH
      Z(13,M)=XNO
      Z(14,M)=XNH
      Z(15,M)=XNN
      Z(16,M)=XNNO
      Z(17,M)=XNNH3
      Z(18,M)=FIN
      Z(19,M)=XN(K+1)
      DO 701 NA=1,19
      E(NA)=(Z(NA,M)-W(NA,M))/W(NA,M)
 701  E(NA)=ABS(E(NA))
      IF(E(1).LE.0.001.AND.E(7).LE.0.001.AND.E(16).LE.0.0001.AND.E(19).L
     1E.0.001) GO TO 57
      L=0
      DO 702 NB=1,19
 702  W(NB,M)=Z(NB,M)
      GO TO 130
 57   Y(1,M)=T
      Y(2,M)=PHINEW
      Y(3,M)=XNCO2/XN(K+1)
      Y(4,M)=XNH2O/XN(K+1)
      Y(5,M)=XNO2/XN(K+1)
      Y(6,M)=XNN2/XN(K+1)
      Y(7,M)=XNCO/XN(K+1)
      Y(8,M)=XNH2/XN(K+1)
      Y(9,M)=XNC/XN(K+1)
      Y(10,M)=XNCH/XN(K+1)
```

```
      Y(11,M)=XNCH4/XN(K+1)
      Y(12,M)=XNOH/XN(K+1)
      Y(13,M)=XNO/XN(K+1)
      Y(14,M)=XNH/XN(K+1)
      Y(15,M)=XNN/XN(K+1)
      Y(16,M)=XNNO/XN(K+1)
      Y(17,M)=XNNH3/XN(K+1)
      Y(18,M)=L
      Y(19,M)=K
      BB=10.0
49    CONTINUE
      WRITE(6,501)P,TIN,F,FIN,TR,CR
501   FORMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC COMBUSTION CF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MOLE FRACTIONS FOR VARYING',//,6X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MOLE FRACTICN.****** (EXHAUST GAS RECIRCULATION )*****',//,10X,
     5'FRACTION OF GAS RECIRCULATED  F=',F8.5,5X,'FIN=',F8.4,5X,'TR=',F6
     6.1,5X,'CR=',F6.2)
      WRITE(6,500)((Y(I,M),M=1,5),I=1,19)
 500  FORMAT(///,10X,'T',5(1X,F14.3),//,8X,'PHI ',5(1X,F14.3),//,8X,'CO2'
     1,5(1X,E14.7),//,8X,'H2O',5(1X,E14.7),//,9X,'O2',5(1X,E14.7),//,9X,
     2'N2',5(1X,E14.7),//,7X,'  CC',5(1X,E14.7),//,8X,' H2',5(1X,E14.7),
     3//,9X,'C ',5(1X,E14.7),//, 7X,'C2H2',5(1X,E14.7),//, 8X,'CH4',5(1X
     4,E14.7),//,9X,'CH',5(1X,E14.7),//,9X,'O',5(1X,E14.7),//,9X,'H',5(1
     5X,E14.7),//,10X,'N',5(1X,E14.7),//,9X,'NO',5(1X,E14.7),//,8X,'NH3'
     6,5(1X,E14.7),//,10X,'L',5(9X,F6.1),//,10X,'K',5(9X,F6.1))
      IF(NP.GT.5) GO TC 503
      WRITE(6,502)P,TIN,CR
502   FCRMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC COMBUSTION OF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MOLE FRACTIONS FCR VARYING',//,6X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MOLE FRACTION.*********(STANDARD CARBURETION)*********',//,10X,
     5'CR=',F6.2)
      WRITE(6,500)((X(I,M),M=1,5),I=1,19)
C
C     ARRAY W HAS BEEN USED AGAIN TO MINIMISE THE  STORAGE LOCATIONS
C
503   DO 506 ND=1,5
      DO 505 NC=1,19
      W(NC,ND)=(Y(NC,ND)-X(NC,ND))/X(NC,ND)
505   CONTINUE
506   CCNTINUE
```

```
      WRITE(6,501)P,TIN,F,FIN,TR,CR
      WRITE(6,500)((W(I,M),M=1,5),I=1,19)
48    CONTINUE
47    CONTINUE
46    CONTINUE
45    CONTINUE
      RETURN
      END
      FUNCTION XKP1(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP1=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP2=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP3(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP3=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP4(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP4=10.0**CONSTT
      RETURN
      END
```

```
      FUNCTION XKP5(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP5=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP6(T,J)
      DIMENSICN H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP6=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP7(T,J)
      CIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP7=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP8(T,J)
      CIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP8=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP9(T,J)
      DIMENSICN H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CCNSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP9=10.0**CONSTT
      RETURN
```

```
      END
      FUNCTION XKP10(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP10=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP11(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP11=10.0**CONSTT
      RETURN
      END
      FUNCTION PHCO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHCO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-94052.0-2238.1
      RETURN
      END
      FUNCTION PHH2O(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHH2O=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-57798.0-2367.7
      RETURN
      END
      FUNCTION PHO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2069.8
      RETURN
      END
      FUNCTION PHN2(T,J)
```

```
      [illegible]
      [illegible]
      [illegible]
      [illegible]
      END
```

```
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHN2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2072.3
      RETURN
      END
      FUNCTION PHCO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHCO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-26415.7-2072.6
      RETURN
      END
      FUNCTION PHH2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHH2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2023.8
      RETURN
      END
      FUNCTION PHOH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHOH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+10060.0-2106.2
      RETURN
      END
      FUNCTION PHO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+59159.0-1607.4
      RETURN
      END
      FUNCTION PHH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
```

```
     1+H(7)*(T**6)+52089.0-1481.2
      RETURN
      END
      FUNCTION PHN(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
         PHN=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+112750.0-1481.0
      RETURN
      END
      FUNCTION PHNO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
        PHNO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+21600.0-2194.2
      RETURN
      END
      FUNCTION PHC(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
         PHC=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+171698.0-1558.9
      RETURN
      END
      FUNCTION RHC7H(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
151   FORMAT(5E14.7)
       RHC7H=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-44885.0
      RETURN
      END
```

APPENDIX G

COMPUTER PROGRAM IV

1. Exhaust Gas Recirculation
2. $\phi \geq 1.0$

```
C      AGARWAL V.K. (DEPT. OF MECH. ENG. UNIVERSITY OF OTTAWA)
C
C      EXHAUST GAS RECIRCULATICN
C
C      FOR NEXT PHI,APPROXIMATION OF MAJOR CONSTITUENTS HAS BEEN TAKEN
C      FROM PREVIOUS VALUE OF PHI,SO PHI=1.0 IS TO BE RUN FIRST
C
C      ANALYSIS FOR HEPTANE AS FUEL FOR VARIOUS VALUES OF PRESSURES
C
C      COMPOSITION OF AIR BY VOLUME ASSUMED N2IS TO O2 = 3.76 IS TO 1
C
C      PRODUCT COMPOSITICN ANALYSIS
C
C      CCMPOSITION OF TRACES ASSUMED ZERO AND MAJOR CONSTITUENTS FOUND
C
C      COMPUTING TRACES COMPCSITION
C
C      PHI IS EITHER EQUAL TC OR GREATER THAN ONE
C
C
C      ***********************************************************
C      DESCRIPTION OF NCMANCLATURE USED IN THE PROGRAM
C      ***********************************************************
C
C      PREFIX  X  IS USED TO CCNVERT FLOATING PT. VARIABLE INTO AN INTEGE
C
C      K AFTER  X  -- EQUILIBRIUM CONSTANT
C
C      N AFTER  X  -- NUMBER CF MOLES
C
C     EXAMPLES
C       XK(N)...... EQUILIBRIUM CCNSTANT
C
C       XNKP....... EQLILIBRIUM
C
C       XNCO2...... NC. CF MOLES OF CO2
C
C       XNNO....... NO. CF MOLES OF NO
C
C       XN(K+1).... TCTAL # MCLES
C
C       REAENT..... REACTANT ENTHALPY OF FRESH CHARGE
C
C       PROENT..... PRODUCT ENTHALPY OF EXHAUST GAS
```

```
C
C     PENTLO..... LOW PRODUCT ENTHALPY (EGR FRACTION ENTHAPY )
C
C  GENERAL
C
C        TIN:-   INTAKE AIR TEMPERATURE
C
C        J   :-  TAKING CARE OF DATA CARD READING
C
C        P   :-  PRESSURE
C
C        MA  :-  CONTROLLING  INITIAL GUESS OF XNCO
C
C        MB  :-  SUBSEQUENT FLAME TEMP. CCNVERGENCE
C
C        MM  :-  DATA CARC REACING
C
C        L   :-  COUNT FOR # CF ITERATIONS FOR FLAME TEMPERATURE
C
C        K   :-  COUNT FOR # OF ITERATIONS FOR COMPOSITIONS OF PRODUCTS
C
C        MP  :-  MP=0   FOR STANDARD CARBURETION
C
C     NP :-  PRINTS STANDARD CARBURETION RESULTS ONLY WHEN
C            TIN OR CR IS ALTERED
C
C     **********************
C     FIRST ITERATION
C     **********************
      DIMENSION Y(20,4),XK(11),XN(95),A(17),X(20,4),W(20,4),Z(20,4),
     1ER(20)
      YMC=0.0
      MM=1
      J=1
      TIN=300.0
      CR=8.0
      P=CR**1.3
      NP=0
      TR=100.0
      DC 47 JB=1,4
      TR=TR+200.0
      FIN=0.0
      DC 48 JA=1,4
      FIN=FIN+0.1
```

```
      A(1)=0.7
      PHI=0.9
      BB=10.0
      G=7.5
C
C     FUEL SYMBOL IS CXXHYY
C
C
C     C7H16 (HEPTANE) IS THE FUEL IN THIS PROGRAM
C
C     THEREFORE   XX=7.0   YY=16.0
C
C     ZZ= STOICHIOMATIC # OF MOLE OF OXYGEN
C
C     STOICHIOMATIC EQ'N IS C7H16+11(O2+3.76 N2) = 7CO2+8H2O+11*3.76**N2
C     THEREFORE    ZZ=11.0
C
      XX=7.0
      YY=16.0
      YYY=YY/2.0
      ZZ=11.0
      DO 49 M=1,4
      MP=0
      MB=0
      MA=1
      PHI=PHI+0.1
      L=0
C
C     T=2500.0-PHI*200.0 HAS BEEN FOUND TO GIVE GOOD INITIAL GUESS FOR T
C
      T=2500.0-PHI*200.0
C
C     LOOP 19 (SKIPPING LOOP 8&9 VIA 7 ) CALCULATES FINAL FLAME
C     TEMPERATURE & EXHAUST COMPONENTS FOR STANDARD CARBURETION
   19 RO2=ZZ/PHI
      XNCO=A(MA)
      XNN2=3.76*RO2
      XNCO2=XX-XNCO
      XNH2O=G
      GO TO 6
   22 MA=MA+1
      IF(MA.GT.15.AND.MP.EQ.1) GO TO 56
      IF(MA.GT.15) GO TO 55
      YMC=YMC+1.0
```

```
      S=YMC/2.0
      IA=S
      WRITE(6,183)YMC,S,IA,MA
 183  FORMAT(/,10X,'YMC,S,IA,MA ARE AS FOLLOWS',/,10X,2(F15.5),/,10X,2(I
     115))
      IF(S-IA) 181,181,182
 181  A(MA)=A(MA-1)+0.1*YMC
      XNCO=A(MA)
      GO TO 24
 182  A(MA)=A(MA-1)-0.1*YMC
  24  XNCO=A(MA)
C
C      XNCO IN LOOP 7  COMES FROM THE ITERATION FOR WHICH TEMP. ITERATION
C         HAS BEEN DONE
C
C      IF MA CHANGES EVEN THEN XNH2O IS BEING TAKEN FROM PREVIOUS ITERATI
C
C      SINCE FUELIS C7H16   SO  A1=7.0  A2=16.0
C
         XNH2O=(A2-2.0*XNH2-XNH-XNOH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
         XNCO2=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
          XNN2=(A4-XNN-XNNO-XNNH3)/2.0
      WRITE(6,17)A1,A2,A3,A4,XNCO2,XNH2O,XNCO,XNN2
 17   FORMAT(/,5X,'FOR STANDARD CARBURETION,A1,A2,A3,A4 & XNCO2,XNH2O,XN
     UCO,XNN2 ARE AS FOLLOWS',/,4(5X,F20.7))
       XNCO1=A1-XNCO2-XNC-2.0*XNCH-XNCH4
        XNCO21=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
       WRITE(6,191)XNCO1,XNCO21
 191   FORMAT(5X,'XNCO1=',F10.4,10X,'XNCO21=',F10.4)
       XNCO=(XNCO+XNCO1)/2.0
       XNCO2=(XNCO2+XNCO21)/2.0
        XNCO=A1-XNCO2-XNC-2.0*XNCH-XNCH4
       WRITE(6,17)A1,A2,A3,A4,XNCO2,XNH2O,XNCO,XNN2
  6    A1=XX
       A2=YY
       A3=RO2*2.0
       A4=XNN2*2.0
C
C      WHEN GAS IS RECICULATED,INITIAL REACTANTS ARE --------------
C
C        (1-F)C7H16+(1-F)RO2(O2+3.76N2)+F(PRODUCTS WITHOUT RECIRCULATION)
C
       GO TO 7
C
```

```
C     LOOP 8 CALCULATES FINAL FLAME TEMPERATURE & EXHAUST COMPONENTS
C             FOR ***EGR***
C
8     C1=(1.0-FIN)*(R1+RO2*R2+3.76*RO2*R3)
      D2=PENTLO
C
C     FOR A GIVEN F CALCULATIONS ARE DONE ONLY ONCE BETWEEN @ 8&9
C
 9    REAENT=D1+F*D2
C
C     FOR A GIVEN FIN CALCULATIONS ARE DONE REPEATEDLY BETWEEN @ 8&9
C
C     CALCULATING VALUES OF EQUILIBRIUM CONSTANTS
C
 7    XN(1)=XNCO2+XNH2O+XNCO+XNN2
      XK(1)=XKP1(T,J)
      XK(2)=XKP2(T,J)
      XK(3)=XKP3(T,J)
      XK(4)=XKP4(T,J)
      XK(5)=XKP5(T,J)
      XK(6)=XKP6(T,J)
      XK(7)=XKP7(T,J)
      XK(8)=XKP8(T,J)
      XK(9)=XKP9(T,J)
      XK(10)=XKP10(T,J)
      XK(11)=XKP11(T,J)
      K=0
      C=0.0
      CC=0.0
 40   K=K+1
      IF(K.GT.25) J=J+1
      IF(K.GT.25) GO TO 22
      B=P/XN(K)
      XNO2=((XK(1)*XNCO2/XNCO)**2.0)/B
      XNH2=(XNCO*XNH2O)/(XNCO2*XK(2))
      XNC=(XNCO**2.0)/(XNCO2*XK(3))
      IF(FIN.GE.0.5.AND.MP.GE.1) GO TO 474
      XNCH=XNH2*XK(4)*(XNC*B)**2
      XNCH4=(XNCO*XNH2*XK(5)/XNH2O)*(B*XNH2)**2
      GO TO 42
 474  XNCH=0.0
      XNCH4=0.0
 42   XNOH=XNH2O*XK(6)*((B*XNH2)**(-0.5))
      XNO=XK(7)*((B/XNO2)**(-0.5))
```

```
      XNH=XK(8)*((B/XNH2)**(-0.5))
      XNN=XK(9)*((B/XNN2)**(-0.5))
      XNNO=XK(10)*(XNO2*XNN2)**(0.5)
      XNNH3=XK(11)*B*XNH2*(XNN2*XNH2)**(0.5)
      XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
     1H+XNN+XNNO+XNNH3
      TEST=(XNH2-C)/XNH2
      TEST1=(XNCO-CC)/XNCO
      D=ABS(TEST)
      E=ABS(TEST1)
      C=XNH2
      CC=XNCO
      IF(MB.EQ.1) GO TO 33
      IF(D.LE.0.050.AND.E.LE.0.050.AND.K.GE.5) GO TO 51
      GO TO 34
33    IF(D.LE.0.005.AND.E.LE.0.002.AND.K.GE.5) GO TO 51
      IF(D.LE.0.005.AND.E.LE.0.005.AND.K.GE.5.AND.MP.EQ.1) GO TO 51
C
C     ***********************
C     SUBSEQUENT ITERATIONS
C     ***********************
C
34     XNCO=A1-XNCO2-XNC-2.0*XNCH-XNCH4
        XNH2O=(A2-2.0*XNH2-XNH-XNOH-2.0*XNCH-3.0*XNNH3-4.0*XNCH4)/2.0
        XNCO2=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
         XNN2=(A4-XNN-XNNO-XNNH3)/2.0
       IF(K.GT.25)WRITE(6,25)XNCO2,XNH2O,XNO2,XNN2,XNCO,XNH2,TEST,TEST1,K
25     FORMAT('  XNCO2=',F6.3,2X,'XNH2O=',F6.3,2X,'XNO2=',F6.3,2X,'XNN2='
      1,F6.3,2X,'XNCO=',F6.3,2X,'XNH2=',F6.3,2X,'TEST=',E14.7,2X,'TEST1='
      2,E14.7,2X,'K=',I3)
       XNCO1=A1-XNCO2-XNC-2.0*XNCH-XNCH4
        XNCO21=(A3-XNCO-XNH2O-2.0*XNO2-XNOH-XNO-XNNO)/2.0
       XNCO=(XNCO+XNCO1)/2.0
       XNCO2=(XNCO2+XNCO21)/2.0
        XNCO=A1-XNCO2-XNC-2.0*XNCH-XNCH4
       IF(XNCO.LE.0.0) XNCO=0.5
       IF(K.GT.25)WRITE(6,25)XNCO2,XNH2O,XNO2,XNN2,XNCO,XNH2,TEST,TEST1,K
       XN(K+1)=XNCO2+XNH2O+XNN2+XNO2+XNCO+XNH2+XNC+XNCH+XNCH4+XNOH+XNO+XN
      1H+XNN+XNNO+XNNH3
C
C      XN(TOTAL) IS THE  # OF TOTAL MOLES USED FOR THE SUBSEQUENT ITERATI
C
       GO TO 40
C
```

```
C      ***********************************
C      ITERATIONS FOR ADIABATIC TEMPERATURE
C      ***********************************
C
 51    L=L+1
       IF(MM.EQ.1) J=1
       IF(L.GT.10.AND.MP.GE.1) GO TO 561
       IF(L.GT.10) GO TO 551
       GO TO 140
 130   TS=T
       T=TR
 140   P1=PHCO2(T,J)
       P2=PHH2O(T,J)
       P3=PHO2(T,J)
       P4=PHN2(T,J)
       P5=PHCO(T,J)
       P6=PHH2(T,J)
       P7=PHOH(T,J)
       P8=PHO(T,J)
       P9=PHH(T,J)
       P10=PHN(T,J)
       P11=PHNO(T,J)
       P12=PHC(T,J)
       PROENT=XNCO2*P1+XNH2O*P2+XNC2*P3+XNN2*P4+XNCO*P5+XNH2*P6+XNC*P12+X
      1NOH*P7+XNO*P8+XNH*P9+XNN*P10+XNNO*P11
       IF(ABS(T-TR).LE.0.01) PENTLC=PROENT
       IF(ABS(T-TR).LE.0.01) GO TO 52
       IF(MP.GE.1) GO TO 106
C
C      REACTANT ENTHALPY =H(C7H16)+RO2*H(O2)+3.76*RO2*H(N2)
C
       R1=RHC7H(TIN,J)
       R2=PHO2(TIN,J)
       R3=PHN2(TIN,J)
       REAENT=R1+RO2*R2+3.76*RO2*R3
C
C      APPROXIMATE SP. HEAT ASSUMED 500  CAL/GM MOLE OF FUEL
C
 106   AA=PROENT-REAENT
       AB=ABS(AA)
       T1=T-(AA/500.0)
       P11=PHCO2(T1,J)
       P22=PHH2O(T1,J)
       P33=PHO2(T1,J)
```

```
      P44=PHN2(T1,J)
      CP1=(P1-P11)
      CP2=(P2-P22)
      CP3=(P3-P33)
      CP4=(P4-P44)
      IF(ABS(T-T1).LE.0.001) GO TO 159
      CP=(XNCO2*CP1+XNH2O*CP2+XNO2*CP3+XNN2*CP4)/(T-T1)
      CP=ABS(CP)
      TNEW=T-(AA/CP)
      DIFF=TNEW-T
      BB=ABS(DIFF)
      GO TO 161
  159 BB=0.0
C
C     CP CALAULATIONS DO NOT INCLUDE  CO H2 AND OTHER  SPICIES
C
C     NORMALIZATION T2=(T+TNEW)/2 HAS BEEN DONE TO ACHIEVE RAPID CONVERGENCE
C      IF DIFFERENCE BETWEEN T AND TNEW IS LARGE ENOUGH
C
  161  IF(MP.GE.1) GO TO 163
       IF(AB.LT.50.0.AND.BB.LT.0.2) GO TO 55
       GO TO 164
  163  IF(AB.LT.50.0.AND.BB.LT.0.2) GO TO 56
  164  T2=(T+TNEW)/2.0
       MM=MM+1
       J=J+1
       MB=1
       IF(ABS(T-TNEW).LE.10.0) GO TO 53
       T=T2
       IF(MP.GE.1) GO TO 9
       GO TO 7
   53  T=TNEW
       IF(MP.GE.1) GO TO 9
       GO TO 7
  551  WRITE(6,562)
  562  FORMAT(//,5X,'TEMPERATURE ITERATION IS NOT CONVERGING RAPIDLY.')
   55  X(1,M)=T
       IF(K.GT.25) K=K-1
       X(2,M)=PHI
       X(3,M)=XNCO2/XN(K+1)
       X(4,M)=XNH2O/XN(K+1)
       X(5,M)=XNO2/XN(K+1)
       X(6,M)=XNN2/XN(K+1)
       X(7,M)=XNCO/XN(K+1)
```

```
      X(8,M)=XNH2/XN(K+1)
      X(9,M)=XNC/XN(K+1)
      X(10,M)=XNCH/XN(K+1)
      X(11,M)=XNCH4/XN(K+1)
      X(12,M)=XNOH/XN(K+1)
      X(13,M)=XNO/XN(K+1)
      X(14,M)=XNH/XN(K+1)
      X(15,M)=XNN/XN(K+1)
      X(16,M)=XNNO/XN(K+1)
      X(17,M)=XNNH3/XN(K+1)
      X(18,M)=L
      X(19,M)=K
      X(20,M)=MA
      NP=NP+1
      A(1)=XNCO
      G=XNH2O
      IF(MP.EQ.0) GO TO 130
52    MP=MP+1
      T=TS
      F=(FIN*4.76*RO2)/(XN(K+1))
      IF(MP.EQ.1)    L=0
      GO TO 8
561   WRITE(6,562)
56    IF(MP.GT.1) GO TO 700
C
C     ARRAYS W & Z TAKE CARE OF CONTINUOUS EGR(STEADY STATE)
C
      W(1,M)=T
      PHINEW=(1.0-FIN)*PHI
      W(2,M)=PHINEW
      W(3,M)=XNCO2
      W(4,M)=XNH2O
      W(5,M)=XNO2
      W(6,M)=XNN2
      W(7,M)=XNCO
      W(8,M)=XNH2
      W(9,M)=XNC
      W(10,M)=XNCH
      W(11,M)=XNCH4
      W(12,M)=XNOH
      W(13,M)=XNO
      W(14,M)=XNH
      W(15,M)=XNN
      W(16,M)=XNNO
```

```
      W(17,M)=XNNH3
      W(18,M)=FIN
      W(19,M)=XN(K+1)
      L=0
      GO TO 130
  700 Z(1,M)=T
      PHINEW=(1.0-FIN)*PHI
      Z(2,M)=PHINEW
      Z(3,M)=XNCO2
      Z(4,M)=XNH2O
      Z(5,M)=XNO2
      Z(6,M)=XNN2
      Z(7,M)=XNCO
      Z(8,M)=XNH2
      Z(9,M)=XNC
      Z(10,M)=XNCH
      Z(11,M)=XNCH4
      Z(12,M)=XNOH
      Z(13,M)=XNO
      Z(14,M)=XNH
      Z(15,M)=XNN
      Z(16,M)=XNNO
      Z(17,M)=XNNH3
      Z(18,M)=FIN
      Z(19,M)=XN(K+1)
      DO 701 NA=1,19
      ER(NA)=(Z(NA,M)-W(NA,M))/W(NA,M)
  701 ER(NA)=ABS(ER(NA))
      IF(ER(1).LE.0.005.AND.ER(7).LE.0.005.AND.ER(16).LE.0.0010.AND
     1.ER(19).LE.0.005) GO TO 57
      L=0
      DO 702 NB=1,19
  702 W(NB,M)=Z(NB,M)
      GO TO 130
   57 Y(1,M)=T
      Y(2,M)=PHINEW
      Y(3,M)=XNCO2/XN(K+1)
      Y(4,M)=XNH2O/XN(K+1)
      Y(5,M)=XNO2/XN(K+1)
      Y(6,M)=XNN2/XN(K+1)
      Y(7,M)=XNCO/XN(K+1)
      Y(8,M)=XNH2/XN(K+1)
      Y(9,M)=XNC/XN(K+1)
      Y(10,M)=XNCH/XN(K+1)
```

```
      Y(11,M)=XNCH4/XN(K+1)
      Y(12,M)=XNOH/XN(K+1)
      Y(13,M)=XNO/XN(K+1)
      Y(14,M)=XNH/XN(K+1)
      Y(15,M)=XNN/XN(K+1)
      Y(16,M)=XNNO/XN(K+1)
      Y(17,M)=XNNH3/XN(K+1)
      Y(18,M)=L
      Y(19,M)=K
      Y(20,M)=MA
141   IF(MA.GT.15)WRITE(6,142)PHI
142   FCRMAT(//,'  ITERATION FOR PHI=',F4.1,'IS NOT CONVERGING')
 49   CONTINUE
      WRITE(6,501)P,TIN,F,FIN,TR,CR
 501  FCRMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC COMBUSTION CF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MCLE FRACTIONS FOR VARYING',//,6X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MOLE FRACTICN.****** (EXHAUST GAS RECIRCULATICN )*****',//,10X,
     5'FRACTION OF GAS RECIRCULATED  F=',F8.5,5X,'FIN=',F8.4,5X,'TR=',F6
     6.1,5X,'CR=',F6.2)
       WRITE(6,500)((Y(I,M),M=1,4),I=1,20)
  500 FCRMAT(///,10X,'T',4(4X,F14.3),//,8X,'PHI',4(4X,F14.3),//,8X,'CO2'
     1,4(4X,E14.7),//,8X,'H2O',4(4X,E14.7),//,9X,' O2',4(4X,E14.7),//,9X,
     2'N2',4(4X,E14.7),//,7X,'  CO',4(4X,E14.7),//,8X,' H2',4(4X,E14.7),
     3//,9X,'C ',4(4X,E14.7),//, 7X,'C2H2',4(4X,E14.7),//, 8X,'CH4',4(4X
     4,E14.7),//,9X,'OH',4(4X,E14.7),//,9X,'O',4(4X,E14.7),//,9X,'H',4(4
     5X,E14.7),//,10X,'N',4(4X,E14.7),//,9X,'NO',4(4X,E14.7),//,8X,'NH3'
     6,4(4X,E14.7),//,10X,'L',4(9X,F9.1),//,10X,'K',4(9X,F9.1),//,9X,'MA
     7',4(9X,F9.1))
       IF(NP.GT.5) GC TC 503
       WRITE(6,502)P,TIN,CR
  502  FORMAT(1H1,5X,'FLAME TEMP. AND PRODUCT COMPOSITION FOR THE ADIABAT
     1IC CCMBUSTION CF HEPTANE/AIR MIXTURE AT A PRESSURE OF',//,F9.1,' A
     2TMOSPHERE  AND  A INITIAL REACTANT TEMP. OF',F7.1,' DEGREE KELVIN.
     3MOLE FRACTIONS FOR VARYING',//,6X,'EQUIVALENCE RATIOS COMPOSITION
     4IN MCLE FRACTICN.*********(STANCARD CARBURETION)*********',//,10X,
     5'CR=',F6.2)
       WRITE(6,500)((X(I,M),M=1,4),I=1,20)
C
C      ARRAY W HAS BEEN USED AGAIN TO MINIMISE THE STORAGE LOCATIONS
C
 503   DO 506 ND=1,5
       DO 505 NC=1,20
```

```
      W(NC,ND)=(Y(NC,ND)-X(NC,ND))/X(NC,ND)
  505 CONTINUE
  506 CONTINUE
      WRITE(6,501)P,TIN,F,FIN,TR,CR
      WRITE(6,500)((W(I,M),M=1,4),I=1,20)
   48 CONTINUE
   47 CONTINUE
      RETURN
      END
      FUNCTION XKP1(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP1=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP2=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP3(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP3=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP4(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP4=10.0**CONSTT
      RETURN
```

```
      END
      FUNCTION XKP5(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP5=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP6(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(F(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP6=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP7(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP7=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP8(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP8=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP9(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) REAC(1,151)(H(I),I=1,7)
  151 FCRMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP9=10.0**CONSTT
```

```
      RETURN
      END
      FUNCTION XKP10(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP10=10.0**CONSTT
      RETURN
      END
      FUNCTION XKP11(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      CONSTT=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)
      XKP11=10.0**CONSTT
      RETURN
      END
      FUNCTION PHCO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHCO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-94052.0-2238.1
      RETURN
      END
      FUNCTION PHH2O(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
       PHH2O=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-57798.0-2367.7
      RETURN
      END
      FUNCTION PHO2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHO2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2069.8
      RETURN
      END
```

```
      FUNCTION PHN2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHN2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2072.3
      RETURN
      END
      FUNCTION PHCO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHCO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-26415.7-2072.6
      RETURN
      END
      FUNCTION PHH2(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHH2=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-2023.8
      RETURN
      END
      FUNCTION PHOH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHOH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+10060.0-2106.2
      RETURN
      END
      FUNCTION PHO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
        PHO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+59159.0-1607.4
      RETURN
      END
      FUNCTION PHH(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
```

```
      PHH=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+52089.0-1481.2
      RETURN
      END
      FUNCTION PHN(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHN=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+112750.0-1481.0
      RETURN
      END
      FUNCTION PHNO(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHNO=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+21600.0-2194.2
      RETURN
      END
      FUNCTION PHC(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      PHC=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)+171698.0-1558.9
      RETURN
      END
      FUNCTION RHC7H(T,J)
      DIMENSION H(7)
      IF(J.EQ.1) READ(1,151)(H(I),I=1,7)
  151 FORMAT(5E14.7)
      RHC7H=H(1)+H(2)*T+H(3)*(T**2)+H(4)*(T**3)+H(5)*(T**4)+H(6)*(T**5)
     1+H(7)*(T**6)-44885.0
      RETURN
      END
```