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AMMONIA IN DIESEL ENGINES

A Thesis

Presented for the

Master of Science

Degree

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Gestur Valgardsson

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To My Parents:

Valgardur Ó. Breidfjörd

and

Jóna Gestsdóttir

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ABSTRACT

Recent concern over Iceland's dependence on imported oil products has brought new emphasis on synthetic nonpetroleum fuels such as hydrogen, methanol, and anhydrous ammonia. This study was undertaken to document the performance of a compression ignition engine fueled with anhydrous ammonia; and, to derive a mathematical model to predict the general behavior of anhydrous ammonia as a compression engine fuel.

The engine used, Caterpillar D330c, 4 cylinder, 425 cu in, equipped with 17.5:1 compression ratio and precombustion chambers was not in any way modified to accommodate the unique combustion properties of the ammonia.

All tests were conducted with the engine running at the speed of 1500 rpm. Fuel-oil fueled engine tests were conducted to establish the baseline performance. Among results established for different engine loads were: the relationship between the fuel-oil and ammonia consumption; the thermal efficiency of the engine running for variable ammonia consumption; and, the relationship between induction air and ammonia consumption. Pressure-traces from the engine cylinder were also obtained.

The main findings of this study were that only moderate amounts of ammonia could be substituted for the fuel-oil. The limiting factor is the high rate of pressure rise in the cylinder, which in some cases was as high as 200 psi/deg. It is believed that this

high rate of pressure increase is caused by abnormally high rate of release of chemical energy. It is shown that in order to secure satisfactory operation of the engine the rate of pressure increase should not exceed 90 psi/deg, during combustion. The thermal efficiency at full load increased slightly, 3%, with increases in ammonia consumption, but at low loads the thermal efficiency decreased by as much as 35%.

No emission tests were conducted, but it is estimated that as much as 40% of the ammonia consumed by the engine is not burned.

A mathematical model based on the constant volume combustion cycle was derived. The model was then used to predict the behavior of performance factors with increasing fractions of ammonia in the fuel-air mixture. Results of the calculations are presented in the form of graphs.

Results of this model indicate that for low ammonia fueling (0-25% by weight) the performance factors of the engine should not deviate significantly from those obtained with fuel-oil. This was substantiated by the experiment. However, for higher ammonia fueling rates the difference becomes significant. Because of the limited amount of fuel-oil that could be replaced by the ammonia, the ability of the mathematical model to predict the performance of the engine for higher ammonia fueling rates could not be fully investigated experimentally.

It is believed that the abnormal rate of pressure increase is caused by the exothermic reaction between the fuel and the oxygen,

which in turn is caused by heterogeneous combustion of the ammonia within the cylinder. Therefore, it is proposed that future work be aimed toward investigating the combustion mechanics of the ammonia-air mixture within the cylinder. Also, means by which more regular combustion of the ammonia-air mixture can be achieved should be investigated.

In addition, since it is known that the combustion properties of ammonia are greatly improved by enriching the ammonia-air mixture with hydrogen, it is proposed that the possibilities of partially dissociating the ammonia outside the engine should be investigated.

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NOMENCLATURE

Symbol	Definition
C_p	Specific heat at constant pressure.
C_v	Specific heat at constant volume.
c_{v_1}	Molar specific heat of the fresh NH_3 and air mixture at state-point (1).
c_{p_2}	Molar specific heat of the residual at state-point (1).
CR	Compression ratio V_1/V_2
dm	Differential injection of fuel-oil, Eq. X-4.
dP	Differential change in pressure.
dU	Differential change in internal energy.
dV	Differential change in volume.
H	Total enthalpy.
H_{rp}	Enthalpy of reaction, Eq. III-11.
H_p	Enthalpy of the reacting mixture.
H_r	Enthalpy of the reactant mixture.
h	Specific enthalpy.
h_{H_2O}	Specific enthalpy of H_2O.
h_{N_2}	Specific enthalpy of N_2.
h_{NH_3}	Specific enthalpy of NH_3.
h_{O_2}	Specific enthalpy of O_2.
$h_{C_{10}H_{22}}$	Specific enthalpy of $C_{10}H_{22}$.
h_{CO_2}	Specific enthalpy of CO_2.
$ISFC_a$	Indicated specific fuel consumption of NH_3, Eq. IV-6.

Symbol	Definition
$ISFC_o$	Indicated specific fuel consumption of $C_{10}H_{22}$, Eq. IV-6.
k	Defined as c_p/c_v.
M_a	Actual number of moles of NH_3 and air in the cylinder before injection of fuel-oil.
M_x	Actual number of moles of residual in the cylinder during combustion.
M_t	Actual number of moles of NH_3 air and fuel-oil in the cylinder after injection.
N_{po}	Defined by Eq. III-31.
N_{tp}	Total number of moles of product, Eq. III-37. Note: $N_{tp} = N_{op}$.
n_a	Number of moles of NH_3 in Eq. III-1.
n_o	Number of moles of $C_{10}H_{22}$ in Eq. III-1.
n_i	i = 1, 2, ... , 10. Number of moles of each specie in Eq. III-1. i = 1 refers to CO_2; i = 2 refers to CO; i = 3 refers to O_2; i = 4 refers to O; i = 5 refers to NO; i = 6 refers to N_2; i = 7 refers to H_2; i = 8 refers to H; i = 9 refers to OH; i = 10 refers to H_2)
P_1	Pressure at state-point (1)
P_2	Pressure at state-point (2).
P_3	Pressure at state-point (3).
P_4	Pressure at state-point (4)

Symbol	Definition
P_5	Pressure at state-point (5)
$dP/d\theta$	Rate of pressure increase.
p_i	Partial pressure of constituent i.
Q	Heat transfer to the control-volume, Eq. X-4.
Q_{ch}	Release of chemical energy.
Q_c	Transfer of heat to the cylinder.
R	The Universal gas constant.
S	Entropy.
s	Specific entropy.
(Δs_o^j)	Change in entropy of constituent i, when going from state-point o to j.
T_1	Temperature at state-point (1).
T_2	Temperature at state-point (2).
T_3	Temperature at state-point (3).
T_4	Temperature at state-point (4).
T_5	Temperature at state-point (5).
U	Internal energy.
U_2	Internal energy of the NH_3, $C_{10}H_{22}$, air and residual at state-point (2).
U_a	Internal energy of NH_3 at state-point (2).
U_o	Internal energy of $C_{10}H_{22}$ at state-point (2).
U_{air}	Internal energy of air at state-point (2).
U_r	Internal energy of residual at state-point (2).
U_3	Internal energy of the product mixture at state-point (2).

Symbol	Definition
U^i_{cm}	Initial energy of the control mass at V_{tdc}, Eq. III-59.
U^f_{cm}	Internal energy of control mass at V_{bdc}, Eq. III-62.
U_{rp_a}	Heat of reaction of NH_3 at constant volume combustion, Eq. IV-3.
U_{rp_o}	Heat of reaction for $C_{10}H_{22}$ at constant volume combustion, Eq. IV-3.
u	Specific internal energy.
u_{NH_3}	Specific internal energy of NH_3.
$uC_{10}H_{22}$	Specific internal energy of $C_{10}H_{22}$.
V	Volume.
V_1	Volume at state-point (1). Note: $V_1 = V_3$.
V_2	Volume at state-point (2). Note: $V_2 = V_4$.
V_{bdc}	Volume at bottom dead center.
V_{tdc}	Volume at top dead center.
W_s	Piston work.
W_{cm}	Work performed by the mixture on the control volume, Eq. III-61.
W_{net}	Net work output, Eq. IV-1.
W_{exp}	Expansion work, Eq. IV-1.
W_{comp}	Compression work, Eq. IV-1.
Y	Number of moles of oxygen in Eq. III-1.
Y_{cc}	Chemically correct amount of Y.
Y_{min}	Minimum number of moles of oxygen necessary to convert all the carbon to carbon monoxide.

Greek Symbols	Definition
	Extent of reaction.
$d\xi/dt$	Rate of reaction of component mr.
	Efficiency.
η_t	Thernal efficiency, defined by Eq. IV-3.
η_{vol}	Volumetric efficiency, defined by Eq. IV-4.
$\phi(T)$	Defined by Eq. III-46.

Superscripts	
j	Denotes state-point (j), Eqs. III-47, III-49, III-50.
i	Denotes initial state, Eq. III-59.
f	Denotes final state, Eq. III-62.

Subscripts	
i	Denotes constituent in the gas mixture.
o	Denotes reference state, Eq. III-44, or property of n-Decane, Eq. III-10.
j	Denotes state-point, Eqs. III-46 to III-53.
1	Denotes state-point (1), Figure II-1.
2	Denotes state-point (2), Figure II-1.
3	Denotes state-point (3), Figure II-1.
4	Denotes state-point (4), Figure II-1.
5	Denotes state-point (5), Figure II-1.
tdc	Denotes top dead center.
bdc	Denotes bottom dead center.
net	Net amount of property.

Subscripts	Definition
comp	Compression.
exp	Expansion.
NH_3	Property for ammonia.
$C_{10}H_{22}$	Property for n-Decane.
CO_2	Property for carbon dioxide.
CO	Property for carbon monoxide.
N_2	Property for nitrogen.
O_2	Property for oxygen.
H_2O	Property for water vapor.

CHAPTER I

INTRODUCTION

Recent concern in Iceland regarding the availability of oil supplies has brought new emphasis on synthetic, nonpetroleum fuels. Since Iceland possesses few fossil energy sources and has to rely on imported oil products, finding a suitable substitute is of economic importance. The country is rich in hydropower and geothermal energy resources in relation to the size of its population of 230,000. At this time only 10% of the hydropower potential (estimated at 28 TWh/year)[1] and even less of the geothermal potential (estimated at more than 100 TWh/year) have been harnessed [1].[2] The presently available geothermal energy is utilized mostly for space heating. The presently utilized hydropower and geothermal energy constitutes nearly one-half of the energy used in the country. The remainder comes from imported oil products. Figure I-1 shows the energy flow diagram for the Icelandic economy.

At present, refined oil imports to Iceland amount to approximately 600,000 metric tons/year. Table I-1 shows how the oil products are being used within the economy [1].

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[1] TWh/year = 10^{12} Wh/year.

[2] Numbers in square brackets refer to numbers in reference list.

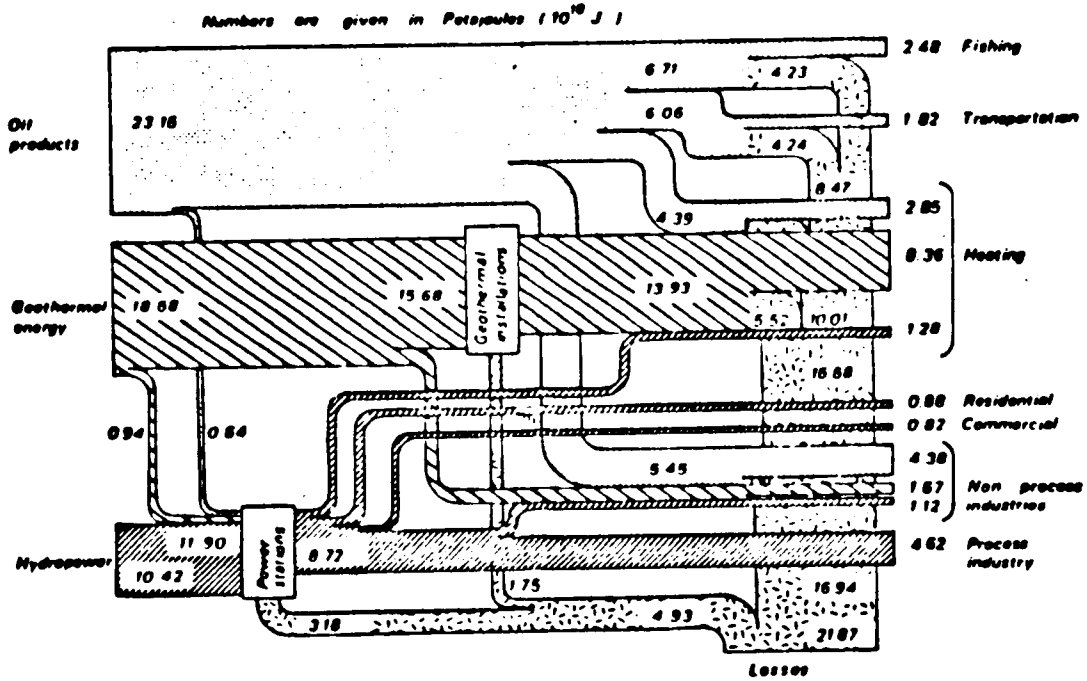


Figure I-1. Energy flow diagram for Iceland's economy.

Extracted from A. Valfells and B. Arnason, "The Role of Hydrogen in Iceland's Fuel Strategy," Science Institute, University of Iceland, Reykjavik, Iceland, 1979.

Table I-1. Present Imports of Oil Products to Iceland.

Item	%	TWh/Year
Transport	33.3	2.14
Fishing Fleet	25.0	1.61
House Heating	16.6	1.07
Industry	25.1	1.62
Total	100.0	6.44

Source: A. Valfells and B. Arnason, "The Role of Hydrogen in Iceland's Fuel Strategy," Science Institute, University of Iceland, Reykjavik, Iceland, 1979.

About 25% of the imported oil products are used by the fishing fleet. Trawlers, which account for 90,000 metric tons/year, used to be fueled by coal before it was gradually replaced by more convenient and less expensive oil. In the last 10 years more viscous (viscosity: 2.5-3.0 Engler) and less expensive oil has been used and it may be assumed that this will continue for the near future. However, the fishing boats, which presently use about 60,000 metric tons/year, are less easily converted to burn this heavier oil.

Efforts have been made to find practical alternative fuels for reciprocating engines and even though many fuels have been proposed, none of them is able to replace the hydrocarbon fuels without some penalty. In light of Iceland's unique energy situation, it appears from other studies [1,2,3,4] that among several possible fuels hydrogen and ammonia may be feasible replacements for some of the hydrocarbon fuels used in Iceland. Because of the well-known storage problem associated with hydrogen, ammonia is emerging as the promising

replacement for Iceland's hydrocarbon fuels. In light of this, it has been proposed by the Science Institute of Iceland that an extensive investigation of the possible use of ammonia be conducted.

Present Study

The present study was primarily meant as an initial investigation of the possible usage and behavior of anhydrous ammonia as a fuel in a compression ignition engine. The engine used was a Caterpillar D330 engine equipped with 4 cylinder 4.75x6.0, 425 cu in, 17.5:1 compression ratio, and precombustion chambers. See Appendix F for further details.

Of prime interest is the possible reduction in fuel-oil consumption when ammonia is fed into the engine's intake manifold. This is termed "fumigation." Also of interest was development of a computer code which could be used to predict performance parameters of engines running simultaneously on ammonia and fuel-oil.

In the course of this work it became apparent that less fuel-oil could be replaced by the ammonia than had been anticipated, the limiting factor being the tendency of the engine to knock when the amount of ammonia exceeded specific values for each load condition. Therefore, in order to obtain information about the probable causes of the engine's tendency to knock, a cylinder pressure pick-up was installed to permit measurements of the cylinder pressure trace.

Properties of Ammonia and n-Decane

Table I-2 permits a comparison between some combustion-related properties of ammonia and n-Decane (which is chosen to represent typical fuel-oil for internal combustion engines).

As shown, the heating value of fuel-oil is about 2.3 times that of ammonia. However, the stoichiometric air-fuel ratio for ammonia is 6.06:1 as compared to a much larger ratio of 15.1:1 for fuel-oil. Also, from the table, it can be concluded that for equal volumes of stoichiometric air-fuel mixture, the energy content of the ammonia-air mixture is about 80% of that obtained for fuel-oil. Note, however, that it cannot be concluded that the power output of a compression ignition engine fueled with ammonia should be about 80% of that obtained with fuel-oil as this is affected by (among other things) the differences in combustion kinetics and also on the means by which the two fuels are introduced to the engine.

There are basically three performance-related factors which have to be considered when ammonia is to be burned in reciprocating engines. They are: high minimum ignition energy; low flame speed; and narrow flammability limits.

Compared to conventional hydrocarbon fuels, ammonia is difficult to ignite. Buckley and Husa [5] reported that the minimum ignition energy was 680 mJ. Vercamph et al. [6] have shown that the ignition energy required is only 8 mJ. Furthermore, Vercamph has shown that a relatively small amount of hydrogen (4.0% by volume) reduces the required energy level to that of hydrocarbons (0.3 mJ). In addition,

Table I-2. Properties Pertinent to the Combustion of Ammonia and n-Decane.

	Ammonia	n-Decane	Data Sources
Chemical formula	NH_3	$C_{10}H_{22}$	
Density (liq) [kg/m^3]	823.6	870.6	a
Boiling point 1 atm [C]	-33.3	174.0	a
Freezing point 1 atm [C]	-77.7	-29.7	a
Vapor press. (25 C) [MN/m^3]	1.0	--	a
Heat of vaporization (20 C) [kJ/kg]	1373.0	263.0	a
Heat of combustion (lower-value-gaseous prod) [kJ/kg]	18790.0	44333.0	a,b
Stoichiom. air/fuel ratio	6.06	15.1	b,a
Stoichiom. heat release by weight [kJ/kg air]	3100.0	2930.0	
Stoichiom. heat release by volume [kJ/m^3 mixture]	2879.0	3599.0	
Octane rating-research	130+	116+	c
Minimum ignition energy 1atm; stoichiom. mixture [mJ]	680.0	0.3	e
Flammability limit % stoichiom. fuel-air ratio	75/153	52/421	e,a
Flame speed [cm/sec]	33.0	100.0	d

[a]R. E. Bolz and G. L. Tuve, Handbook of Tables for Applied Engineering Science, Boca Raton, Florida: CRC Press, Inc., 1976.

[b]W. Cornelius, L. W. Huellmantel, and H. R. Mitchell, "Ammonia as an Engine Fuel," SAE Transactions, Vol. 74, 1966, Paper 650072.

[c]T. J. Pearsall and C. G. Garbedian, "Combustion of Anhydrous Ammonia in Diesel Engines," SAE Transactions, 1967, Paper 670947.

[d]E. S. Starkman and G. S. Samuelson, "Flame-Propagation Rates in Ammonia-Air Combustion at High Pressure," 11th Symposium on Combustion, The Combustion Institute, 1967, pp. 1037-1045.

[e]F. J. Vercamph, M. C. Hardin, and J. R. Williams, "Ammonia Combustion Properties and Performance in Gas Turbine Burners," 11th Symposium on Combustion, The Combustion Institute, 1967, pp. 985-992.

there is experimental evidence [3,7] that the same ignition energy reduction can be achieved by injecting a small amount of fuel-oil into the ammonia. Another method used to promote combustion is to incorporate a spark-ignition system in the engine. Starkman [8] successfully operated a Diesel engine equipped with a relatively simple high energy spark-ignition system. In general, it can be deduced from the literature that problems associated with high ignition energy can be overcome by one or more of the methods mentioned.

Considerable differences exist between the flame speeds of the various air-fuel mixtures. For all fuels the flame speeds are low near the inflammability limits (both on the rich and the lean side) and have a maximum near the stoichiometric mixture [9]. Typical values of the flame velocity relative to the unburned mixture for many hydrocarbon fuels range between 50-150 cm/sec [9,10,11]. On the other hand, Vercamph [6] and Pearsall [3] have shown that the flame speed of ammonia (at atmospheric pressure and stoichiometric air-fuel ratio) should be expected to be lower than those for the hydrocarbons.

Klaus Bro and Sunn Pedersen [12] conducted experiments with an engine using fuel-oil as an ignition promoter and methanol, ethanol, methane, and ammonia as the main fuels. Their results revealed that the low flame speed of ammonia may be responsible for the large amount of unburned ammonia typically found in the exhaust gas. Furthermore, they state that because of the low flame speed there is reason to believe that the combustion of ammonia takes place only in

a volume confined to the pilot-fuel spray area. Therefore, since only the pilot-fuel and the ammonia within the pilot-fuel volume burn, decreased efficiency and increased emissions of unburned fuel result (the latter originating from the volume where the combustion does not reach). This effect, if true, may explain the tendency of the ammonia to knock, in spite of its high octane rating (130+) [7]. The portion of the ammonia which never gets to burn successfully gets highly compressed and may, therefore, experience erratic combustion which manifests itself in audible knock in the cylinder.

There are two types of limits generally associated with laminar flame propagation. One type governs the ability of the mixture to support flame propagation; and the other is concerned with flow conditions. The first type includes flammability limits and the quenching distance, and the second the phenomena of flash-back, blowoff, and the onset of turbulence.

If an adequate ignition source is introduced to a stoichiometric amount of fuel-oxidizer mixture the mixture spontaneously burns and, even if the source is removed, the flame propagation would continue. There are mixtures, however, which will not self-support the flame after the ignition source is removed. These mixture ratios fall in the lean and rich end of the concentration range. The leanest and the richest concentrations which will self-support a flame are called the lean and the rich flammability limits, respectively.

As can be observed from Table I-2, the flammability range of ammonia is considerably narrower than for n-Decane. This means that the ammonia-air mixture is less suited to sustain combustion once the initial ignition source is removed. In the literature there is no report of any immediate remedy for this deficiency of ammonia as a fuel. In addition, the presence of "inert" gases, such as CO_2 and N_2, acts to narrow the limit. Studies by Vercamph et al. [6] and Pearsall et al. [3,7], however, indicate that hydrogen enrichment of the ammonia-air mixture acts to widen the limit. Also, it is known [11] that the flammability limits for fuels are widened as the oxygen content of the oxidizer is increased. The influence of elevated pressure is to narrow the limits [11]. Therefore, if the possibility of hydrogen enrichment or partial dissociation of the ammonia is excluded it can be concluded that the variables that influence the width of the flammability limit can in practice not be altered. Furthermore, the influence of pressure counteracts the influence it has on the compression ignition and the ability of ammonia to work with high compression ratios. Hence, it can be concluded that this deficiency cannot be readily removed.

Another property of interest is ammonia's high heat of vaporization. The heat of vaporization of ammonia is about 4.5 times that of typical fuel-oil and since the engine consumes about 2.3 times as much ammonia by weight (for equal output of power) the ammonia-fueled engine requires about 10.4 times as much heat for vaporization than its oil-fueled counterpart. This leads to the

conclusion that it may be necessary to install a vaporizer to vaporize the ammonia before it is introduced to the engine. This problem, however, is easily solved since the cooling system of the engine provides a readily available source of energy. This high heat of vaporization can partly explain the difficulties experienced with liquid injection of ammonia to engines, since in this case the cooling effect will reduce the temperature rise after compression, thus reducing the probability of successful compression ignition.

Literature Survey

Among the first large-scale practical uses of ammonia as a fuel was the Gazamo Process [13], which utilized ammonia as a fuel for transportation vehicles in Belgium during 1943. In the Gazamo Process the engines were supplied with a mixture of ammonia vapor and coal gas. The hydrogen released from the goal gas was used to promote combustion of the ammonia. The control of proportions and flows was accomplished manually by the operator of the vehicle. This program, promoted by shortages of hydrocarbon fuels created by World War II, was terminated when the shortages were relieved.

In 1961, a U.S. Army-sponsored program was initiated at the Allison Division of General Motors Corporation [2,4] to determine if a method could be found for the indirect use of nuclear energy as a source of vehicle propulsion power. The concept conceived for this purpose was termed the "Energy Depot." One of the initial investigations was to compile the characteristics and availability of

potential fuels. The evaluation of a number of possible fuels revealed that ammonia was a promising substitute for conventional fuels. This selection was based on its ease of production, ease of handling and storage, and its safety in reciprocating engines.

During the sixties a large number of experiments were conducted, both in connection with the Energy Depot concept and as a consequence of the oil crises in 1974.

Lutra et al. [14] performed an experiment with a small, Petter AV1, diesel engine (Max bhp 6). The ammonia was evaporated outside the engine and then introduced to the engine with the intake air. Ignition was initiated by using pilot fuel. The results reveal that an overall improvement in engine performance was experienced, with a considerable increase in thermal efficiency, at all loads and speeds.

Gray et al. [15] investigated the use of both liquid and gaseous ammonia in a CFR cetan engine, but they were only able to substitute a rather modest amount of ammonia for fuel-oil. The best performance was obtained when the ammonia was injected and vaporized in a long chamber. Heating elements installed on the chamber enabled control of the vapor temperature. They also tried direct cylinder injection of liquid ammonia, using separate ammonia injectors on each cylinder. With this setup satisfactory combustion occurred. However, with this setup it was necessary to increase the compression ratio to 30 for reliable ignition. Sticking of the pintles in the ammonia injectors, due to carbon formation on the surfaces, was also

experienced and ammonium hydroxide caused lubrication problems. The study, however, revealed that material compatibility could be achieved.

Starkman et al. [8] used liquid injection of ammonia into the cylinder of a diesel engine, but a spark ignition system had to be installed. A similar experiment, conducted by Pearsall et al. [3,7], revealed that the liquid injection form of operation results in inferior performance when compared to the vapor approach with gaseous ammonia fed to the intake air and ignited with the pilot fuel. Comparisons between the performance of the pilot fuel ignition and spark ignition systems, however, revealed some advantages of the spark ignition.

As mentioned above, Bro and Pedersen [12] conducted experiments in which ammonia was used as a replacement fuel. They were successful in replacing a relatively large percentage (50-60% by heat content) of fuel-oil with ammonia by injecting a gaseous ammonia into the intake air and heating the mixture at 120 C. Ignition was provided by the pilot fuel. Within the range of relative fuel-air ratios normally employed with fuel-oils, the efficiency for the ammonia burning engine was about 15% less than when using oil. At higher ammonia fueling rates, however, the efficiency exceeded the fuel-oil efficiency. Of the four alternate fuels tested, the performance of the ammonia was judged to be the poorest, primarily because of the large amount of ammonia passing through the engine unburned.

CHAPTER II

ANALYTICAL STUDY

This part of the work is concerned with the prediction of compression ignition engine performance using ammonia as the main fuel, and n-Decane ($C_{10}H_{22}$) as the pilot fuel. The inclusion of the pilot fuel simulates the conditions in a real engine. In the real engine the pilot fuel is injected into the cylinder through the conventional fueling system and therefore does not enter the ideal operating cycle until the compression stroke is completed. On the other hand, the ammonia is introduced into the intake air, and therefore has to be considered during the intake and compression strokes.

The theoretical prediction of performance for many thermodynamic systems may be carried out with satisfactory accuracy using relatively simple approaches. However, for systems which involve transient combustion processes the analysis can be quite involved, as the following indicates.

One of the major problems associated with performance predictions of internal combustion engines is the determination of the composition and corresponding thermodynamic properties of the working fluid at different points in the cycle. A well-known problem is the determination of the amount of chemical species such as CO_2 and H_2O which will dissociate at the temperatures and pressures encountered in the cycle. Since the extent to which such dissociation

proceeds is dependent both on the temperature and the pressure of the working fluid, and since both of these variables change substantially during the cycle, the composition of the working fluid should be expected to vary also.

At the outset of a thermodynamic analysis of internal combustion engines, it is necessary to make some assumptions regarding how the working fluid composition is to be determined throughout the cycle. Thermodynamic principles state that, given enough time, any reacting fluid will come to a state of chemical equilibrium. Furthermore, given any two of the thermodynamic variables (temperature, pressure, volume, energy, etc.) and the initial composition the composition is fixed and can be calculated. A common assumption is that during the combustion process ample time is allowed for the working fluid to react in such manner that at every instant of time there exists continuous chemical equilibrium within the fluid. That is, the working fluid may be treated as an equilibrium mixture at every instant of time. In this work the "law" of conservation of matter is used along with the "second law" of thermodynamics to calculate the equilibrium composition of the working fluid. This assumption is often referred to as the "shifting equilibrium" assumption.

In addition to the necessary assumptions mentioned above, others have to be made. The combustion process actually requires time for completion. The mechanisms involved in flame propagation in the combustion chamber are complex, and thus the theoretical evaluation of the time necessary to complete combustion is outside the scope of

this work. It will be assumed that every finite change of composition occurs instantly.

Another problem which must be addressed when modeling a combustion process is that of determining the heat transfer from the working fluid to the surroundings. During one cycle of any internal combustion engine there is a net transfer of heat from the working fluid. The heat transfer is important for satisfactory operation of the engine as interior surfaces of the combustion chamber (walls, heads, and piston faces) must be maintained at safe operating temperatures. The effect of this heat transfer is to reduce the power output. In this work, however, heat transfer will be neglected. If heat transfer and finite combustion time are neglected it is to be expected that the theoretical performance will be greater than experimental data obtained from real engines; however, it is believed that the inclusion of these assumptions will still permit the model to make quantitative and qualitative evaluations of how the engine responds to changes in operating conditions. This requires that the absolute magnitude of the heat transfer and the influence of finite combustion time are weak functions of system parameters such as compression ratio and manifold pressure. In this case if real engine performance data are known for one engine, the predicted values may be corrected by scaling factors to account for the effects of heat transfer and finite combustion time, thus yielding proper values for the engine.

In this work it was desired to predict the performance of a diesel engine using both ammonia and n-Decane as its fuel. The real engine, which the model was to imitate, would operate by introducing gaseous ammonia into the intake manifold of the engine. Combustion of the mixture is then initiated by injection of a small amount of fuel-oil (pilot oil) which is injected into the engine cylinder using the original oil injection system.

Since at the outset it was assumed that the amount of the pilot oil injected would constitute only a fraction of that of the ammonia (both on weight and energy bases), it was assumed that the combustion of the mixture would more closely approach constant volume rather than constant pressure combustion.

The objective of the work here is therefore to predict the performance of an engine operated on ammonia and pilot fuel. The theoretical model employed is similar to the traditional Otto cycle, except that at the end of the compression stroke a finite amount of n-Decane is injected to the combustion chamber thereby introducing additional energy into the cycle. The combustion and the expansion events are assumed to proceed in full chemical equilibrium with the chemical composition determined by the "law" of conservation of matter and the Second Law of Thermodynamics. The effects of heat transfer and finite combustion time are neglected. Finally, because of the high temperatures reached in the combustion chamber, ideal gas behavior is assumed.

The evaluation of all thermodynamic properties used in this work is based on references 16, 17, and 18.

Theoretical Techniques Applied

The cycle used as a model for this analysis is based on the Otto cycle. In Figure II-1 P-V and T-S diagrams for the cycle are presented in their simplest forms. The cycle consists of: induction of fresh air mixed with ammonia (6-1); compression of the ammonia air mixture (1-2); introduction of pilot oil, at 2; constant volume combustion (2-3); isentropic expansion of the combustion products (3-4); opening of the exhaust valve (4-5); and, finally, expulsion of exhaust products during the exhaust stroke (5-6).

The second figure shows the temperature versus entropy relationship for the cycle.

The analysis of this cycle has been conducted using the Dec-10 digital computer. The specific analytical methods are described in more detail below.

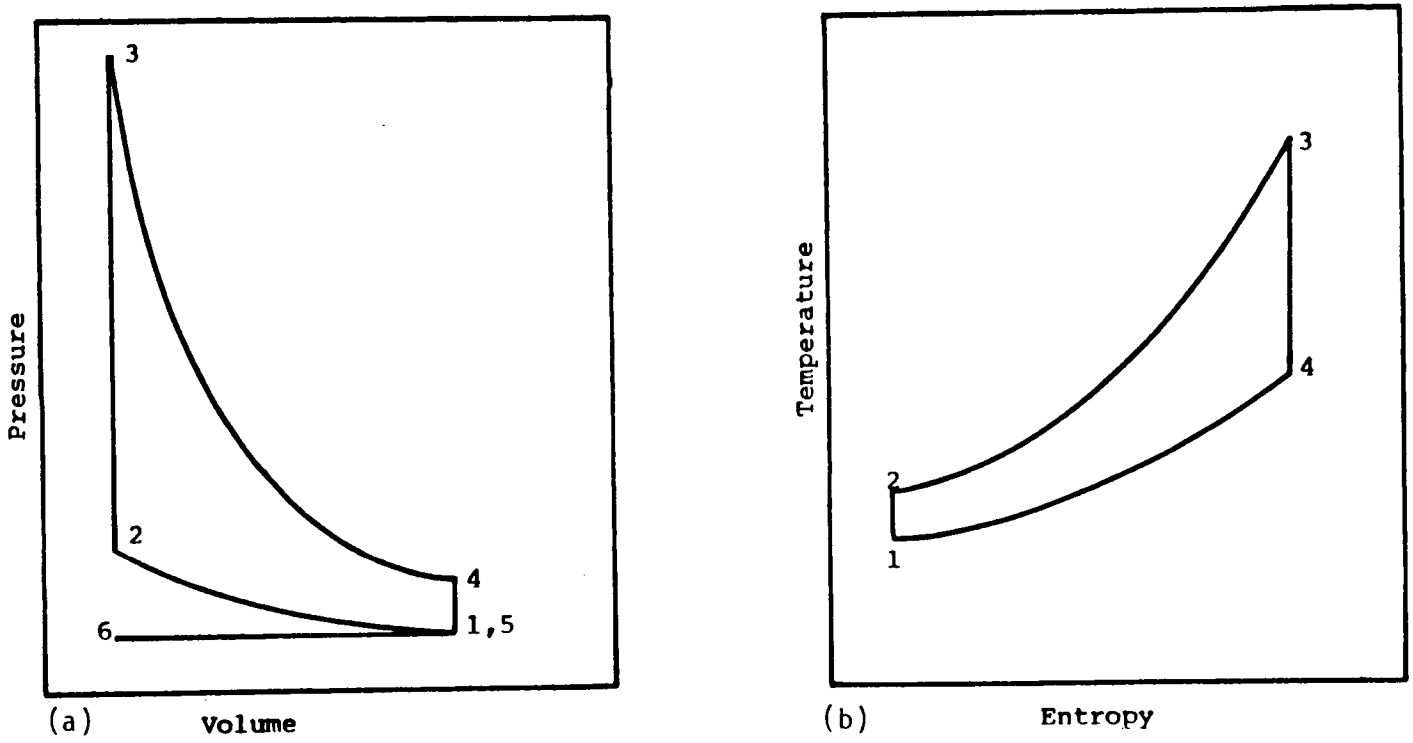


Figure II-1. The proposed combustion cycle. (a) P-V diagram; (b) T-S diagram.

CHAPTER III

THE CYCLE MODEL

The Combustion Equation

The analysis begins by examining the chemical equation which describes the combustion process. Denoting by n_a and n_o the number of moles of ammonia and pilot-oil, respectively, and by 4.76Y the number of moles of air, the equation can be written:

$$n_a NH_3 + n_o C_{10}H_{22} + Y(O_2 + 3.76N_2) \rightleftharpoons$$
$$n_1 CO_2 + n_2 CO + n_3 O_2 + n_4 O + n_5 NO + \qquad \text{(III-1)}$$
$$n_6 N_2 + n_7 H_2 + n_8 H + n_9 OH + n_{10} H_2O$$

The numerical system n_i, i = 1,2, ... , 10 has been adopted to designate the number of moles of the product gases.

The case when the stoichiometric amount of air, denoted by $4.76Y_{cc}$, oxidizes the fuel is included as a special case in this equation, i.e., only n_1, n_6 and n_{10} are different from zero.

The Compression Process

When ammonia is considered as an engine fuel careful consideration has to be given to the condition of the fuel when it enters the engine. Since ammonia has a high latent heat of vaporization and a low stoichiometric air-fuel ratio when compared with

conventional hydrocarbon fuels, the condition of the ammonia (i.e., whether it is in liquid or vapor phase) has an important influence on the performance of the engine. In this analysis, however, only the case where gaseous ammonia is introduced to the engine is considered. It is assumed that the ammonia is vaporized in a vaporizer, heated either by the cooling water of the engine or by another energy source. The temperature of the ammonia air mixture at the inlet to the cycle will be denoted by T_m.

The theoretical model employed in the analysis of the compression stroke is that of an ideal gas-mixture with constant specific heats. The initial temperature, T_1, is determined by the relative amounts of fresh mixture of ammonia and air, and the fraction, M_x, of combustion products at temperature T_5 remaining in the combustion chamber from the previous cycle. The exact values of T_5 and M_x are not known initially, so values have to be estimated to start the calculation. When the value for T_1 has been determined, the compression stroke can be evaluated. The influence of pressure on specific heats is neglected based on the ideal gas assumption. The relationship between temperature and volume for the isentropic compression of ideal gases can be used.

$$T_2 = T_1(V_1/V_2)^{(k-1)} = T_1(CR)^{(k-1)}$$

$$\text{where } k = c_p/c_v = c_p/(c_p-R) \qquad \text{(III-2)}$$

If there are M_a moles of fresh charge in the cylinder, and M_x moles

of the residual, then the specific heat of the fluid in the cylinder can be evaluated as follows.

$$c_p(T_1) = (M_a c_{p_1} + M_x c_{p_2})/(M_a + M_x) \qquad \text{(III-3)}$$

where c_{p_1} is the molar specific heat of the fresh ammonia air mixture, and c_{p_2} is the molar specific heat of the fresh ammonia air mixture, and c_{p_2} is the molar specific heat for the residual, all evaluated at T_1. The value for c_{p_1} can be evaluated as follows:

$$c_{p_1} = (n_a c_{P_{NH_3}} + Y c_{p_{O_2}} + 3.76 c_{P_{N_2}})/(n_a + 4.76Y) \qquad \text{(III-4)}$$

The composition of the residual has to be known in order to calculate the value of c_{p_2}. Therefore, the following assumptions were made. Based on the relatively low temperature at state-point (1), it is assumed that the gases will not experience any dissociation. Further, in order to simplify the calculations, it is assumed that the residual gases will not contain NH_3. Since the residual gases only account for about 2% of the total volume in the combustion chamber it is expected that these two simplifying assumptions do not affect the results to any great extent. Under this assumption the composition of the residual gases can be determined by a simple mole balance and the species which have to be considered are dependent on the number of moles of oxygen present in Eq. III-1. Therefore, if the number of moles of oxygen, Y, is larger than necessary to oxidize all the fuel

to CO_2, H_2O and N_2, the excess oxygen will appear in the residual. In this case the value of c_{p_2} is calculated as follows:

$$c_{p_2} = (10n_o c_{p_{CO_2}} + (Y-Y_{cc})c_{p_{O_2}} + (11n_o + 3/2n_a)c_{p_{H_2O}} + (3.76Y + n_a/2) + (3.76Y + n_a/2)c_{p_{N_2}})/N_{po} \quad \text{(III-5)}$$

$$\text{where } N_{po} = (10n_o + (Y-Y_{cc}) + (11n_o + 3/2n_a) + (3.76Y + n_a/2)$$

On the other hand, if the number of moles of oxygen is lower than necessary to convert all the carbon moles to CO_2 the residual gas will be assumed to consist of CO_2, CO, H_2O and N_2. The value of c_{p_2} in this case will be evaluated as follows:

$$c_{p_2} = (2(Y-Y_{min})c_{p_{CO_2}} + 2(Y_{cc} - Y)c_{p_{CO}} + (11n_o + 3/2n_a)c_{p_{H_2O}} + (3.76Y + n_a/2)c_{p_{N_2}})/N_{po} \quad \text{(III-6)}$$

$$\text{where } N_{po} = (2(Y-Y_{min}) + 2(Y_{cc} - Y) + (11n_o + 3/2n_a) + (3.76Y + n_a/2))$$

In the last equation (III-6), Y_{min} denotes the minimum number of moles of oxygen necessary to convert all the carbon to carbon monoxide.

$$Y_{min} = Y_{cc} - 5n_o = 5n_o + (22n_o + 3n_a)/4 \quad \text{(III-7)}$$

It was noted during the construction of the program that only minor changes in results were experienced if the compression stroke were divided into a number of smaller steps, and the above relationships were used to evaluate c_p at the prevailing temperature for each step. Therefore, in order to decrease the actual computation time, the one step approach was used.

The Combustion Process

The combustion process is initiated by the introduction of a specific amount of pilot fuel to the combustion chamber. Since the energy content of this fuel may constitute a significant part of the total internal energy of the mixture, it would give erroneous results if it were neglected. Contrary to the conventional Otto cycle in which the ignition energy of the spark is commonly neglected, the pilot fuel contribution to the total chemical energy of the system has to be included in the calculations for this cycle. In this work, it is assumed that the pilot fuel enters the combustion chamber at a fixed temperature (490 K). It should be noted that although a specific temperature was chosen, the particular value is not considered important in terms of the total energy of the pilot charge.

After the pilot fuel has entered the combustion chamber, the combustion of the fuel is assumed to occur instantly at constant volume. This assumption is made since it seems reasonable to assume that constant pressure control of the cycle is impossible with presumably most of the fuel present in the cylinder at the outset of combustion.

For constant volume adiabatic combustion from state-point (2) to point (3), the equations describing the process are:

$$dU = 0 \tag{III-8}$$

$$dV = 0 \tag{III-9}$$

The two equations (III-8 and III-9), together with knowledge of the composition at state-point (2), completely determine the composition and properties of the products at state-point (3).

Integrating the energy equation (III-8) between state-points (2) and (3) gives:

$$U_2(T_2,V_2) = U_a(T_2) + U_o(T_f) + U_{air}(T_2) + U_r(T_2) = U_3(T_3,V_3=V_2) \tag{III-10}$$

where U_a denotes the contribution of ammonia to the total internal energy of the mixture, and U_o, U_{air}, and U_r denote the contributions from oil, air, and residual gases, respectively.

Just after compression, all the necessary properties at state-point (2) (the temperature T_2, V_2 and composition) have been calculated, or are assumed known, so calculation of the total internal energy of the working fluid (U_2) at state-point (2) is possible.

The working fluid present is composed of ammonia, air and residual from the previous cycle. Based on the relatively low temperature at state-point (2), it is assumed that the residual gases will not experience any dissociation at the prevailing temperature.

Therefore, the composition of the gases can be determined by a simple mole balance. Under this assumption the composition of the residual gases is determined by the number of moles of oxygen present in Eq. III-1. If the number of moles of oxygen Y are larger than necessary to oxidize all the fuel to CO_2, H_2O and N_2 the excess oxygen will appear in the residual. On the other hand, if the number of moles of oxygen is lower than necessary to convert all the carbon moles to CO_2, the residual gas will be assumed to consist of CO_2, CO, H_2O and N_2. With the mole fractions of each constituent available from the governing equation (III-1), U_2 can now be evaluated.

Each of the terms in Eq. III-10 will now be treated in more detail, beginning with the term for ammonia.

The enthalpy value of the ammonia is first evaluated at T = 298.15 K using the definition of the heat of reaction at constant pressure.

$$H_{rp} = H_p(298.16) - H_r(298.16) \qquad \text{(III-11)}$$

From the stoichiometric equation governing the combustion of ammonia,

$$NH_3 + 0.75\ O_2 \rightarrow 1.5\ H_2O + 0.5\ N_2 \qquad \text{(III-12)}$$

the two terms on the right side of Eq. III-11 can be written:

$$H_p(298.16) = 1.5h_{H_2O} + 0.5h_{N_2} \qquad \text{(III-13)}$$

$$H_r(298.16) = h_{NH_3} + 0.75h_{O_2} \qquad \text{(III-14)}$$

Substituting these results into Eq. III-11 yields:

$$H_{rp_{NH_3}}(\text{gas},dp=0) = 1.5h_{H_2O} + 0.5h_{N_2} - h_{NH_3} - 0.75h_{O_2} \qquad \text{(III-15)}$$

In these last equations $H_{rp_{NH_3}}$ denotes the heat of reaction for ammonia; h_{H_2O}, h_{N_2} and h_{O_2} the enthalpy values at 298.16 K of gaseous water, nitrogen and oxygen.

The last expression, III-15, can be manipulated to yield the enthalpy value for ammonia at 298.16 K.

$$h_{NH_3} = - H_{rp_{NH_3}} + 1.5h_{H_2O} + 0.5h_{N_2} - 0.75h_{O_2} \qquad \text{(III-16)}$$

In order to evaluate the internal energy of the ammonia, use was made of the relationships

$$h - u = R\,T \qquad \text{(III-17)}$$

Thus,

$$u_{NH_3}(298.16) = h_{NH_3}(298.16) - 298.16\,R \qquad \text{(III-18)}$$

In order to evaluate the internal energy value at T_2, the following relationships were used:

$$h_i(T_2) - h_i(298.16) = \int_{298.16}^{T_2} c_{pi}(t)\,dt \qquad \text{(III-19)}$$

For the purpose of this work the specific heat values were formulated as linear functions of temperature, i.e.,

$$c_{p_i}(T) = a_i + b_i T \qquad \text{(III-20)}$$

where the constants a_i and b_i were determined for each species (see Appendix D, Table D-2). Substituting these results into Eq. III-19 gives:

$$h_{NH_3}(T_2) - h_{NH_3}(298.16) = a_{NH_3}(T_2 - 298.16) + \frac{1}{2} b_{NH_3}(T_2^2 - 298.16^2) \qquad \text{(III-21)}$$

or, if use is made of III-17,

$$u_{NH_3}(T_2) = h_{NH_3}(T_2) - h_{NH_3}(298.16) - R(T_2 - 298.16) + u_{NH_3}(298.16)$$

In order to evaluate the internal energy of the n-Decane an approach is used similar to that used for ammonia. However, since the n-Decane enters the combustion volume in liquid form property values for the liquid phase should be used. It is also assumed that the liquid n-Decane behaves as an incompressible fluid.

Based on the stoichiometric combustion of $C_{10}H_{22}$

$$C_{10}H_{22} + 15.5\ O_2 \rightarrow 10\ CO_2 + 11\ H_2O \qquad \text{(III-22)}$$

the two terms on the right hand side of Eq. III-11 can now be written.

$$H_p(298.16) - 10h_{CO_2} + 11h_{H_2O} \qquad \text{(III-23)}$$

$$H_r(298.16) = h_{C_{10}H_{22}} + 15.5h_{O_2} \qquad \text{(III-24)}$$

The expressions for H_{rp} of $C_{10}H_{22}$, and the enthalpy, now become:

$$H_{rp_{C_{10}H_{22}}}(liq,dp=0) = 10h_{CO_2} + 11h_{H_2O} - 15.5h_{O_2} - h_{C_{10}H_{22}} \qquad \text{(III-25)}$$

or

$$h_{C_{10}H_{22}} = - H_{rp_{C_{10}H_{22}}} + 10h_{CO_2} + 11h_{H_2O} - 15.5h_{O_2}$$

The internal energy of liquid n-Decane becomes:

$$u_{C_{10}H_{22}}(298.16) = h_{C_{10}H_{22}}(298.16) - Pv \qquad \text{(III-26)}$$

The last term on the right is assumed to be negligible, based on the specific volume of the fluid, therefore the expression for the internal energy becomes

$$u_{C_{10}H_{22}}(298.16) = h_{C_{10}H_{22}}(298.16) \qquad \text{(III-27)}$$

In order to evaluate the internal energy value at T_f, the same numerical procedure is used as before. However, keeping in mind that the n-Decane is behaving as an incompressible liquid it is not necessary to distinguish between c_p and c_v, and therefore the symbol c

is used to represent both. Consequently, the internal energy of the n-Decane, at T_f, can be evaluated from:

$$h_{C_{10}H_{22}}(T_f) - h_{C_{10}H_{22}}(298.16) = \int_{298.16}^{T_f} c(T)dT \qquad \text{(III-28)}$$

Since the specific heats of liquids are relatively weak functions of temperature and pressure [16], it is assumed that the specific heat of n-Decane is constant. Therefore, Eq. III-28 becomes

$$u_{C_{10}H_{22}}(T_f) - u_{C_{10}H_{22}}(298.16) - c(T_f - 298.16) \qquad \text{(III-29)}$$

References [9] and [17] give c = 314. [kJ/kmol K]. Substituting into Eq. III-29 yields:

$$u_{C_{10}H_{22}}(T_f) = 313.822(T_f - 298.16) + u_{C_{10}H_{22}}(298.16) \qquad \text{(III-30)}$$

Note should be made that it is through this last equation that the influence of the entrance temperature of the pilot-oil, T_f, enters into the calculations.

As mentioned before, it was assumed that the residual gases consisted of either CO_2, O_2, H_2O and N_2 or CO_2, CO, H_2O and N_2, depending on the amount of oxygen. For the case when the number of moles of oxygen is larger than necessary to convert all the carbon to CO_2, the internal energy of the mixture can be evaluated as follows:

$$u_r(T_2) = (10n_o u_{CO_2} + (Y-Y_{cc})u_{O_2} + (11n_o + 3/2n_a)u_{H_2O} + (3.76Y + n_a/2)u_{N_2})/N_{po} \quad \text{(III-31)}$$

where $N_{po} = (10n_o + (Y-Y_{cc}) + (11n_o + 3/2n_a) + (3.76Y + n_a/2))$

On the other hand, if the number of moles of oxygen is lower than necessary to convert all the carbon to CO_2, the residual gas will be assumed to consist of CO_2, CO, H_2O and N_2 and the internal energy in this case is evaluated as follows:

$$u_r(T_2) = (2(Y-Y_{min})u_{CO_2} + 2(Y_{cc}-Y)u_{CO} + (11n_o + 3/2n_a)u_{H_2O} + (3.76Y + n_a/2)u_{N_2})/N_{po} \quad \text{(III-32)}$$

where $N_{po} = (2(Y-Y_{min}) + 2(Y_{cc}-Y) + (11n_o + 3/2n_a) + 3.76Y + n_a/2))$

where Y_{min} is defined by III-7.

The mole numbers, n_i, are available from the governing chemical equation (III-1).

At this point it is convenient to regroup the different energy terms and define the internal energy of the ammonia-air mixture per mole of the mixture.

$$u_{a\text{-}air} = (n_a u_{NH_3} + Yu_{O_2} + 3.76u_{N_2})/(n_a + 4.76Y) \quad \text{(III-33)}$$

Assuming that there are M_a number of moles of ammonia-air mixture, and M_x moles of residual in the combustion chamber at the

end of compression, the total number of moles of ammonia, air and pilot-oil will be given by M_t:

$$M_t = M_a\left(1 + \frac{n_o}{(n_a + n_o + 4.76Y)}\right) \qquad \text{(III-34)}$$

where n_o, n_a and Y are mole numbers from the combustion equation (III-1). The internal energy content of the mixture at state-point (2) is then given by

$$U_2(T_2,V_2) = M_t((n_a + 4.76Y)u_{a\text{-}air} + n_o u_{C_{10}H_{22}})/(n_a + n_o + 4.76Y) + M_x u_r \qquad \text{(III-35)}$$

At the outset a value for M_x is assumed, and the value for M_t can be estimated from the ideal gas law, i.e.,

$$M_t = (P_1\ V_{bdc})/(R\ T_m) \ \ldots \text{ first estimate} \qquad \text{(III-36)}$$

After analyzing one cycle, the values of M_t and M_x can be re-evaluated. The values are then compared to those from the previous cycle and calculations halted when acceptable agreement is obtained.

In order to evaluate the internal energy of the product gases U_3, the composition and the temperature at state-point (3) have to be known. Based on the ideal gas assumption, knowledge of these two variables is enough to fix the internal energy.

The equilibrium composition of the combustion products was formulated as a function of two conditions: volume and temperature,

i.e., $n_i = f(V,T)$, to be explained in Chapter VI. Also, the internal energy of each species was formulated to be given as a function of temperature (see Appendix D). With the functional relationship of U and n_i on T known, the iteration for T_3 can be performed.

As mentioned before, iteration is necessary to produce the solution. The method employed in this work was as follows: In accordance with Eq. III-9, the constant volume condition $V_2 = V_3$ was imposed on the system. A bisection algorithm was then employed to iterate for the value of $T = T_3$, which satisfied Eq. III-10. Flow diagrams of the algorithm are presented in Appendix B.

Both the evaluation of the equilibrium composition (Chapter VI) and the property values (Appendix D) are treated in greater detail below.

After the value of T_3 has been found the corresponding pressure is calculated by:

$$P_3 = P_2(T_3/T_2)N_{tp}\left(\frac{C_m}{M_t + M_x}\right); \qquad \text{(III-37)}$$

where

$$N_{tp} = \sum_{i=1}^{10} n_i; \quad C_m = \left(\frac{M_t}{n_a + 4.76Y}\right) + \left(\frac{M_x}{N_{tp}}\right)$$

The Expansion

With the state at the end of combustion known, calculations of the expansion process and the mechanical work can be performed. It is assumed that the expansion is isentropic.

It is reasonable to assume that during expansion, when cooling of the product gases is experienced, some changes in the composition will also be experienced. The extent to which this process will occur is not very easily determined. In this work two different cases were considered.

If it is assumed that at the end of combustion the products are in chemical equilibrium, two different extreme cases during expansion can be considered. When the volume of the combustion chamber is varied at a finite rate, the system will adjust to the new conditions by performing an irreversible process, resulting in not only time dependent changes of thermodynamic variables, but also spatial gradients, created by the movement of the piston throughout the volume of the system. A detailed description of the process, therefore, requires the application of equations outside the scope of this work. However, assuming that the influence of the spatial gradient can be neglected, the process can be modeled as reversible.

Even with this idealization only two extreme cases can be analyzed effectively. However, it is felt that these extreme cases bracket the actual process in the cylinder. The two extreme cases are characterized by the relation of the time rate of change of the extent of reaction, defined by Eq. III-38 to the rate of change of volume (dV/dt), i.e., the rate with which product gases are being formed to the rate with which the volume of the combustion chamber is changed during the expansion stroke.

$$-dm_r/N_r = dm_p/N_p = d\xi \qquad \text{(III-38)}$$

In this last equation, dm_r and dm_p are differential changes in reacting and product species, respectively, and N_r and N_p are stoichiometric numbers. Note that the number of the extent of reaction parameters is equal to the number of equations governing the dissociation. However, the following argument applies equally well to each of them. In one extreme it is postulated that

$$d\xi/dt >> dT/dt; \quad d\xi/dt >> dP/dt \tag{III-39}$$

Here the rate of reaction is assumed to be so fast that the system remains in equilibrium at every instant of time. This case is referred to as the shifting equilibrium case. The other extreme is the case when

$$d\xi/dt << dT/dt; \quad d\xi/dt << dV/dt \tag{III-40}$$

Now the external changes occur so fast that the composition of the system remains fixed. Thus during the change in volume, the system responds as if it were in a state of constrained equilibrium. This case is referred to as the frozen composition case. However, for the particular case of modeling a combustion engine cycle the chemical relaxation is not allowed enough time, nor does the shifting of the equilibrium occur fast enough to reach this equilibrium state. Therefore, it is likely that these two cases will bracket the actual cycle.

It is interesting to estimate the influence of these two cases on the performance parameters of the engine. It is recognized that

the shifting equilibrium case will tend to over-estimate the performance figures for the cycle. This can easily be seen if one considers the dissociation equations governing the process. Since all of these equations are endothermic, dissociation results in reduced pressures and temperatures. If recombination were allowed to occur during the expansion, part of the energy which was spent during dissociation would be returned, raising the pressure and temperature; thus, increased mechanical work would result. The frozen composition case, on the other hand, does not include this effect.

Based on these assumptions, the properties of the working fluid at state-point (4) can be determined as follows: The governing equations during expansion are

$$dS = 0 \tag{III-41}$$

$$\Delta V = \text{Specified} \tag{III-42}$$

The differential change in entropy of an ideal gas can be written:

$$ds = c_p dT/T - RdP/P \tag{III-43}$$

It is now desirable to integrate this equation from some reference state, denoted by subscript o, to some other state, denoted by superscript j. From the Gibbs-Dalton Law for ideal gases, each constituent of a mixture of ideal gases behaves as though it exists alone at the temperature and volume of the mixture. Thus, in a gas mixture an ideal gas exerts its partial pressure on the surroundings.

Therefore, the change in entropy of each of the reacting gases between the two states can be found to be

$$(\Delta s_o^j)_i = \left(\int_{T_o}^{T_j} c_p dT/T\right)_i + R \ln(p_{j,i}/P_o) \qquad \text{(III-44)}$$

The integral

$$\int_{T_o}^{T_j} c_p dT/T \qquad \text{(III-45)}$$

will be denoted by

$$\phi(T_j) - \phi(T_o) \qquad \text{(III-46)}$$

Substituting this into Eq. III-44 results in

$$(\Delta s_o^j)_i = (\phi(T_j) - \phi(T_o))_i - R \ln(p_{j,i}/P_o) \qquad \text{(III-47)}$$

where p_i is the partial pressure of the constituent i. The last term, on the right side, accounts for the pressure contribution to the entropy. The dependency of this equation on knowledge of partial pressure, p_i, is transformed to knowledge of the thermodynamic pressure, P_j, of the mixture at state-point j by the equation

$$p_i = n_{i,j} P_j / N t_p \qquad \text{(III-48)}$$

In this last equation the second index on $n_{i,j}$, j, denotes the

state-point (j) where $n_{i,j}$ is to be evaluated; and, Nt_j denotes the total number of moles of the mixture. Substituting this into Eq. III-47 gives

$$(\Delta s_o^j)_i = (\phi(T_j) - \phi(T_o))_i - R \ln(n_{i,j}P/P_o Nt_p) \qquad \text{(III-49)}$$

Due to the fact that the calculations involve chemical reactions, the absolute entropy of the gases must be used. If the $\phi(T_o)$ is defined to be the absolute entropy at the reference base T_o and P_o = 1 atm, the absolute entropy of constituent i at some other temperature, T_j, and pressure, P_j, can be calculated from

$$s_i(T_j,P_j) = s_i(T_o,P_o) + (\Delta s_o^j)_i \qquad \text{(III-50)}$$

where $s_i(T_o,P_o)$ denotes the absolute entropy of the gas at the reference state T_o and P_o. The absolute entropy for any gas at temperature T_j and P_j now becomes:

$$s_i(T_j,P_j) = s_i(T_o,P_o) - (\phi(T_o) - R\ln(P_o)) + (\phi(T_j) - R\ln(n_{i,j}P_j/Nt_p) \qquad \text{(III-51)}$$

Most thermodynamic tables fix P_o at 1 atm, thus making $s_i(T_o,P_o) = \phi(T_o)$. With this convention, the absolute entropy of the gas then becomes

$$s_i(T_j,P_j) = \phi(T_j)_i - R\ln(n_{i,j}P_j/Nt_p) \qquad \text{(III-52)}$$

The entropy change for a mixture of 10 components between two states (T_3,P_3) and (T_4,P_4) can now be evaluated from Eq. III-52 to be

$$S_3 - S_4 = \sum_{i=1}^{10} (n_{i,3}\phi(T_3) - n_{i,4}\phi(T_4)_i$$

$$- n_{i,3}R \ln(n_{i,3}P_3/Nt_{p3}) + n_{i,4} R \ln(n_{i,4}P_4/Nt_{p4} \qquad \text{(III-53)}$$

This equation is valid for both constant and variable composition during expansion. For the frozen composition case the pressure term simplifies, since $Nt_{p3} = Nt_{p4}$, and the equation reads

$$S(T_3,P_3) - S(T_4,P_4) = \sum_{i=1}^{10} n_i(\phi(T_3)_i - \phi(T_4)_i - R \ln(P_3/P_4)) \qquad \text{(III-54)}$$

The temperature T_4 which equates Eq. III-53 to zero corresponds to the temperature after the assumed adiabatic and reversible process.

Here again, it is necessary to iterate for the solution. In this case, as before, a bisection algorithm was employed. Figure B-1 (Appendix B) presents a flowchart of the algorithm.

Blow-Down

After the expansion is completed, the total pressure of the gases in the cylinder remains at a pressure which is higher than the exhaust manifold pressure. Therefore, to evaluate the temperature that exists after the exhaust valve has opened, and the pressure in the combustion chamber has reached that of the manifold, it is assumed

that the gases that remain in the cylinder expand isentropically down to a temperature value T_5, and pressure $P_m = P_1$. The equations governing this process are therefore identical to those of III-41 and III-42, and are given here again as Eqs. III-55 and III-56:

$$dS = 0 \qquad \text{(III-55)}$$

$$\Delta P = \text{Specified} \qquad \text{(III-56)}$$

For the relatively lower temperature at state-points (4) and (5), dependence of the specific heat on temperature can be neglected without significant error. The relationship between pressure and temperature for a mixture of ideal gases at the same entropy can therefore be used. Thus, Eq. III-55 becomes:

$$T_5 = T_4(P_5/P_4)^{(k-1)/k} = T_4(P_1/P_4)^{(k-1)/k};\ k = c_p/c_v \qquad \text{(III-57)}$$

Evaluation of T_1

As the piston moves through the exhaust stroke, and begins the intake stroke, a fraction of the combustion products remains in the combustion chamber. This fraction is given by the expression

$$M_x = (P_1\ V_{tdc})/(R\ T_5) \qquad \text{(III-58)}$$

Note, however, that if the engine were equipped with supercharger and valve overlap the residual would be negligible as the fresh charge would blow the residual out of the cylinder.

As mentioned before, it was necessary to assume at the outset a value for both T_1 and M_x. The assumed values can now be compared to those calculated and adjusted accordingly.

Values for T_1 and M_x can now be calculated as follows. Consider Figure III-1a. When the piston moves from V_{bdc} to V_{tdc} most of the exhaust gases are evacuated from the cylinder.

As the exhaust valve closes, the intake valve opens, and a new charge is drawn into the cylinder as the piston moves "slowly" to V_{bdc}. The number of moles of fresh charge of ammonia-air mixture drawn into the cylinder is denoted by M_a. After mixing with the residual gases, the temperature in the cylinder will be T_1. The fuel mixture that will be drawn into the cylinder initially occupies volume V_m in the intake pipe (see Figure III-1b). Placing a control volume around $M_a + M_x$, moles of mixture as shown, the initial internal energy of the control mass is given by

$$U_{cm}^{i} = M_x u_p(T_5) + M_a((n_a u_a(T_m) + Y u_{O_2}(T_m) + 3.76 Y u_{N_2}(T_m))/(n_a + 4.76Y)) \tag{III-59}$$

As the piston moves through the length of the stroke, work amounting to

$$W_s = P_1(V_{bdc} - V_{tdc}) \tag{III-60}$$

will be done by the gases in the cylinder, while work amounting to

$$W_{cm} = P_1 V_m \tag{III-61}$$

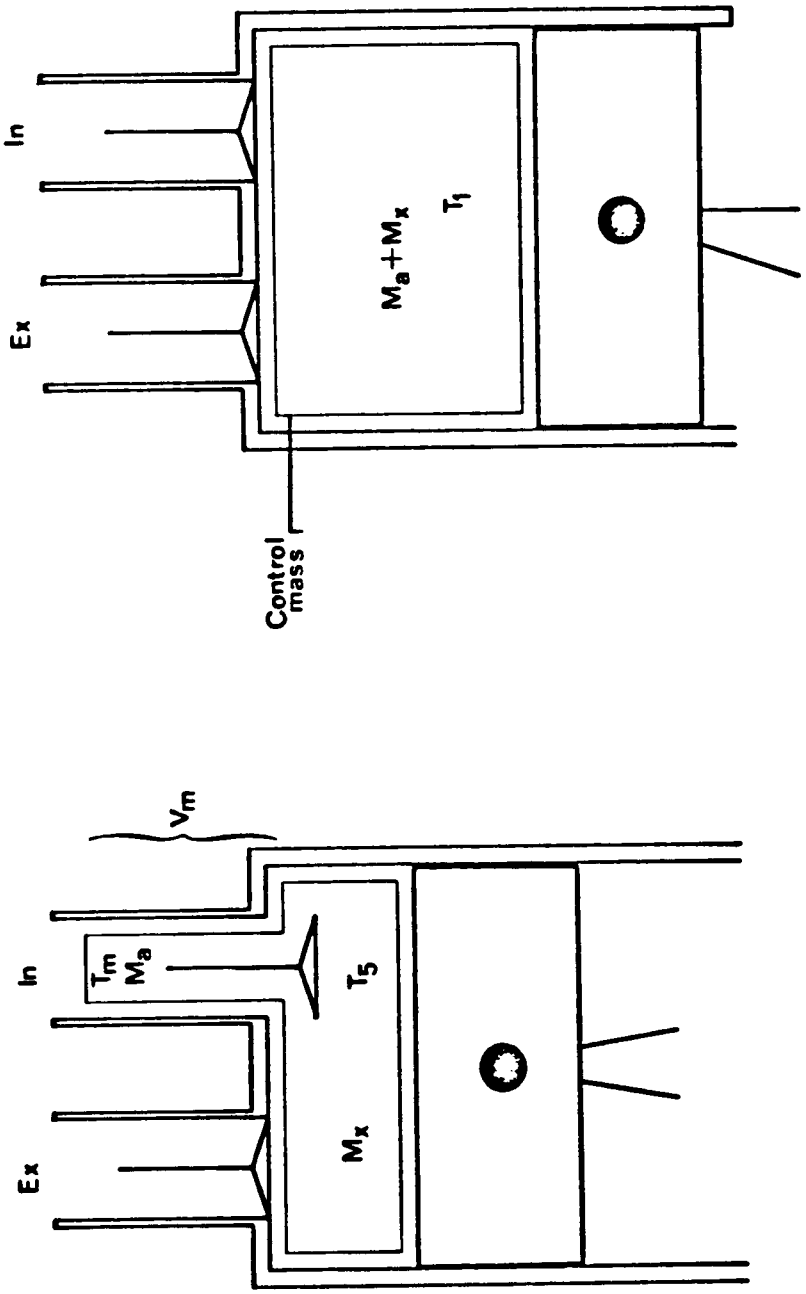


Figure III-1. Control volume for calculation of T_1.

is done on the control mass by the ammonia-air mixture behind M_a. At the V_{bdc} the energy in the control mass has now changed to

$$U_{cm}^f = M_x u_p(T_1) + M_a((n_a u_a(T_1) + Y u_{O_2}(T_1) + 3.76 Y u_{N_2}(T_1))/(n_a + 4.76Y)) \quad \text{(III-62)}$$

Combining these four equations yields

$$U_{cm}^f = U_{cm}^i + W_s + W_{cm} \quad \text{(III-63)}$$

Substituting and rearranging equations yields

$$M_x h_p(T_5) + M_a((n_a h_a(T_m) + Y h_{O_2}(T_m) + 3.76 Y h_{N_2}(T_m))/(n_a + 4.76Y))$$
$$= M_x h_p(T_1) + M_a((n_a h_a(T_1) + Y h_{O_2}(T_1) + 3.76 Y h_{N_2}(T_1))/(n_a + 4.76Y)) \quad \text{(III-64)}$$

In this last equation use has been made of the relationship $dh = du + d(pv)$.

Further, making use of the ideal gas relationship $h = c_p T$, and noting that

$$M_a = \frac{P_1 V_{bdc}}{R T_1} - M_x \quad \text{(III-65)}$$

the energy equation reduces to

$$\left(\frac{c_{pp}}{c_{pm}} - 1\right) \frac{T_1^2}{T_m T_5} + \left(CR + \frac{T_m}{T_5} - \frac{c_{pp}}{c_{pm}}\right) \frac{T_1}{T_5} - CR = 0 \quad \text{(III-66)}$$

where c_{pm} is the constant pressure heat capacity of the ammonia-air mixture, and c_{pp} that of the residue gases. This equation is quadratic in T_1, and therefore possesses two solutions. One solution can be disposed as being physically unrealistic. The usable solution is:

$$T_1 = \frac{B + (B^2 - 4AC)^{1/2}}{2A} \qquad \text{(III-67)}$$

where

$$A = (\frac{c_{pp}}{c_{pm}} - 1)/(T_m T_5); \; B = -(CR + \frac{T_m}{T_5} - \frac{c_{pp}}{c_{pm}})/T_m; \; C = -CR$$

With the value of T_1 available, the number of moles of the new charge can now be calculated as

$$M_a = (P_1 \; V_{bdc})/(R \; T_1) - M_x \qquad \text{(III-68)}$$

where M_x is calculated as in Eq. III-58.

To summarize, all the tools are now available to calculate the thermodynamic properties at each state-point on the cycle. From a knowledge of the composition and temperature at state-point (1) the value of T_2 and hence $U_2(T_2)$ can be calculated. The pressure, P_2, at state-point (2) is also readily calculated from the ideal gas relationship. In order to evaluate T_3 knowledge of the composition of the product gases at state-point (3) is needed.

Chapter VI contains an account of the analytical formulation of the problem. With the composition at state-point (3) known, the value of T_3 which equates $U_2(T_2)$ to $U_3(T_3)$ can be found. Then the

values of T_4 and P_4 can be evaluated using the assumption of reversible isentropic expansion from the thermodynamic conditions T_3 and P_3 to T_4 and $V_4 = CR\ V_3$. In this work, Eq. III-52 was employed to iterate for the temperature T_4. The value of T_5 is then evaluated using Eq. III-56.

Since no prior knowledge of T_1 is available, a value for T_1 has to be assumed to start the calculations. After one iteration with this assumed value, more accurate values are produced using Eq. III-67.

The entire process is then repeated until satisfactory agreement has been achieved between consecutive iterations.

In this work it was found that only few iterations were required for changes of less than 1% in the calculated properties. In general, good stability of the program was experienced.

CHAPTER IV

CYCLE PERFORMANCE

When pertinent properties are known at each of the state-points, the calculation of various cycle performance parameters can be done. The first one to be considered is the predicted work output of the cycle.

Work Output

The work output from the cycle is readily calculated by this expression:

$$W_{net} = W_{exp} - W_{comp} = (U_3 - U_4) - (U_2 - U_1) \qquad \text{(IV-1)}$$

where W_{comp} is the compression work of the cycle and W_{exp} is the expansion work. It should be noted that this expression evaluates the indicated work performed by the cycle, but not the work obtainable from the engine's output shaft (the so-called "brake work").

Mean Effective Pressure

The mean effective pressure of the cycle measures the output of the cycle per unit volume of cylinder displacement, and is given by the equation:

$$IMEP = W_{net}/(V_{bdc} - V_{tdc}) \qquad \text{(IV-2)}$$

Thermal Efficiency

The thermal efficiency is defined as that fraction of the total heating value of the fuel which is released as useful work. For this work this expression was used:

$$\eta_t = \frac{W_{net}}{m_a U_{rp_a} + m_o U_{rp_o}} \qquad \text{(IV-3)}$$

where m_a is the mass of ammonia, and m_o the mass of n-Decane in the cylinder during combustion.

The Volumetric Efficiency

The volumetric efficiency is a pertinent parameter in this study. Volumetric efficiency is defined as the ratio of the mass of air inducted to the cylinder to that mass which would exist at V_{disp} at atmospheric conditions.

$$\eta_{vol} = \frac{M_a}{\left(\frac{V_{disp} P_{atm}}{R T_{atm}}\right)} \left(\frac{Y}{n_a + 4.76Y}\right) \qquad \text{(IV-4)}$$

The role that the presence of ammonia in the mixture plays in this parameter is obvious.

Specific Fuel Consumption

The specific fuel consumption is a comparative parameter that indicates the efficiency with which the engine converts the fuel to

work. The parameter is intensive in nature and can therefore be used to compare performance of two different engines. For this work the following expression was used for each fuel:

$$ISFC_a = \left(\frac{n_a}{n_a + n_o + 4.76Y}\right)\left(\frac{M_a + M_x}{W_{net}}\right)17.03 \qquad \text{(IV-5)}$$

$$ISFC_o = \left(\frac{n_o}{n_a + n_o + 4.76Y}\right)\left(\frac{M_a + M_x}{W_{net}}\right)142.0 \qquad \text{(IV-6)}$$

CHAPTER V

THEORETICAL RESULTS

In order to simplify the presentation of the theoretical results it is necessary to fix a number of the thermodynamic variables, some of which may have considerable influence on the performance parameters of the model. For instance, the temperature of the pilot-oil may have considerable influence on the results. The general behavior of this influence should be clear from Eq. III-28. From that equation, it can be concluded that, for realistic temperatures of the pilot-oil, increasing the temperature of the pilot-oil should result in increased power, higher temperature, and also a higher pressure in the cylinder. However, the effect of this parameter is negligibly small; and, it was decided to fix this parameter at 490 K, which is thought to be representative for real engines.

Another parameter which could be considered is the manifold temperature (or the inlet temperature) of the ammonia-air mixture. The effects of this parameter should be similar to those of the pilot-oil temperature. However, the results reveal that the engine performance is less sensitive to manifold temperature. It was decided to fix this value at 300 K.

The third parameter which had to be fixed is the manifold pressure. In this work the value was fixed as 1 atm, which means

that the model is strictly valid only for naturally aspirated engines at wide open throttle or supercharged engines at very low manifold boost pressures.

The results, to be found in Chapter V, are presented for each dependent variable in two different formats. The first format is a set of four graphs, each showing the relationship with either the equivalence ratio or the compression ratio as the independent variable; and maximum pressure; maximum temperature; efficiency; indicated specific fuel consumption; indicated mean effective pressure; volumetric efficiency; or exhaust temperature as the dependent variables. The mass ratio between ammonia and oil is the parameter for each curve. The second format is a set of three graphs, each showing the relative relationship between ammonia and oil, for the same dependent variables as mentioned above.

Peak Cycle Temperature and Pressure

Among the many intermediate parameters that are of interest to the study of engine performance, the peak cycle temperature and pressure, are perhaps the most significant. These parameters indicate, to large extent, the thermal and mechanical stresses that are experienced by the engine.

Peak temperatures and pressures for various equivalence ratios, Y/Y_{cc} (Y/Y_{cc} is defined as the ratio of the stoichiometric fuel/air ratio to the actual fuel/air ratio), are shown on Plates V-1, V-2 and V-3 for compression ratio 15:1. Plate V-1, Figures A, B, C and D,

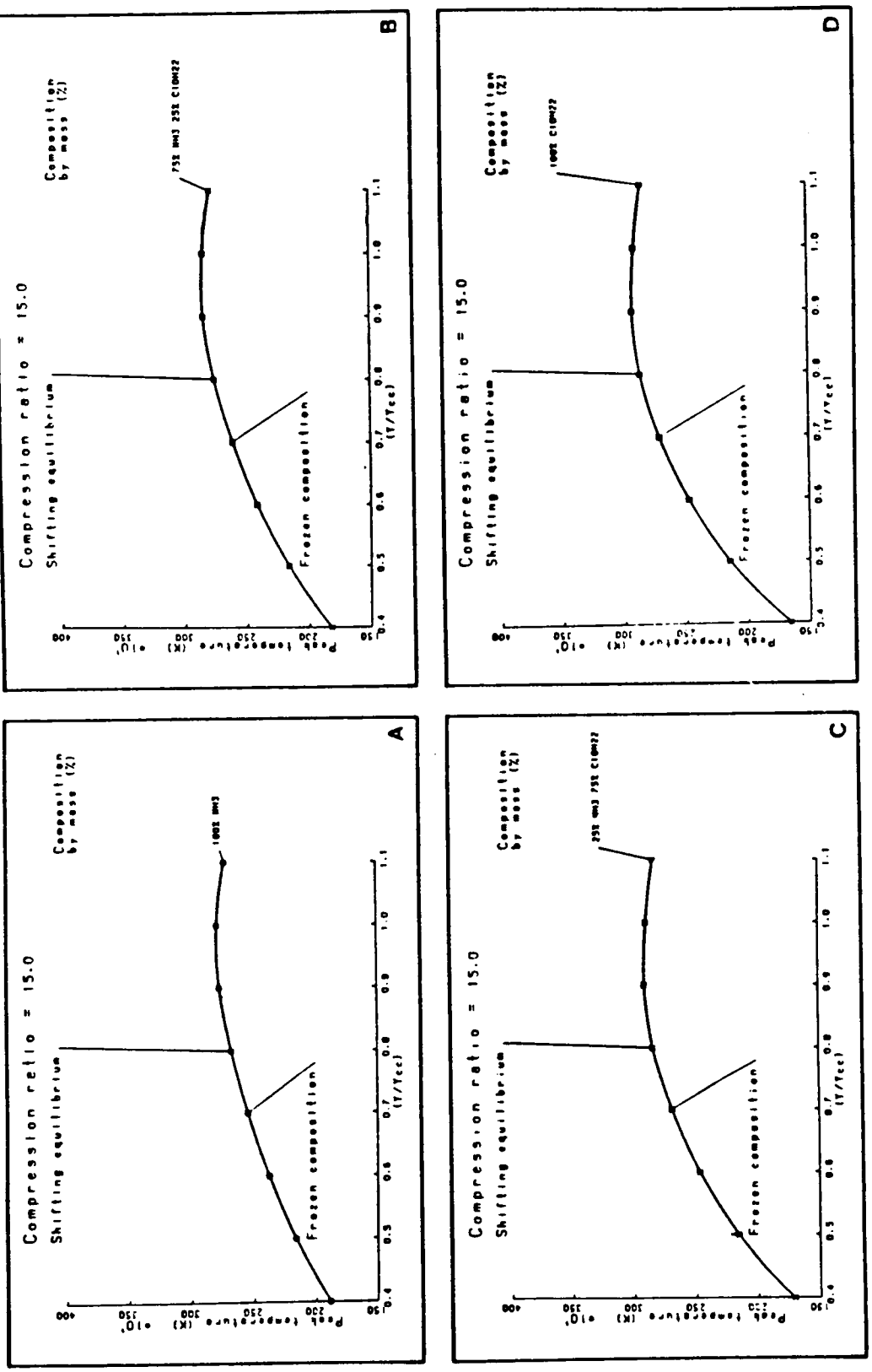


Plate V-1. Peak temperature as a function of equivalence ratio.

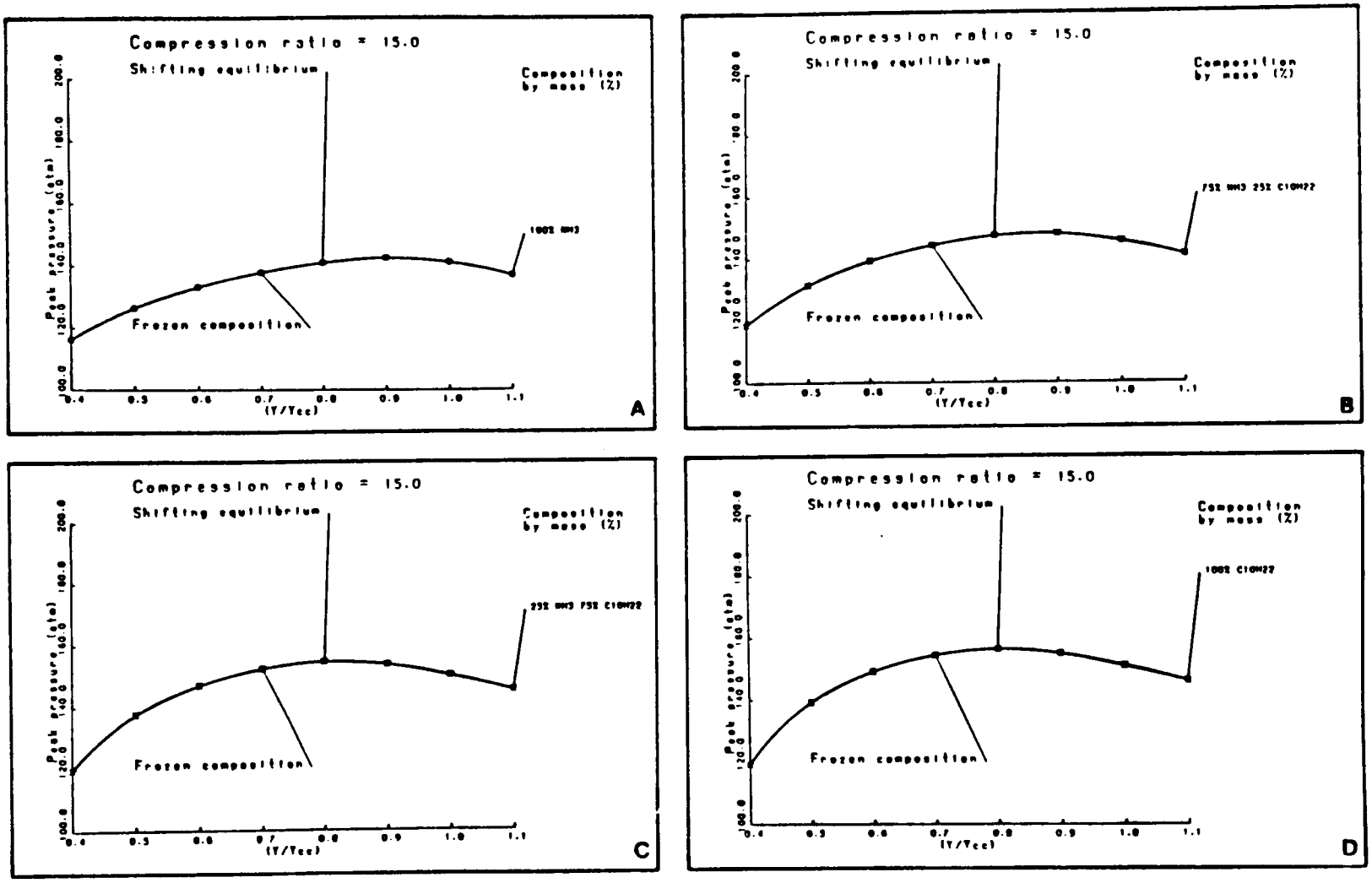


Plate V-2. Peak pressure as a function of equivalence ratio.

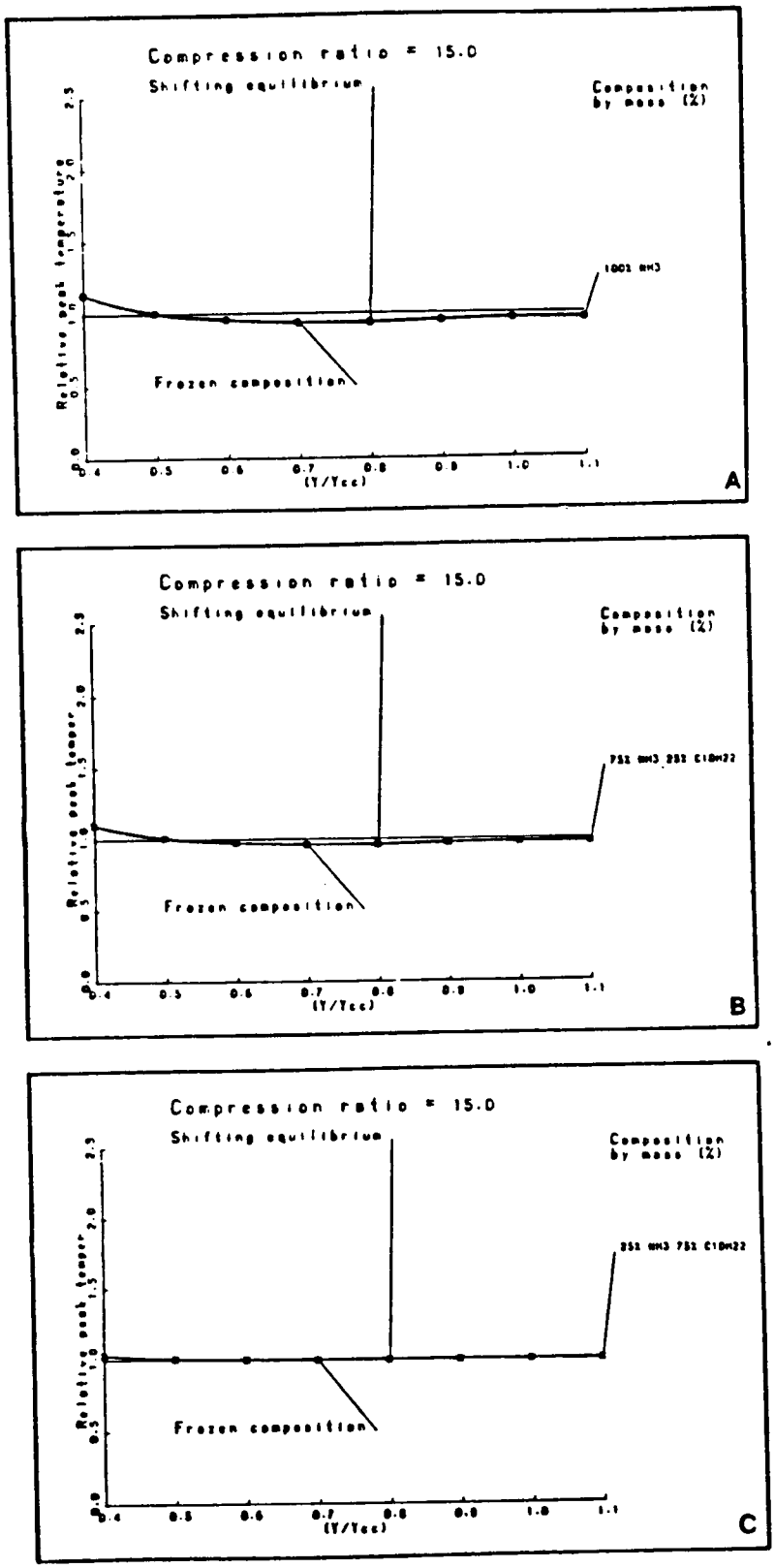


Plate V-3. Peak temperature relative to n-Decane.

indicates that the peak cycle temperatures with n-Decane would be expected to exceed those obtained with ammonia (for equivalence ratios greater than 0.5). The same is true for the peak pressure. No difference is noted between the shifting equilibrium and frozen composition cases.

Plates V-3 and V-4, Figures A, B and C, show the relative relationship between ammonia and oil. The figures show that no significant difference in maximum pressure and temperature should be expected for equivalence ratios above 0.5. However, for equivalence ratios lower than 0.5, the peak temperature, and pressure of the ammonia is higher than for the n-Decane.

From this information, some conclusions can be deduced. For example, the work produced by an engine of given size and compression ratio is dependent upon the cylinder pressure during expansion. An increase in pressure results in a proportionate increase in work output. Therefore, the work output of the ammonia driven engine should be expected to be less than the n-Decane driven, for equivalence ratios greater than 0.5.

Thermal Efficiency

Thermal efficiency is an indication of the degree of utilization of the fuel presented to the engine. On Plate V-5 the influence of the equivalence ratio upon efficiency is presented. The figures reveal that the efficiency to be expected from the ammonia should be above that for n-Decane. Plate V-6, Figures A, B and C,

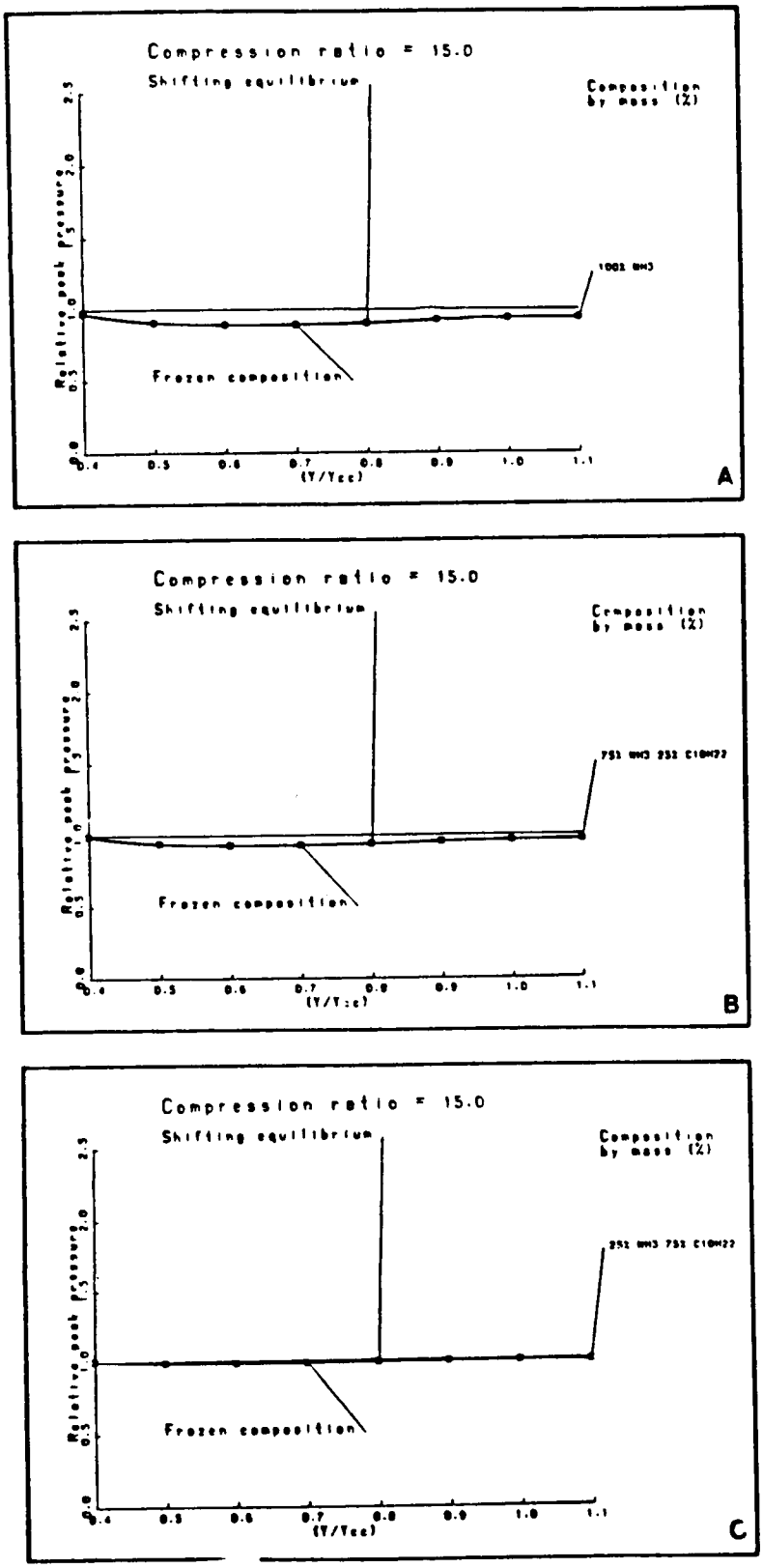


Plate V-4. Peak pressure relative to n-Decane.

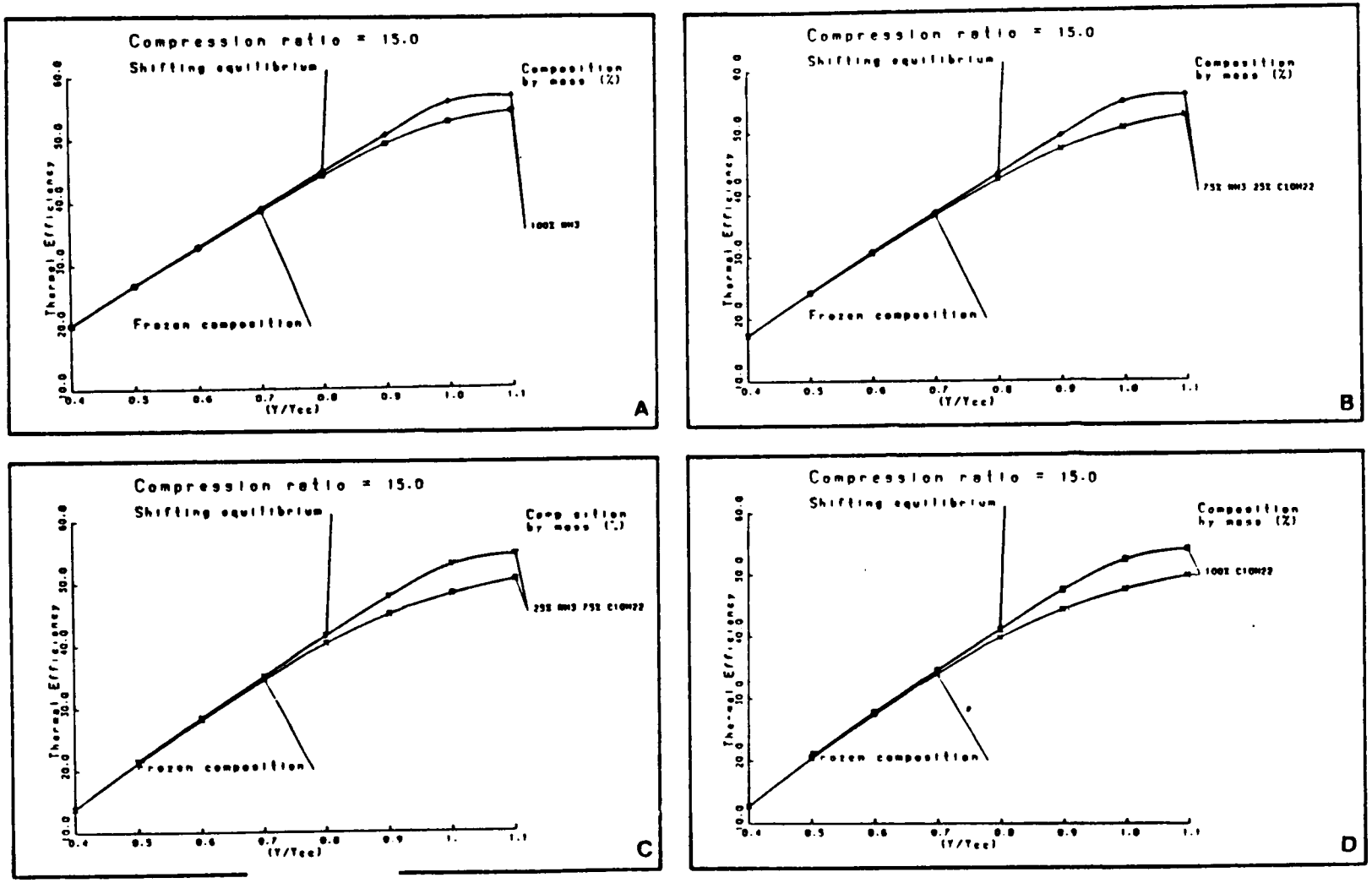


Plate V-5. Thermal efficiency as a function of equivalence ratio.

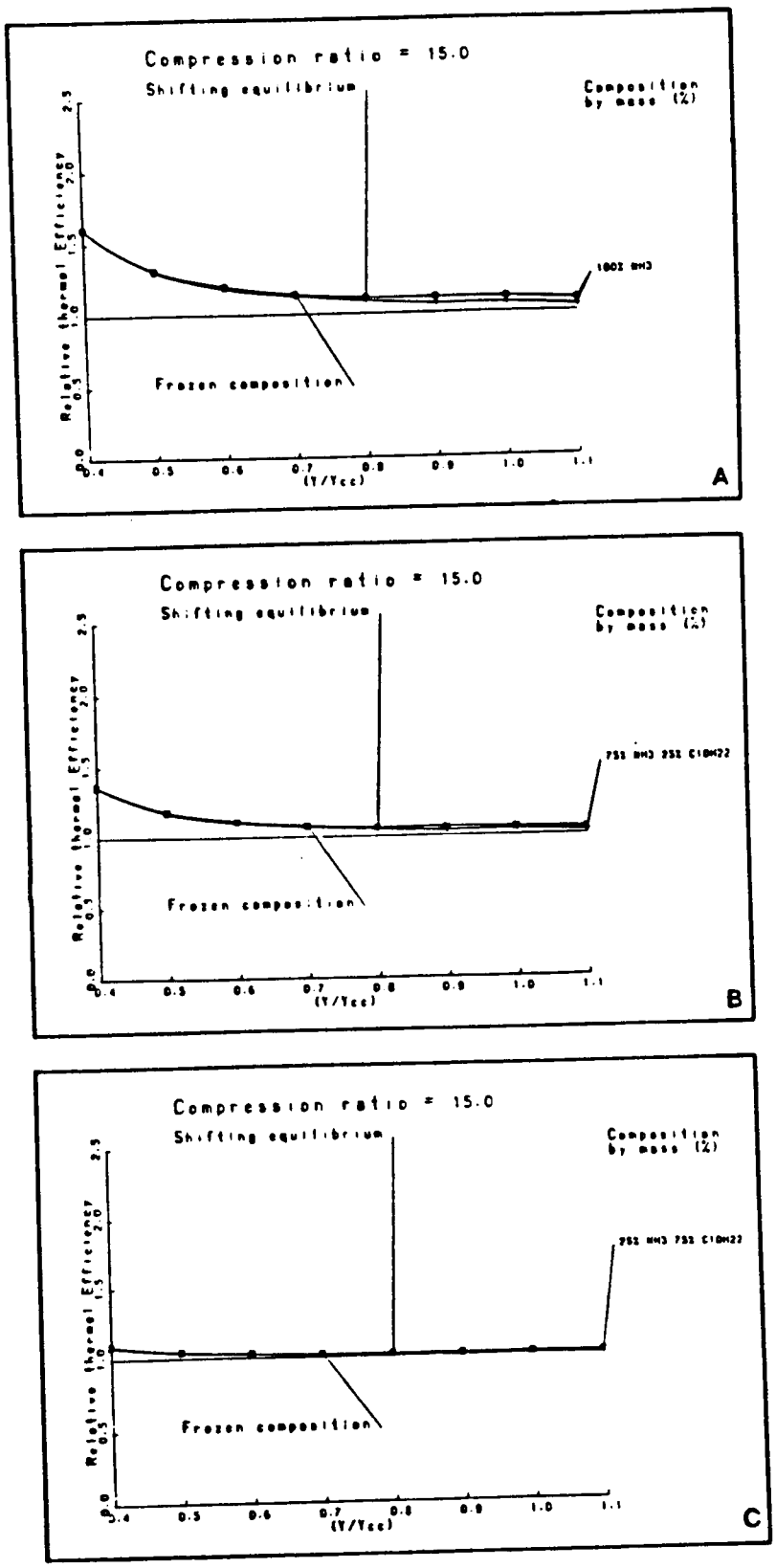


Plate V-6. Thermal efficiency relative to n-Decane.

show the relative relationship. These figures reveal that for low equivalence ratios, burning of ammonia should result in significantly higher efficiency. For instance, the difference is as much as 50% for pure ammonia at equivalence ratio 0.4.

For higher equivalence ratios the difference is less. For example, for pure ammonia at $Y/Y_{cc} = 0.7$ the difference is about 10%, and even less difference is predicted at higher ratios. Since the expected equivalence ratio for real engines is generally low, the difference between the efficiency predicted for n-Decane and ammonia is expected to be significant.

With increasing equivalence ratios (larger than 1.2) the model predicts decreasing efficiency, a result explained by the fact that the excess air is beginning to reduce the combustion temperature.

The Engine Power Output

The best way to express the power output to be obtained from an engine of given volumetric capacity is the mean effective pressure. Plate V-7, which demonstrates theoretical mean effective pressures as a function of equivalence ratio, indicates that the use of ammonia would result in a 5 to 12% reduction in power output relative to the pure n-Decane case. This reduction is explained by the fact that the volumetric efficiency suffers, due to the displacement of induction air by the relative large quantities of ammonia vapor. This difference decreases for decreasing equivalence ratio, and the model even predicts higher mean effective pressures with ammonia for equivalence

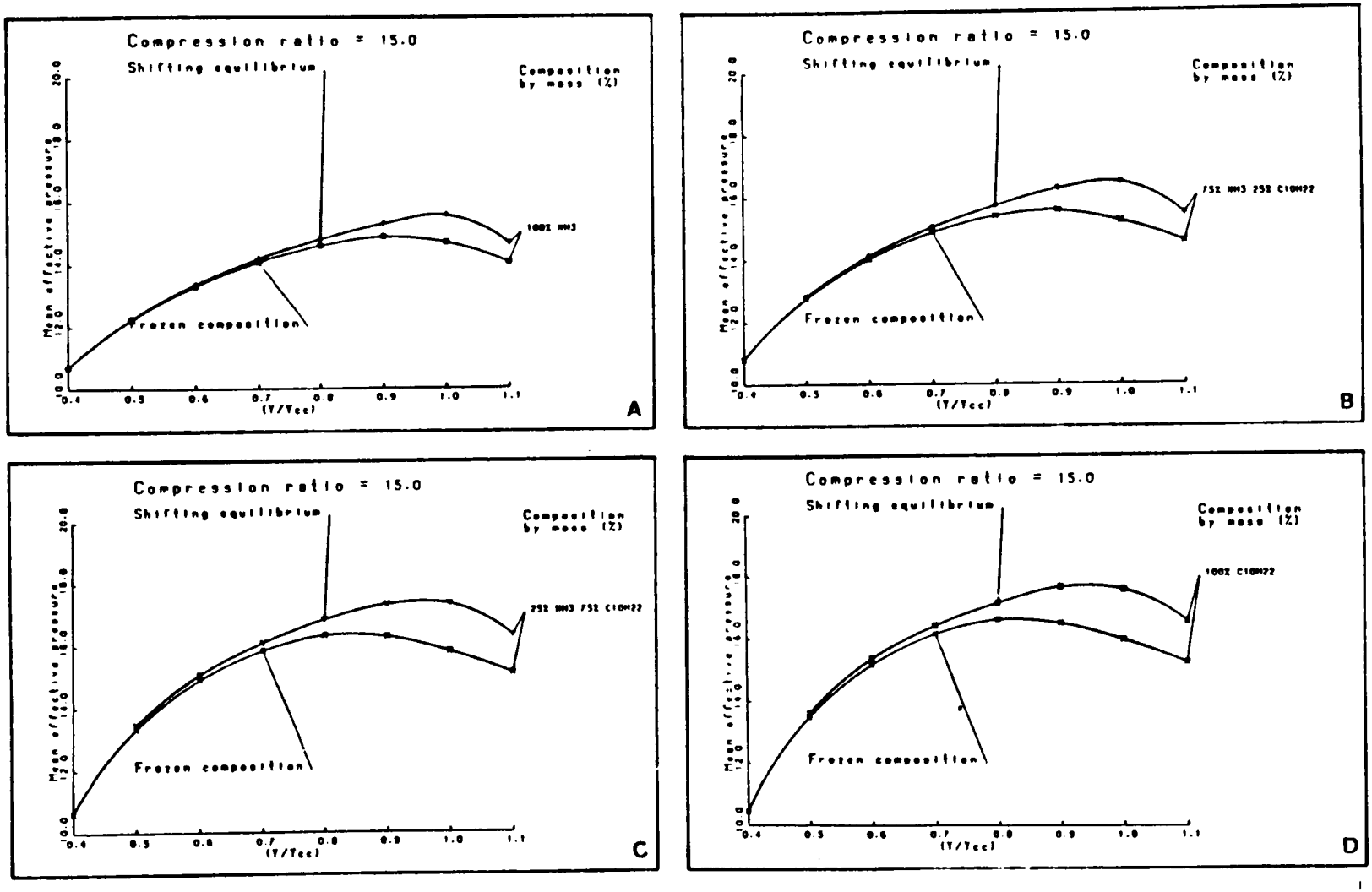


Plate V-7. Indicated mean effective pressure as a function of equivalence ratio.

ratios lower than 0.4. Plate V-8, Figures A, B and C, demonstrates the relative relationships. Figure A predicts lower IMEP for ammonia for all values of Y/Y_{cc}. However, for lower values of Y/Y_{cc} the difference reduces and is eliminated for Y/Y_{cc} lower than 0.4. From Figure B it can be deduced that the predicted IMEP is slightly higher than the pure n-Decane case for low values of Y/Y_{cc}.

A point of interest concerns the difference in results for the two calculation schemes used: frozen composition and shifting equilibrium. For high values of equivalence ratio and values close to the stoichiometric air-fuel ratio, the difference is significant. However, for lower equivalence ratios the difference becomes negligible, and below equivalence ratio = 0.7 there is no significant difference between the two schemes.

Volumetric Efficiency

The volumetric efficiency indicates the charge density obtained from the induction process. Plate V-9 demonstrates the volumetric efficiency for different equivalence ratios (and compression ratio 15:1). The influence of the ammonia in the induction air is obvious, and low volumetric efficiencies (as low as 60%) are to be expected at an equivalence ratio about 0.4. For pure n-Decane the volumetric efficiency was calculated to be about 96%. Plate V-10, Figures A, B and C, demonstrates the relative relationships.

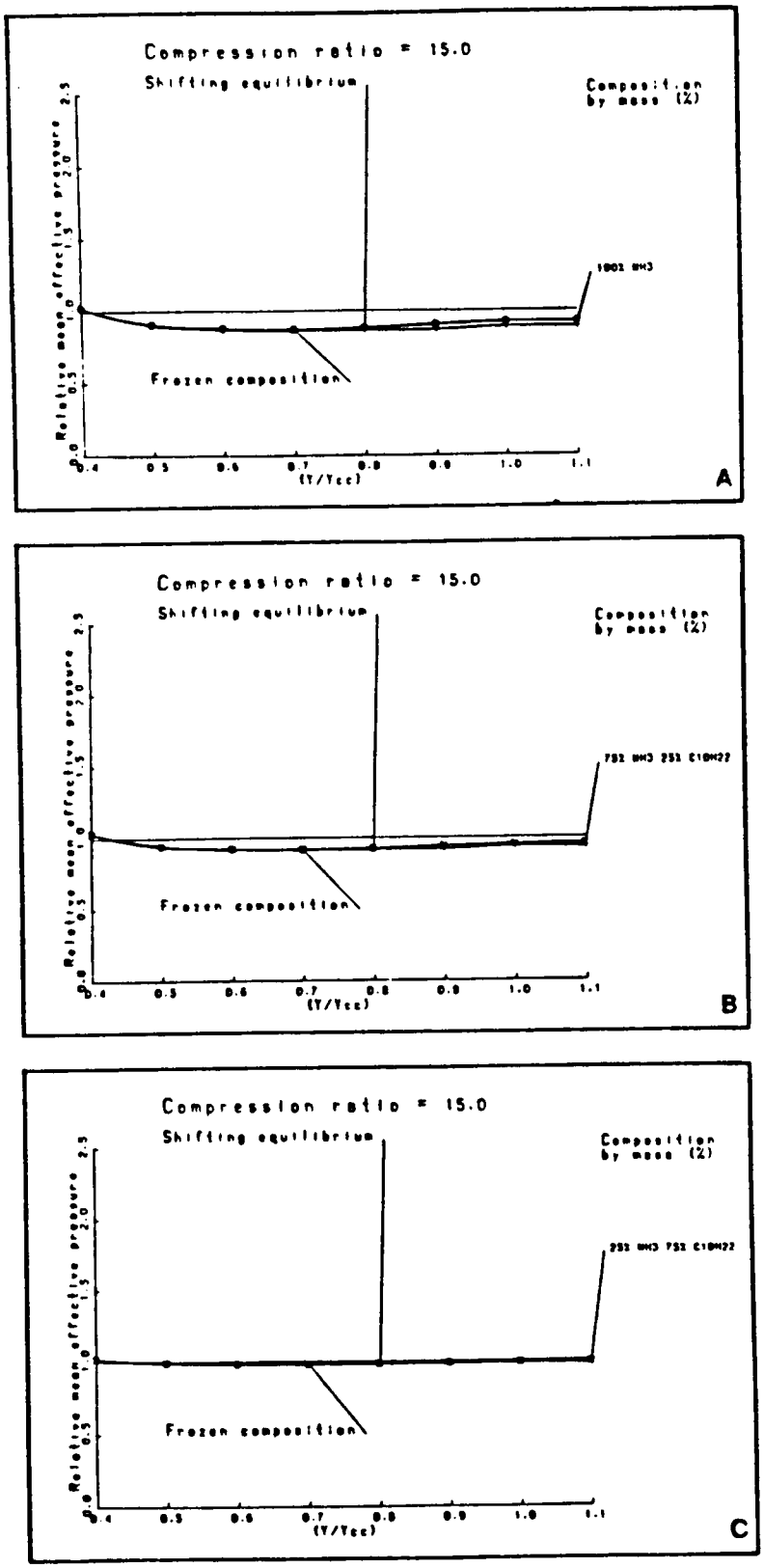


Plate V-8. Indicated mean effective pressure relative to n-Decane.

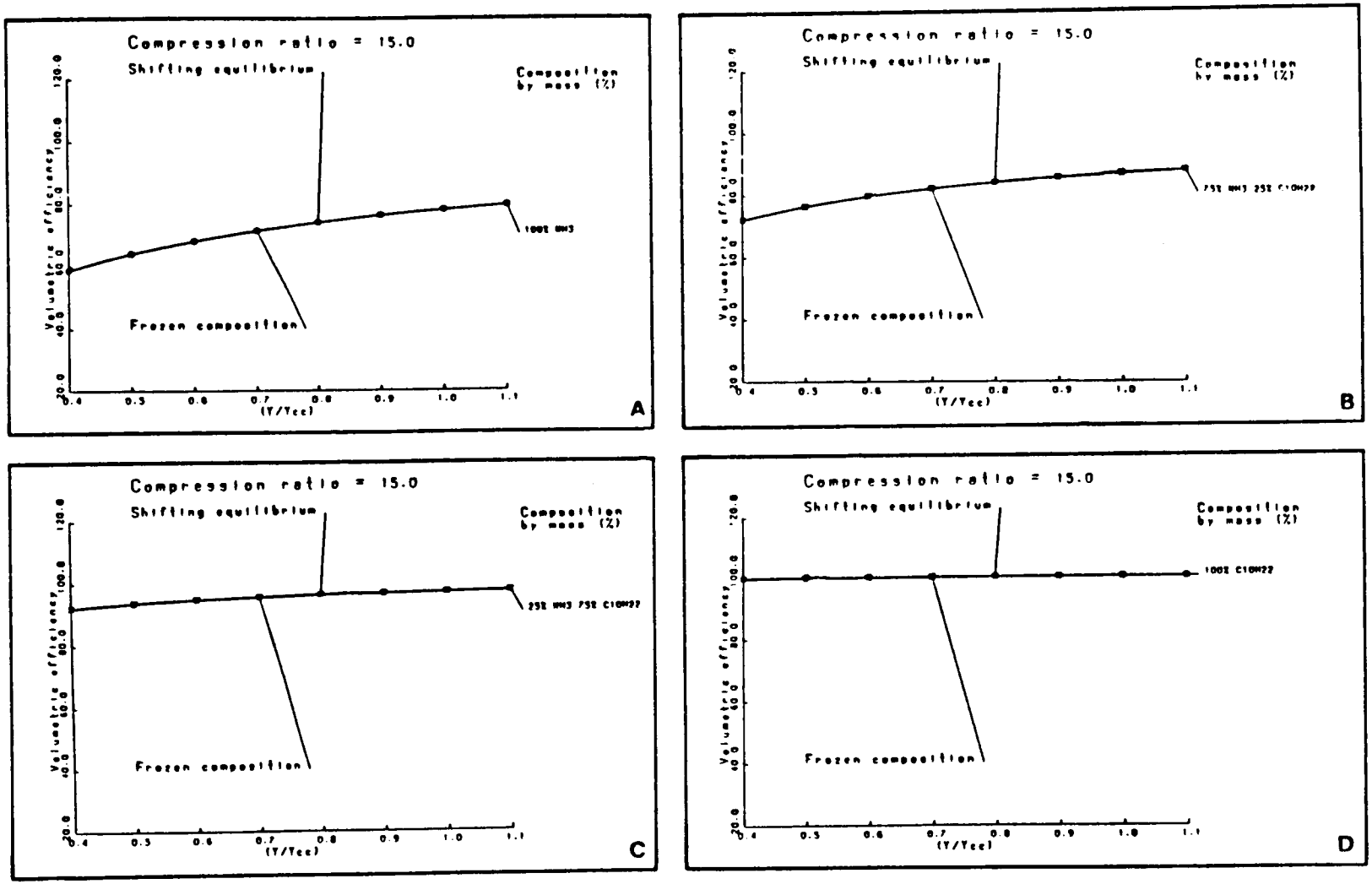


Plate V-9. Volumetric efficiency as a function of equivalence ratio.

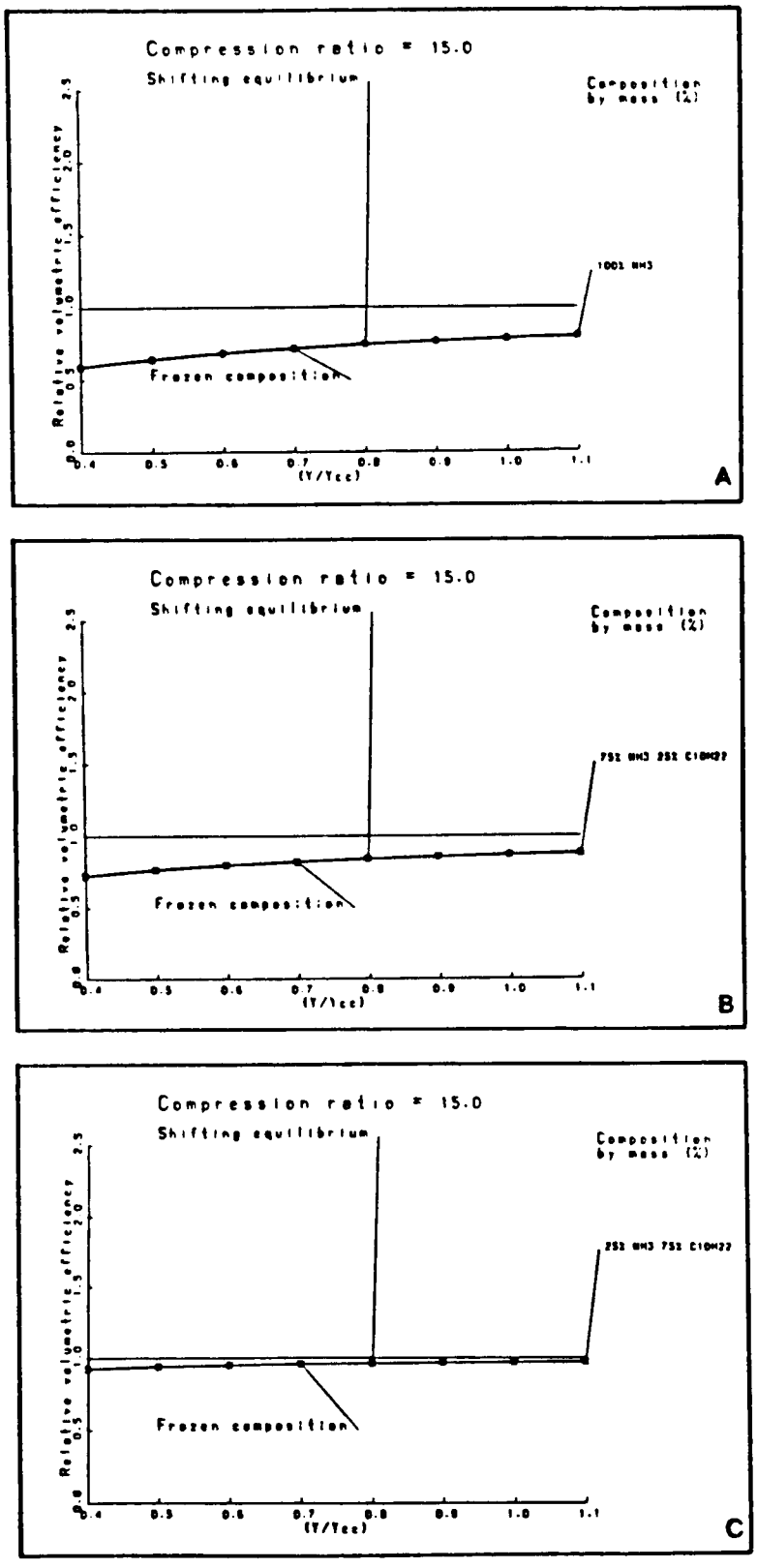


Plate V-10. Volumetric efficiency relative to n-Decane.

Exhaust Temperature

The exhaust temperature of the cycle can be used as an indication of the load to which the engine is exposed. For a particular fuel, the higher the temperature, the larger is the engine load; and, in some engine applications devices are used to monitor the temperature to secure safe operation of the engines. It is, therefore, of interest to estimate the influence the presence of ammonia has on the exhaust temperature, when the engine is run at constant load conditions. Plate V-11, which shows the exhaust temperature as a function of equivalence ratio and compression ratio 15:1, reveals that the exhaust temperature for ammonia is expected to exceed those obtained with n-Decane by as much as 25%, at equivalence ratio 0.4. Note, however, that this comparison is misleading because equal power output is not assumed in this case. For equal power output the difference should be expected to be greater. According to these results, an ammonia fueled engine is expected to run "hotter" than a n-Decane fueled engine; and, devices monitoring the exhaust temperature of the engines must, therefore, accommodate for this higher temperature. Plate V-12 reveals the relative relationship.

Specific Fuel Consumption

When the engine performance is related to the actual power generation, the parameter which may be of the most importance is specific fuel consumption. The theoretically predicted fuel consumption is shown in Plate V-13, Figures A, B and C. From the figures

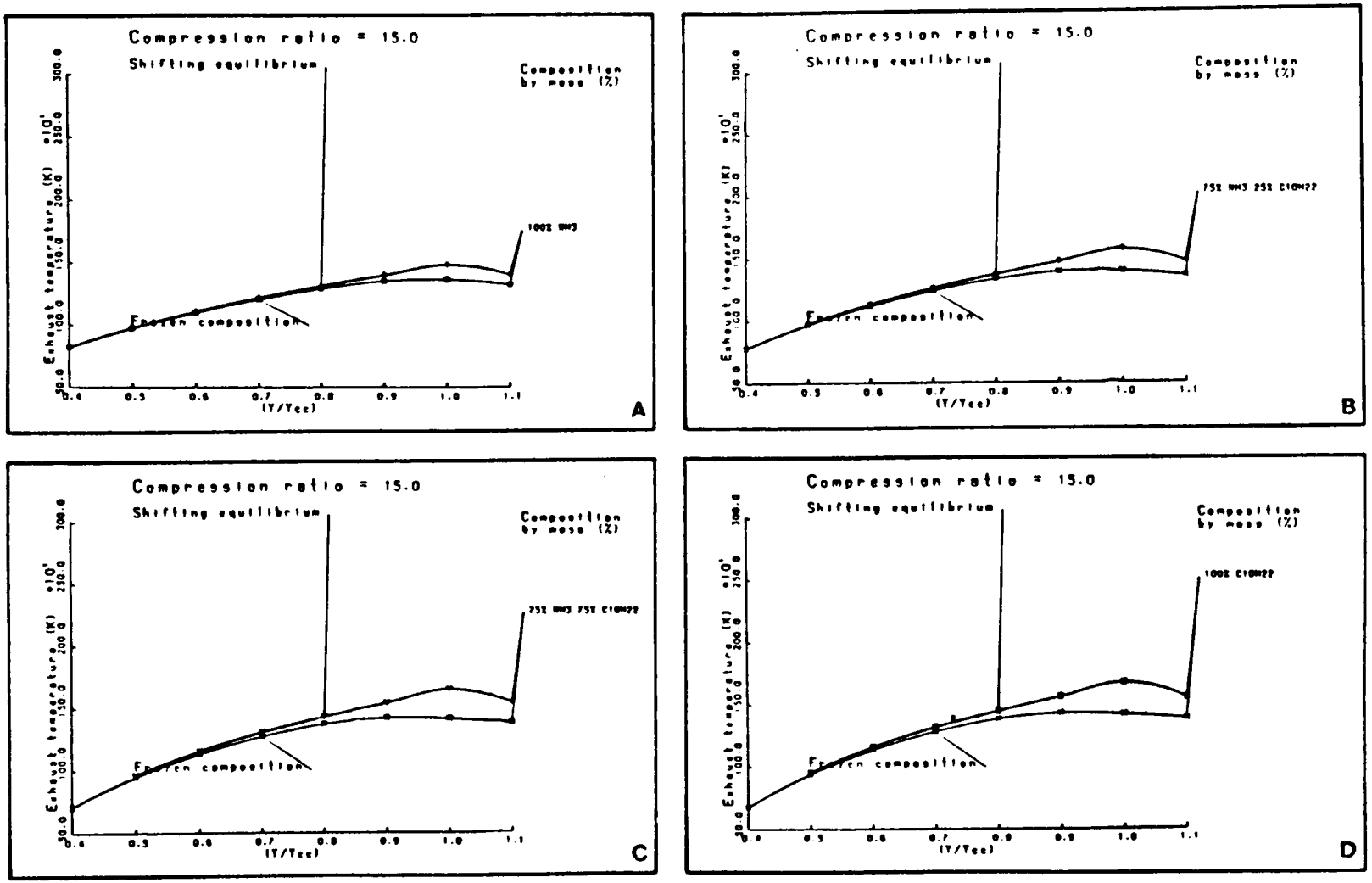


Plate V-11. Exhaust temperature as a function of equivalence ratio.

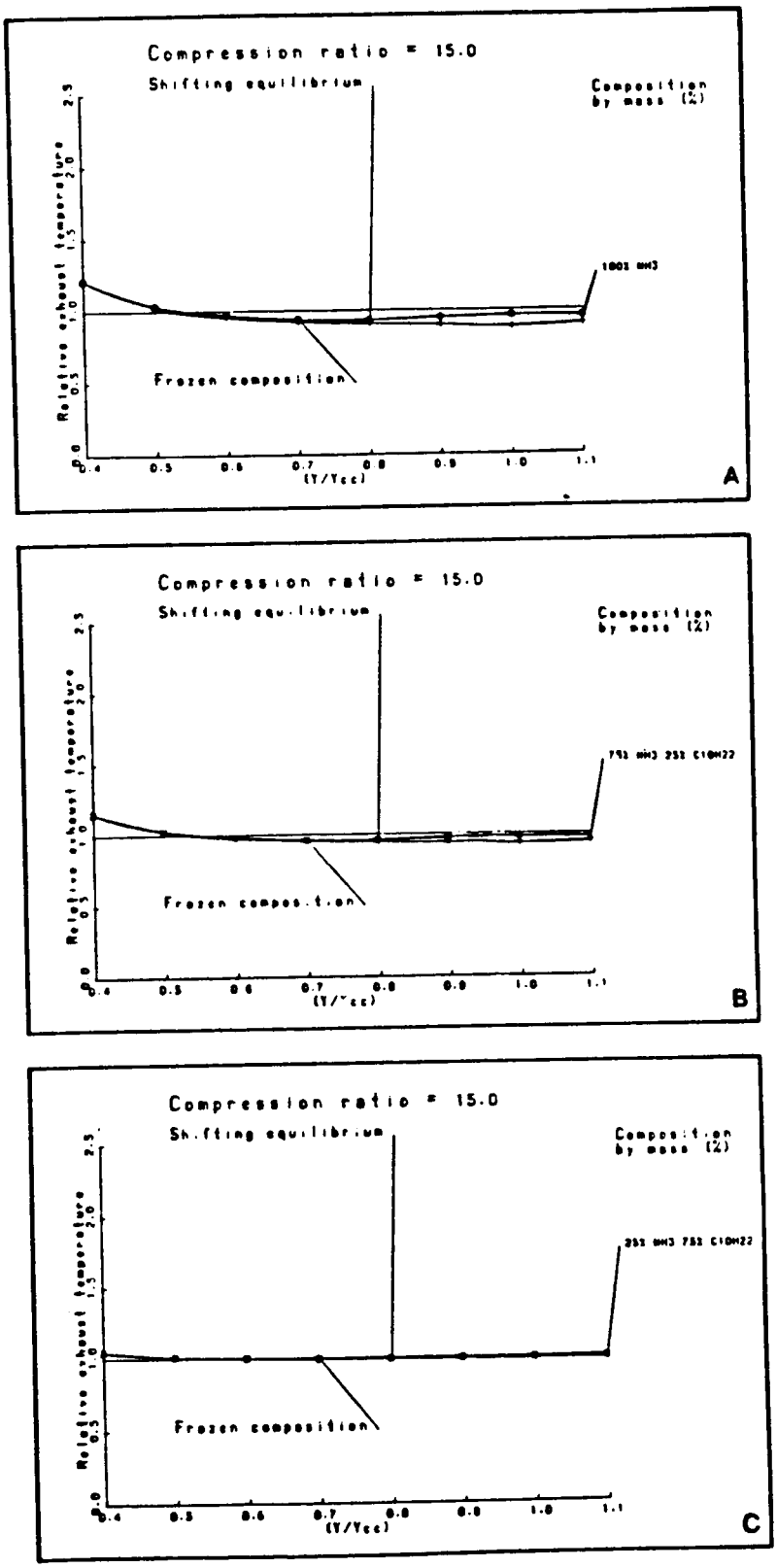


Plate V-12. Exhaust temperature relative to n-Decane.

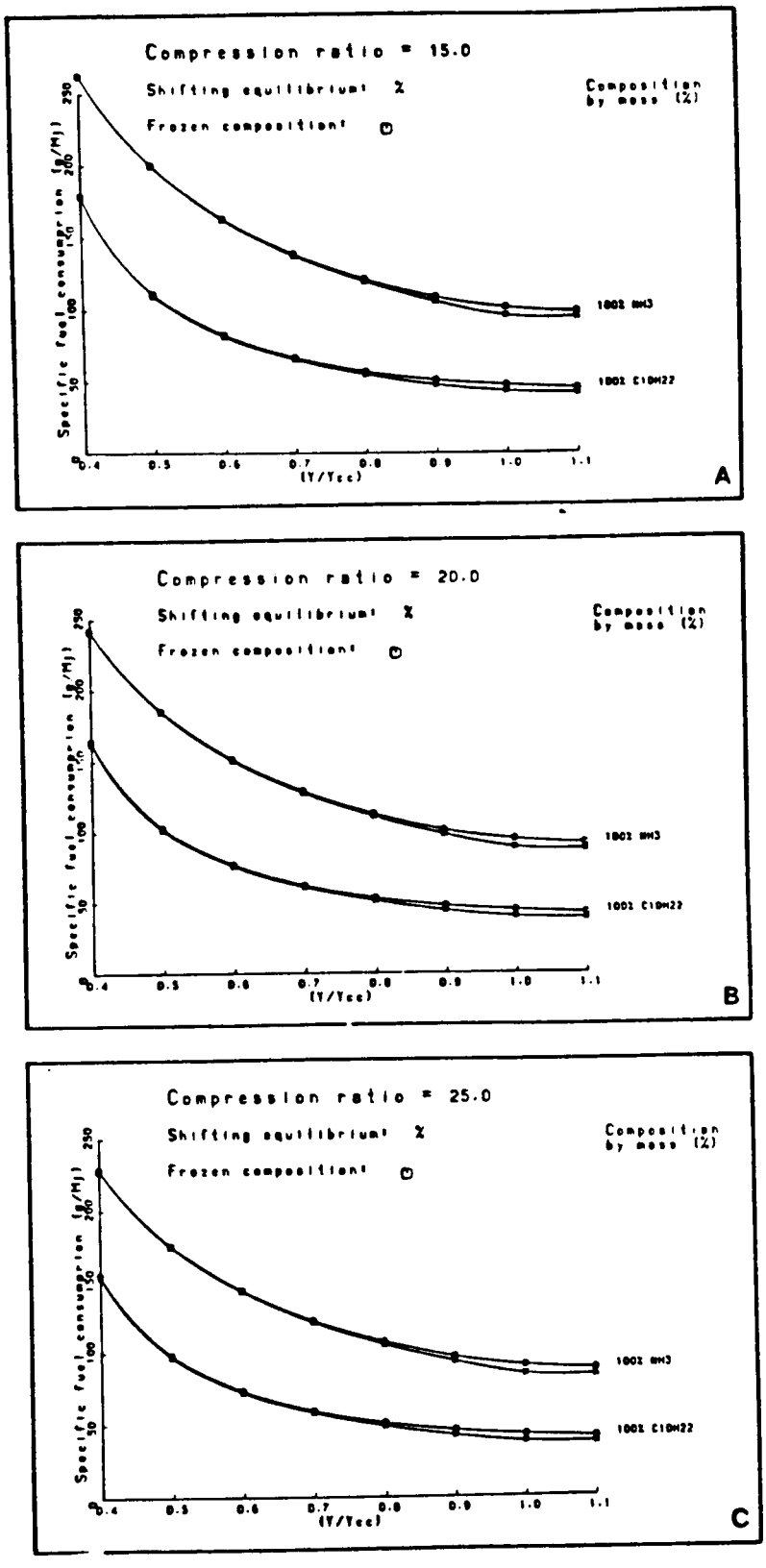


Plate V-13. Indicated specific fuel consumption as a function of equivalence ratio.

it can be deduced that the fuel consumption decreases with higher compression ratios and with higher equivalence ratios. The relative relationship is shown in Plate V-14, Figures A, B and C. These figures reveal that the fuel consumption of ammonia should be expected to exceed that for n-Decane by a factor of about 1.4 to 2.3, depending on the equivalence ratio. Note that this relative relationship is not significantly influenced by changes in compression ratio.

This difference in fuel consumption is primarily a result of the difference in the heating values of ammonia versus n-Decane.

Effect of Compression Ratio

As stated above, a number of parameters had to be fixed in order to reduce the bulk of the material which otherwise would be created. In the literature it has become a common practice to investigate the influence of compression ratio on the predicted results. Plates V-15 through V-19 are presented to reveal the influence of the compression ratio on the performance parameters of the engine.

From these figures the general observation can be made that each of the performance parameters, except the ISFC, increases with increasing compression ratio; the form of the relationships is almost linear. These results are in accordance with the fact that for the temperatures encountered in the combustion cycle the specific heat values of the pertinent gases (of which N_2 is the most common) are close to being constant for each gas. Therefore, based on the ideal gas assumption, the enthalpy of the gases vary linearly with

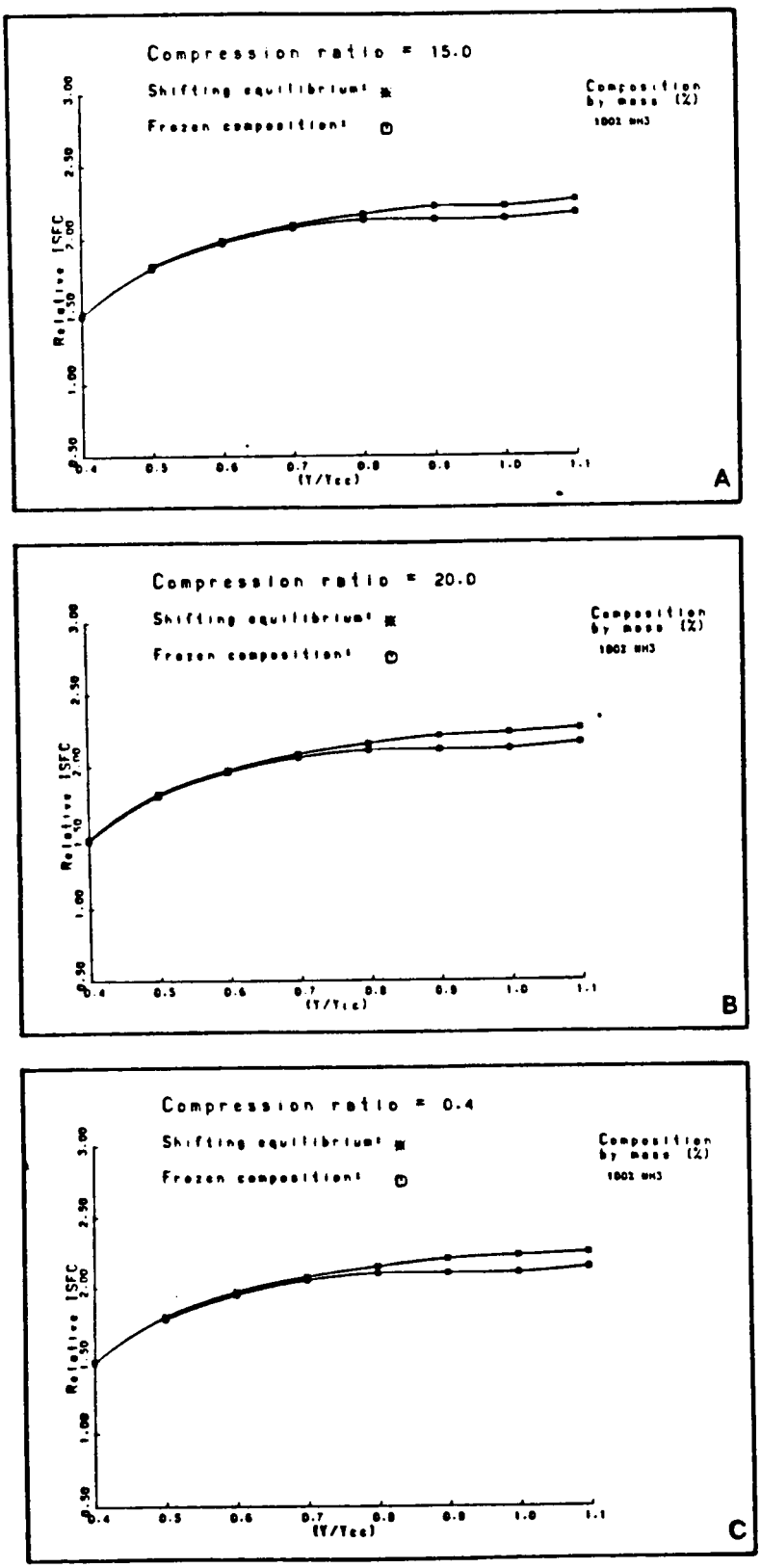


Plate V-14. Relative indicated specific fuel consumption as a function of equivalence ratio.

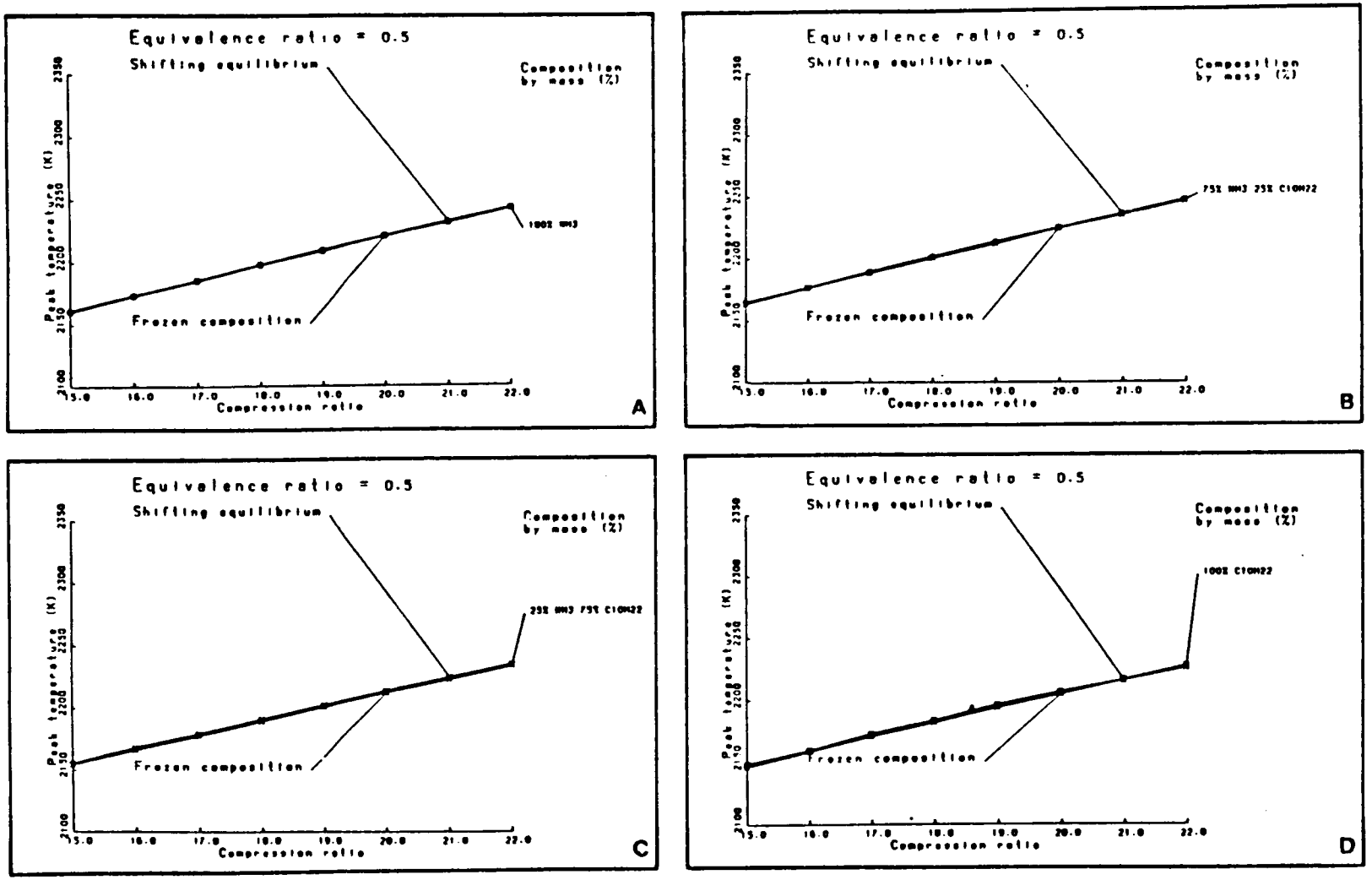


Plate V-15. Peak temperature as a function of compression ratio.

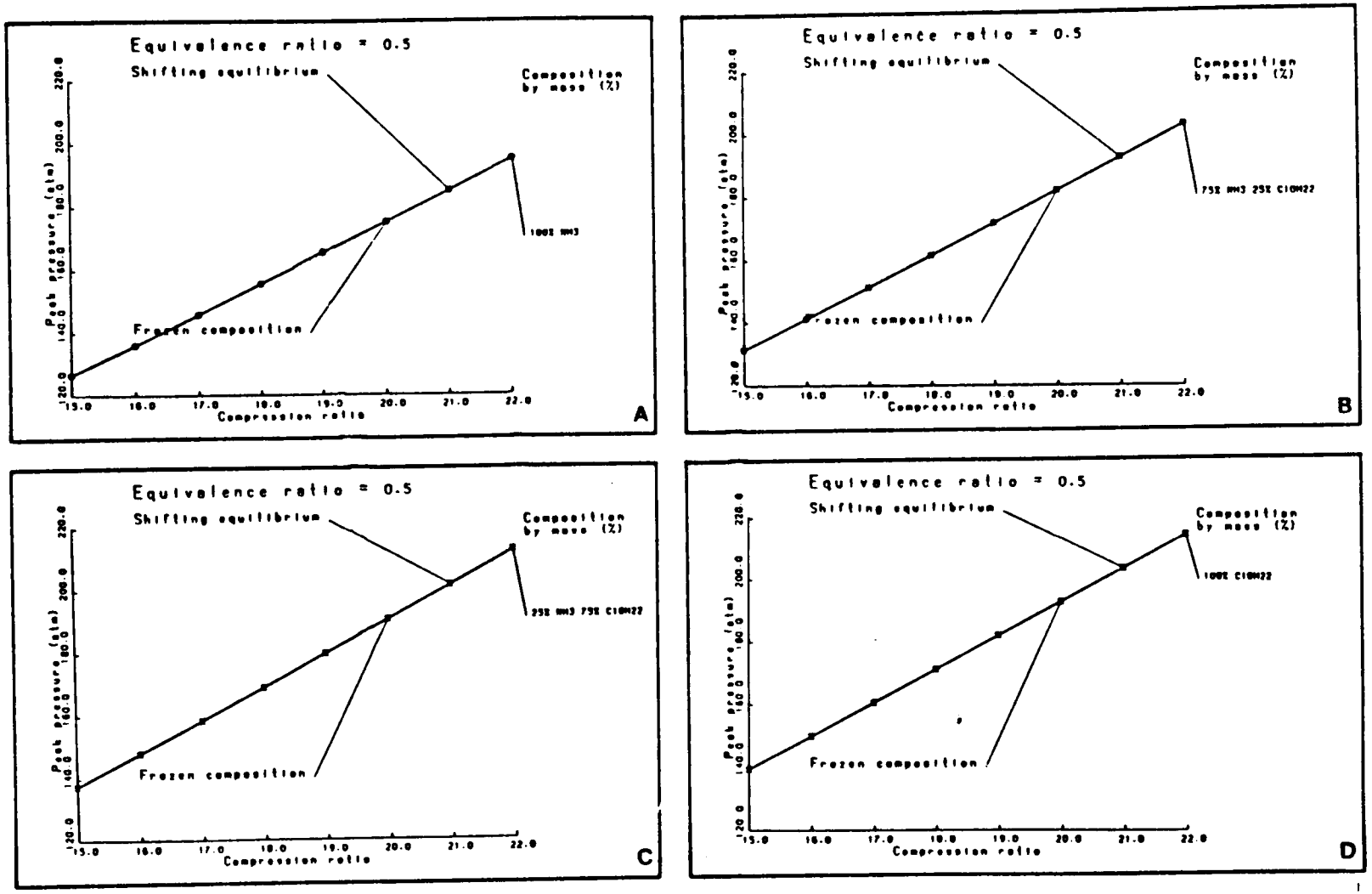


Plate V-16. Peak pressure as a function of compression ratio.

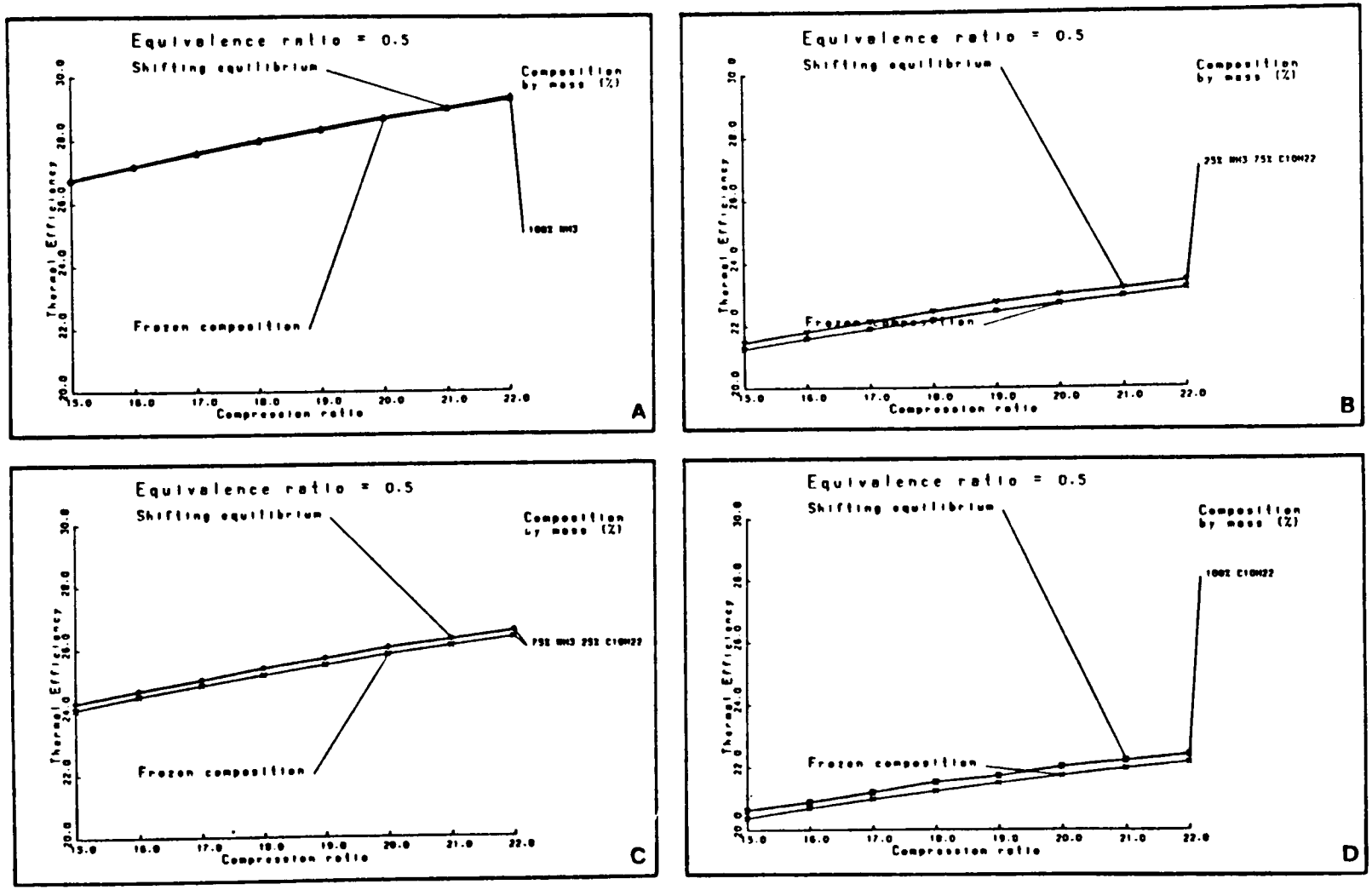


Plate V-17. Thermal efficiency as a function of compression ratio.

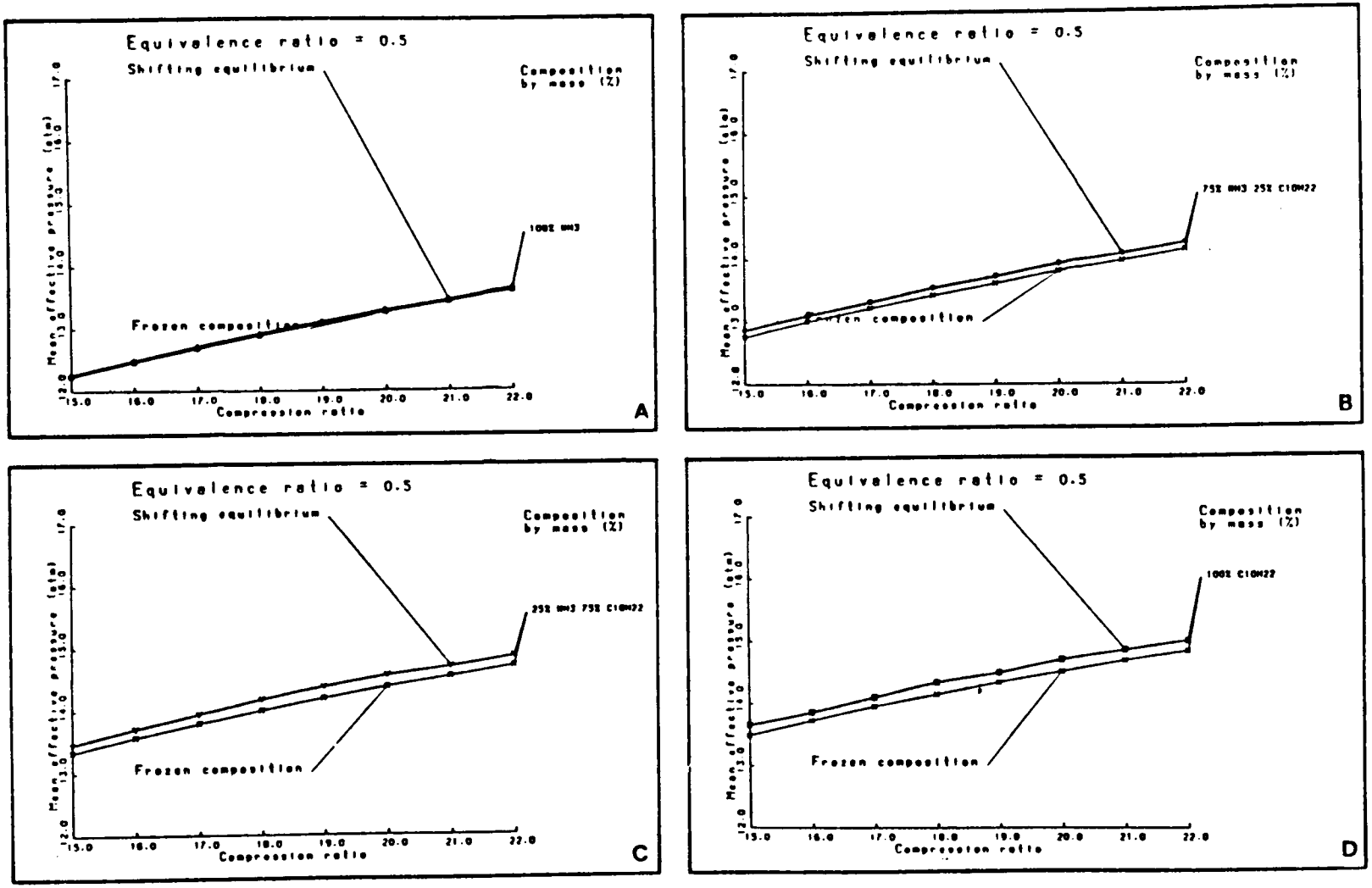


Plate V-18. Indicated mean effective pressure as a function of compression ratio.

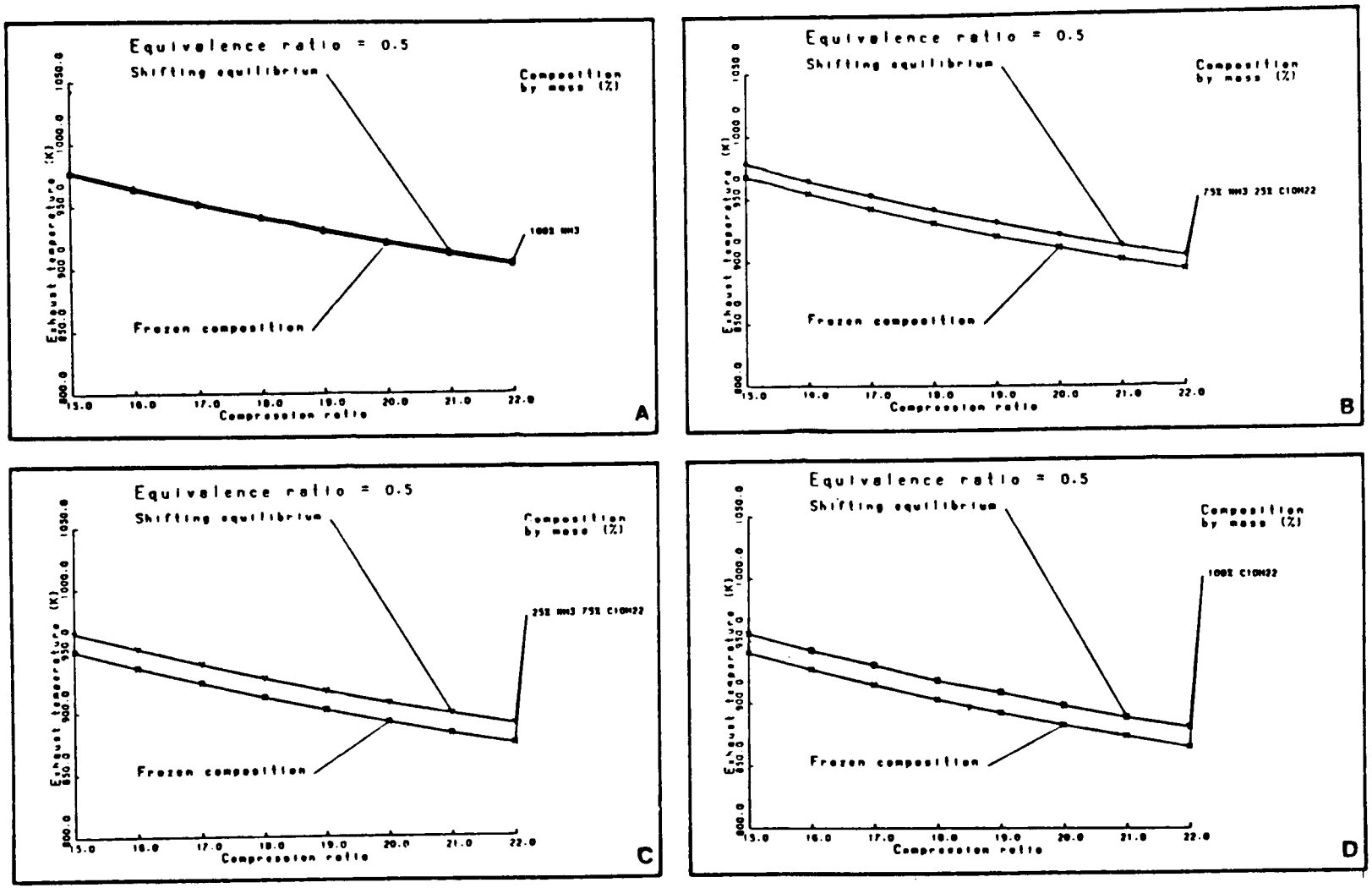


Plate V-19. Exhaust temperature as a function of compression ratio.

temperature. The effect of increasing the compression ratio is largely to increase the temperature of the mixture at the end of the compression cycle. This results, also, in higher energy content of the mixture and hence increases performance parameters, such as power output, maximum temperature, and pressure. This general behavior, reflected in Plates V-15 through V-19, is also experienced in real engines. Note, however, that in the real engine other phenomena which were left out of the present model counteract the influence of the increased compression ratio. Therefore, comparable figures for real engines show a maximum value after which the increase of compression results in decreased performance.

CHAPTER VI

CALCULATION OF CHEMICAL EQUILIBRIUM

In this section the scheme used for the computation of chemical equilibrium is derived. There are in general two reasons for making equilibrium calculations of this type. First, the thermodynamic variables of the system depend on the composition of the product gases following the combustion. Performance calculations are generally straightforward when the composition of the exhaust products is based on assumption of the complete combustion. It is, therefore, natural to inquire whether there is reason to extend the effort to include dissociation calculations of the product gases. The experience shows, that at the prevailing temperatures during the combustion in the constant volume cycle, calculation of performance parameters could give highly misleading performance figures for the cycle if dissociation were ignored.

The second reason for making such calculations is to obtain information about the chemical composition of the product gases since the characteristics of the emissions from internal combustion engines are of general concern.

The subject of this section is to derive the calculation scheme used to calculate the chemical equilibrium composition for a system, containing C, H, O and N atoms. The computational scheme used in this work is one which considers ten different species. It is felt, for

the purpose of this work, that the number of species considered should represent the vast majority of the species which appear in internal combustion engines.

In what follows, the mixture of the product gases is assumed to contain the following species:

$$
\begin{aligned}
&N(1) \text{ moles of } CO_2 \ ; \ N(2) \text{ moles of } CO \ ; \\
&N(3) \text{ moles of } O_2 \ ; \ N(4) \text{ moles of } O \ ; \\
&N(5) \text{ moles of } NO \ ; \ N(6) \text{ moles of } N_2 \ ; \\
&N(7) \text{ moles of } H \ ; \ N(8) \text{ moles of } H_2 \ ; \\
&N(9) \text{ moles of } OH \ ; \ N(10) \text{ moles of } H_2O
\end{aligned}
\qquad \text{(VI-1)}
$$

where N(i), i = 1, 2, ... , 10, are the number of moles of each specie in the combustion equation. This notation, somewhat different from Eq. II-1, should aid in understanding the program code used to carry out the actual calculations.

At the outset, it was recognized that in the limit when no pilot-fuel is being injected to the cycle, the equation system degenerates to a H, O, and N system. Therefore, the formulation of the problem had to tolerate this limiting case, when no carbon atoms are present in the mixture.

The object is, therefore, to calculate 10 mole numbers in the equilibrium state, with V and T known and the resulting system has to be able to accommodate the special case when carbon atoms are absent from the calculations.

In order to close the equation system, ten equations are required. Four equations are supplied by the "law" of conservation of matter, and the remaining six are based on the "second law" of thermodynamics.

Equations for the six reaction constants K_{pi}, i = 1, 2, ... , 6 are derived for the following set of independent reactions:

$$
\begin{aligned}
CO + 1/2\ O_2 &\rightleftharpoons CO_2 && K_{p1} \\
2O &\rightleftharpoons O_2 && K_{p2} \\
O_2 + N_2 &\rightleftharpoons 2NO && K_{p3} \\
2H &\rightleftharpoons H_2 && K_{p4} \\
O + H &\rightleftharpoons OH && K_{p5} \\
H_2 + 1/2\ O_2 &\rightleftharpoons H_2O && K_{p6}
\end{aligned}
\qquad \text{(VI-2)}
$$

The reaction constants K_{pi}, i = 1, 2, ... , 6 are identified with each reaction. To simplify the following discussion, the quantities W_i, i = 1, 2, ... , 6 are defined as follows:

$$W_1 = K_{p1}(P/Nt_p)^{1/2}$$

$$W_2 = K_{p2}(P/Nt_p)$$

$$W_3 = K_{p3} \qquad \text{(VI-3)}$$

$$W_4 = K_{p4}(P/Nt_p)$$

$$W_5 = K_{p5}(P/Nt_p)$$

$$W_6 = K_{p6}(P/Nt_p)^{1/2}$$

where Nt_p is calculated from the following ideal gas relationship:

$$Nt_p = Nt_r(P_i/P_j)(T_j/T_i)(V_i/V_j) \qquad \text{(VI-4)}$$

and where N_{tr} is the total number of moles of reactants; and, the subscripts i and j are used to indicate two different state-points. For example, T_i is the temperature at state-point (i) which precedes state-point (j) in the cycle. For constant volume combustion $(V_i/V_j) = 1$; and, for shifting equilibrium $(V_i/V_j) = CR$, the compression ratio of the cycle.

Further, it should be noted that because for the reaction $O_2 + N_2 \rightarrow 2NO$, there is no net change in the mole numbers between reactants and products, $W_3 = K_{p3}$.

Since only the relative amount of each species in the product gases is of interest any amount of each species can be considered, as long as the relative relationship is preserved. With this in mind, Eq. VI-4 now becomes:

$$Nt_p = (AC+AH+AO+AN)(P_i/P_j)(T_j/T_i)(V_i/V_j) \qquad (VI-5)$$

where the term $Nt_r = (AC+AH+AO+AN)$ denotes the abundance of the reactants in the chemical equation (II-1); and, where AC, AH, AO and AN are the abundances of carbon, hydrogen, oxygen and nitrogen, respectively, calculated from Eq. II-1 as follows:

$$\begin{aligned} AC &= 10\ n_o \\ AH &= 3\ n_a + 22\ n_o \\ AO &= 2\ Y \\ AN &= n_a + 7.52\ Y \end{aligned} \qquad (VI-6)$$

The four conservation of mass equations are given by:

$$\begin{aligned} AC &= N(1) + N(2) \\ AH &= 2(N(8) = N(10)) + N(7) + N(9) \\ AO &= 2(N(1) + N(3)) + N(2) + N(4) + N(5) + N(9) + N(10) \\ AN &= N(5) + 2N(6) \end{aligned} \qquad (VI-7)$$

In the limit when the carbon atom disappears from the system all equations containing carbon atoms in effect disappear from the system of equations. However, because of the nature of these equations (namely, nonlinear) it is possible to manipulate the equations to include this special case.

With this information the set of equations can now be written:

$$AC = N(1) + N(2)$$

$$AH = 2(N(8) + N(10)) + N(7) + N(9)$$

$$AO = 2(N(1) + N(3)) + N(2) + N(4) + N(5) + N(9) + N(10)$$

$$AN = N(5) + 2N(6)$$

$$W_1 = \frac{N(1)}{N(2)\ N(3)^{1/2}}$$

$$W_2 = \frac{N(3)}{N(4)^2} \qquad \text{(VI-8)}$$

$$W_3 = \frac{N(5)^2}{N(3)\ N(6)}$$

$$W_4 = \frac{N(8)}{N(7)^2}$$

$$W_5 = \frac{N(9)}{N(4)\ N(7)}$$

$$W_6 = \frac{N(10)}{N(8)\ N(3)^{1/2}}$$

The first four equations are the mass conservation equations and the last six are the equilibrium equations.

A number of solution schemes have been developed to solve equation systems of this nature [18,19]. For example, the Newton Cranston method [19] is directly applicable to this problem. However, for the

purpose of this work, the following procedure was followed. The equations can be rearranged to give:

$$N(7) = \text{Iteration variable}$$

$$N(8) = W_4 N(7)^2$$

$$N(9) = (AH - N(7) - 2N(8))\left(\frac{B}{B+1}\right)$$

$$N(10) = N(9)\, N(7)(W_6\, W_4\, W_2^{1/2})/W_5$$

$$N(4) = N(9)/(W_5\, N(7))$$

$$N(3) = W_2\, N(4)^2 \qquad \text{(VI-9)}$$

$$N(1) = W_1\left(\frac{N(3)\, AC}{1 + W_1 N(3)^{1/2}}\right)$$

$$N(2) = AC - N(1)$$

$$N(5) = W_3\left(\frac{N(3)}{4}\right)\left(1 + \left(\frac{8\, AN}{W_3 N(3)}\right)^{1/2} - W_3\left(\frac{N(3)}{4}\right)\right.$$

$$N(6) = (AN - N(5))/2$$

and

$$B = W_5 N(7)/(2\, W_2^{1/2}\, W_6\, N(8))$$

In order to close the equation system, the K_{pi}'s functional relationship to the thermodynamic variables is required. The problem is simplified by the fact that for ideal gases K_p is only a function of temperature, i.e., $K_p = K_p(T)$. The functional relationship used in this work is as follows:

$$K_{pi}(T) = EXP(a_i/T + (b_i + c_i/T)\ln(T) + d_i) \qquad \text{(VI-10)}$$

where the constants a, b, c and d are listed in Table D-3 (Appendix D).

The iterations are started with the number of N(7), or H, atoms in the middle of the allowable range, which is simply N(7) = AH/2. From Eqs. VI-9, values for N(i), i = 1, 2, ... , 6, 8, ... , 10, can be calculated. After the values have been evaluated, the number of oxygen atoms, from the present solution, AO_m, can be calculated closing the conservation equation for oxygen. If the value calculated agrees with the right value of AO, the calculations are halted. On the other hand, if the value does not agree within the desired limit, the value of N(7) has to be modified. In this work the following correction scheme was used. If from Eqs. VI-6 the value for N(9) + N(10) in the AO equation is substituted for the corresponding values in the AH equation, and the results differentiated with respect to N(7), i.e., if the quotient dAO/dN(7) is formed, the following results are obtained:

$$dAO/dN(7) = -1 \qquad \text{(VI-11)}$$

From this last equation it can be seen that the differential increase of AO is directly proportional to the same decrease in N(7). Thus, if in the calculation scheme the value of AO_m is larger than AO, then the value of N(7) has to be increased. In the program, a half interval search was used to bracket off the right value, according to the following equation:

$$N_{i+1}(7) = N_i(7) \pm (NH/2^{j+1}) \qquad \text{(VI-12)}$$

The plus sign is used when AO is greater than AO_m, and the minus sign when AO is less than AO_m.

In this program the iteration was halted when the agreement between AO and AO_m was within 0.05%.

Results for Specific Cases

Figure VI-1 is one illustration of the sort of results obtained from the chemical equilibrium composition calculations obtained. In that figure constant volume combustion is assumed, from the initial state Tref = 500K and Pref = 10 atm, and the abundances AC/AH/AO/AN = 10/20/40/0. This figure, thus, represents slightly over-oxidized combustion of n-Decane with oxygen at constant volume.

The special case, when the number of carbon atoms in the system become negligible, is represented in Figure VI-2. Here the case of constant volume combustion is considered from the same reference states as in Figure VI-1. The abundances in this case are AO/AH = 10/20, and can, therefore, be thought of as representing stoichiometric combustion of ammonia and oxygen at constant volume.

The profound influence of temperature is obvious and indicates that at the temperatures shown, dissociation must be considered. However, for temperatures lower than 1500 K no appreciable dissociation is experienced, and use of this fact can be made when appropriate to simplify the calculations.

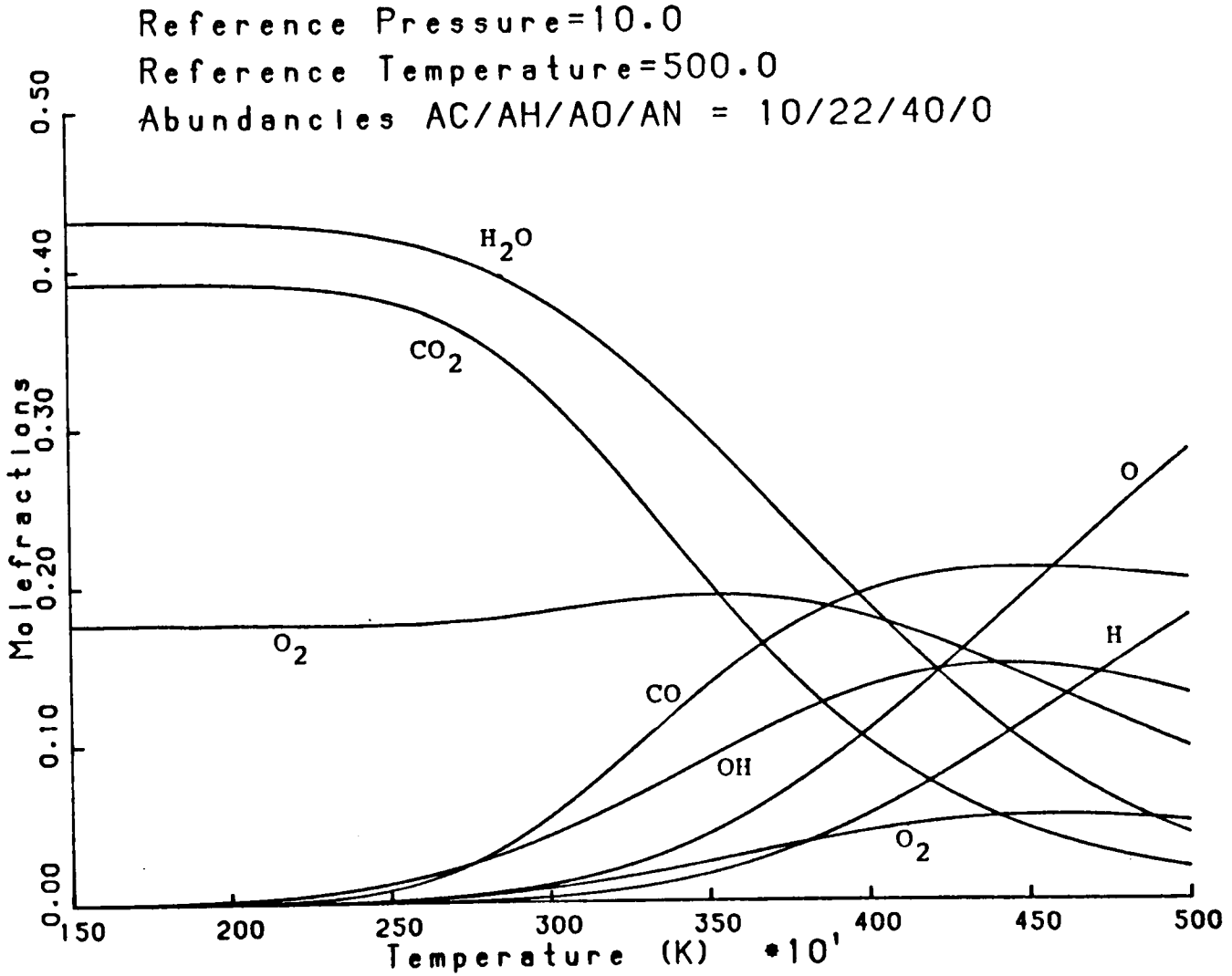


Figure VI-1. Equilibrium composition for C/H/O system. Constant volume combustion.

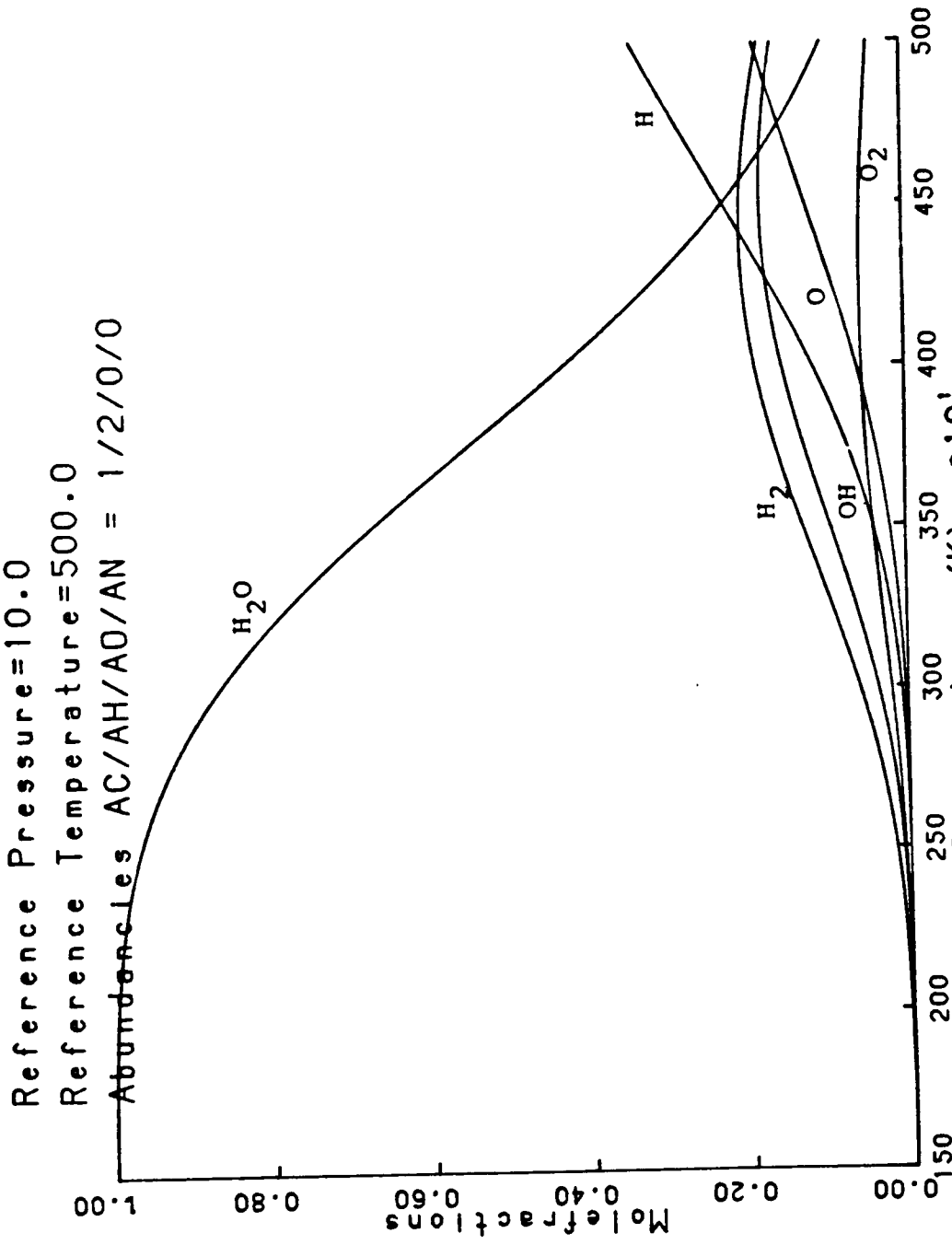


Figure VI-2. Equilibrium composition for H/O system. Constant volume combustion.

It should be noted that the absence of nitrogen greatly exaggerates the change in composition for the mixture as a whole. This can easily be seen when one observes that nitrogen, brought to the combustion by the air, composes about 70 to 80% of the total number of atoms per mole of fuel. Therefore, it is to be expected, when nitrogen is included in the calculations, the general behavior of the C, H, and O atoms, shown in Figures VI-1 and VI-2, will prevail but be somewhat depressed, since nitrogen behaves much like an inert gas over this temperature. Figure VI-3 is an example of results obtained for constant volume combustion, from the same reference states as before, but with nitrogen present.

The influence of pressure also affects the shape of the curves, through Lecatelier's principle. Based on the observation of dissociation equations (VI-2) it is noted that when the equations proceed in the dissociation direction, from right to left, the number of moles increases in general. This means that the effect of increased pressure is to suppress the dissociation of the original species CO_2, H_2O, O_2 and/or CO.

Since the accuracy of the proposed model to a large extent depends on the quality of these calculations, comparisons with other sources [10,18] were made in order to determine the validity of this method. In all cases acceptable agreement was observed.

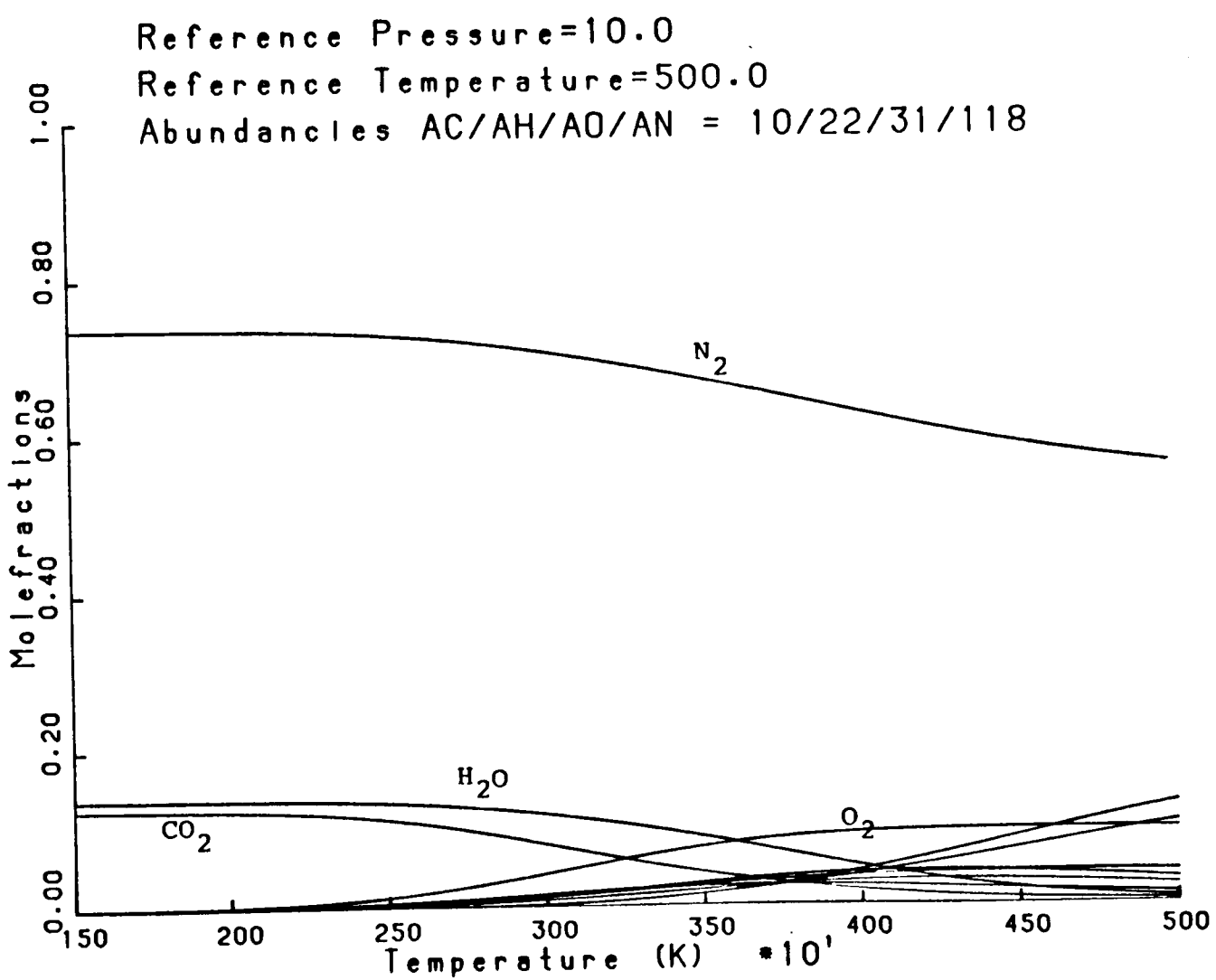


Figure VI-3. Equilibrium composition for C/H/O/N system. Constant volume combustion.

CHAPTER VII

CONCLUSIONS OF THE ANALYTICAL PART

The main purpose of this part of this work was to model the combustion cycle of a diesel engine running on both ammonia and fuel-oil; and, thus obtain a tool by which engine behavior could be predicted when ammonia is injected to the cycle.

The cycle chosen for the model incorporated constant volume combustion. Even though the diesel cycle, at least in theory, is based on constant pressure combustion it was felt that the constant volume cycle would more closely resemble the actual combustion process. This is based on the fact that in the real engine the ammonia and a large part of the fuel-oil that participate in the combustion are present in the combustion chamber at the onset of combustion.

Results of this model show that when increasingly more ammonia is used the performance factors deviate from those obtained with fuel-oil. For example, at equivalence ratios commonly obtained in diesel engines the thermal efficiency of the ammonia fueled cycle should be expected to be about 12% higher than for the cycle running on pure fuel-oil. On the other hand, the power output of the ammonia fueled cycle should be expected to be about 80% of that obtained with fuel-oil.

Caution should be exercised when comparing the theoretical results with those obtained from the engine tests. In addition to

the simplifying assumptions listed earlier, the model did not attempt to model the turbocharger and the precombustion feature of the test engine.

CHAPTER VIII

TEST EQUIPMENT

In this section a description of the system developed to execute the experimental part of this project will be described.

Engine

The engine used for this work was a Caterpillar D330, 4 cylinder, 4.75 in x 6.0 in, 425 cu in, 104 hp @ 1500 rpm, compression ratio 17.5:1. The engine was equipped with precombustion chambers and an impulse turbocharger. See Appendix F for a copy of manufacturer's specification sheets.

Fuel System

Complete fuel supply systems for both the ammonia and the fuel-oil were developed and installed in the engine laboratory (see Figure VIII-1).

In order to provide for safe handling of the ammonia during the test it was necessary to install certain special equipment. A 150-pound main cylinder supplies liquid ammonia to two parallel shell and tube evaporators. In addition to normal fittings, the tank was equipped with a valve system which allowed the ammonia fueling system to be vented between usage.

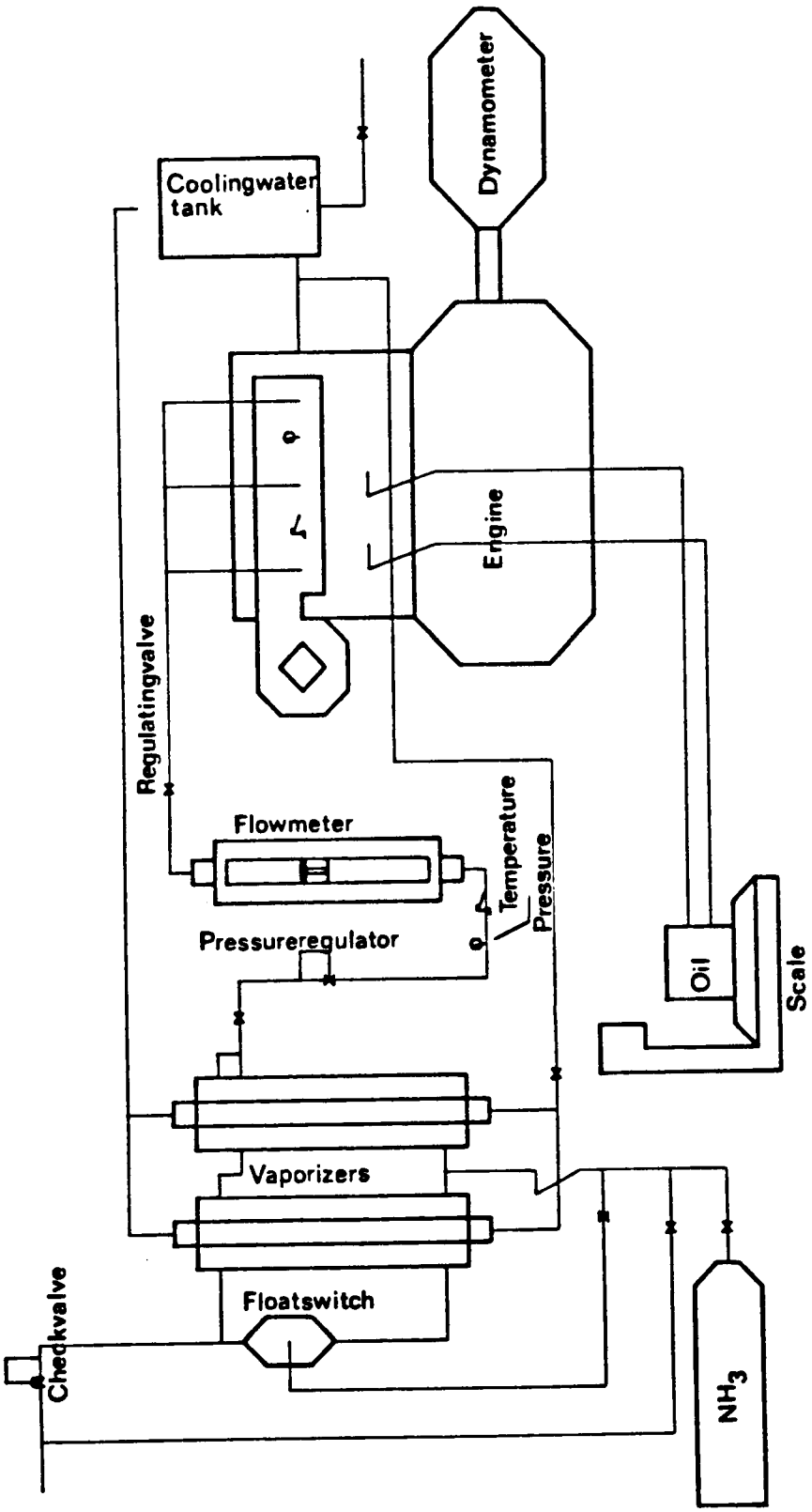


Figure VIII-1. Schematic of the fuel supply system, final version.

The evaporators were provided with heat from the cooling water of the engine. Control of the liquid level in the evaporators was accomplished by employing an electric floatswitch, which operated a solenoid valve on the liquid line from the ammonia tank. The operating pressure in the evaporators was controlled by a pressure regulator valve which controlled the flow rate of water to the evaporators. This arrangement maintained constant operating pressure under all conditions of ambient temperature or ammonia flow rate. Pressure relief valves, set to 150 psig, were mounted on the system to ensure safe operation.

Measurement of the mass flow rate of the ammonia, to be discussed in more detail in Chapter XI, was accomplished with a variable area flowmeter.

Dynamometer

All tests were conducted with the engine coupled to a General Electric DC current, type TLC3544, absorption dynamometer. The torque was measured by a load-cell connected to a strain gauge conditioner amplifier, which gave direct readings of engine torque. Engine speed was determined with the use of a frequency counter, connected to a magnetic pickup excited by the rotating shaft of the dynamometer.

Flowmeter

The mass flow rate of ammonia was measured by a Fisher Porter variable area flowmeter. In order to obtain accurate mass flow rate

measurements, knowledge of the conditions of the ammonia entering the meter have to be known. In order to accomplish this, a pressure regulator was installed to control the pressure of the entering mmonia. A pressure gauge on the outlet from the pressure regulator enabled accurate determination of the prevailing pressure. Measurements of the ammonia temperature after the pressure reduction were accomplished with an iron-constantan thermocouple. This setup enabled accurate determination of the pressure and temperature of the ammonia entering the meter. The meter, originally intended for air flow measurements, was calibrated for ammonia (see Chapter XI).

Oil Flow Rate

A separate fuel line for the oil was installed. The fuel-oil to the engine was taken from a small tank placed on a scale. The mass flow rate of the fuel-oil was determined by recording the time it took the engine to consume a specific amount of oil from the tank. A larger storage tank was then used to replenish the small tank.

Air Flow Rate

The air flow rate to the engine was determined by using a Meriam Laminar Flow Meter, model 50MC2-4, in conjunction with a Meriam, model 40HE35-50, inclined manometer.

Pressure-Time Trace

In order to obtain information about the behavior of the pressure in the engine's cylinders, a pressure transducer was adapted

to the engine. The transducer used was a Kistler Model 603-A. The output from the pressure pickup was amplified by a Kistler Model 503 charge amplifier and displayed on a Tektronix Model 564 dual-beam storage oscilloscope equipped with a dual trace amplifier and 2B67 time base. Photographs of the pressure-time trace were obtained with a Tektronix oscilloscope camera.

Floatswitch

Control of the liquid level in the evaporators was accomplished with a Refrigeration Specialties Co., Model LLX, floatswitch. The switch activated a solenoid valve mounted on the ammonia liquid line from the ammonia tank. Setting the liquid level in the evaporators was done by raising or lowering the floatswitch.

Other Equipment

Other special equipment used for monitoring the engine were stainless steel pressure gauges. These were necessary because of the corrosiveness of ammonia with copper or brass.

All temperatures were monitored using iron-constantan thermocouples. The manifold temperature and the temperature of the air into the laminar flow element were obtained using a Gould Brush, Model 2400, thermocouple reader.

The temperature of the ammonia at the inlet to the flowmeter, and of the ammonia-air mixture in the engine's manifold, was obtained from an Omega, Model 2165A thermocouple reader.

The following table, Table VIII-1, is a detailed listing of the test equipment used in the course of this experiment.

Table VIII-1. Listing of Test Equipment.

Equipment	Description
Air Flow	Merian Laminar Flow Element, Model 50MX2-4, 400 CFM @ 14.7 psia; 8 in H_2O.
Camera	Tektronix Oscilloscope Camera Model C-12, with Polaroid adapter.
Charge Amplifier	Kistler, Model 503.
Dynamometer	General Electric, DC current, Model TLC3544.
Engine	Catepillar D330c, see Appendix F.
Floatswitch	Refrigerator Specialties Co., Model LLX.
Flowmeter	Fisher-Porter Co., Type 10a1700, max SCFM air: 3.3 @ 10.0 psig; 70 F. Max operating pressure 200 psig.
Oscilloscope	Tektronix, Model 564, storage oscilloscope, 3A72 dual trace amplifier and 2B67 time base.
Photographs	Oscilloscope Camera, Model C-12, with Polaroid extension for Type 52. Film used: 3000 ASA film.
Pressure Gauges	Super Gauges, Model 41/2, AD-10593, Range 0-160 psig, stainless steel.
Pressure Regulator	Union Carbide Linde Div., Model R-201-3260.
Pressure Transducer	Kistler, Model 603-A, range 0-5000 psia, 0.365 pcb/psi.
rpm Counter	Hewlett-Packard, Model 5301A, 10 MHz counter, connected to a magnetic switch attached to the dynamometer.
Temperature Manifold and Inlet Air	Gould Brush, Model 2400 Thermocouple Amplifier.
Temperature Ammonia	Omega Engineering, Inc., Model 2165A digital thermocouple reader.
Torque	Load-Cell: BHL Electronics, Model U3G1. Strain-Gauge Conditioner Amplifier: Daytronics Model 857A.

CHAPTER IX

TEST PROCEDURE

Fuel Consumption—Fuel Oil

The mass flow rate of the fuel-oil was measured by placing a small plenum tank, containing the fuel-oil, on a scale and recording the time it took the engine to consume exactly 4, 8, and 16 oz of fuel-oil. Each measurement was initiated by starting a stopwatch when the scale hand passed a predetermined mark on the scale. Then a 4 oz weight was placed on the fuel-oil side of the scale. When the scale hand passed the predetermined mark the second time, the time required for this weight to be consumed by the engine was recorded by measuring the elapsed time since the measurement was started (lap-time), but the watch was not stopped. The second weight 4 oz was then placed on the scale and the time required for the consumption of now a total of 8 oz was recorded. Finally, when the scale hand passed the mark the third time 8 oz were added to the scale, and the time required for consumption of now a total of 16 oz, or 1 lbm. recorded.

This method was employed primarily because it saved time, but in addition it gives a quality check on the measurements, since each elapsed time should ideally be twice the time it took the engine to consume the previous weight. As a guideline, if the difference in the ratio of times was more than 2% the record was rejected and the measurement repeated.

This method yielded consistent values for all weights, with a maximum error of ± 2% within 95% confidence interval for each set of records.

Fuel Consumption—Ammonia

One of the main concerns of this project was the relationship between the fuel flow rates of ammonia and fuel-oil. In order to establish this relationship a means by which the mass flow rate of ammonia could be measured had to be developed. While the measurement of the fuel-oil flow was fairly straightforward, measurement of the ammonia flow rate proved to be much more complicated.

Initially, the same method used for the fuel-oil was tried: i.e., a small ammonia tank was placed on a scale and the flow rate measured in the same way as for the fuel-oil. The accuracy of this method was judged to be unacceptable. The prime reason for the failure of this method was due to the fact that the mass flow rate of ammonia through the evaporators was not steady since the evaporators did not operate under steady state conditions. Thus the liquid flow rate from the ammonia tank was not necessarily instantaneously equal to the vapor flow rate to the engine.

In order to overcome this problem, a liquid level sightglass was placed parallel to the inlet and outlet of the evaporators, thus making an indirect measurement of the flow rate possible. A schematic of this system is shown in Figure IX-1. Measurement of the ammonia flow rate was carried out by filling approximately 50-75% of the

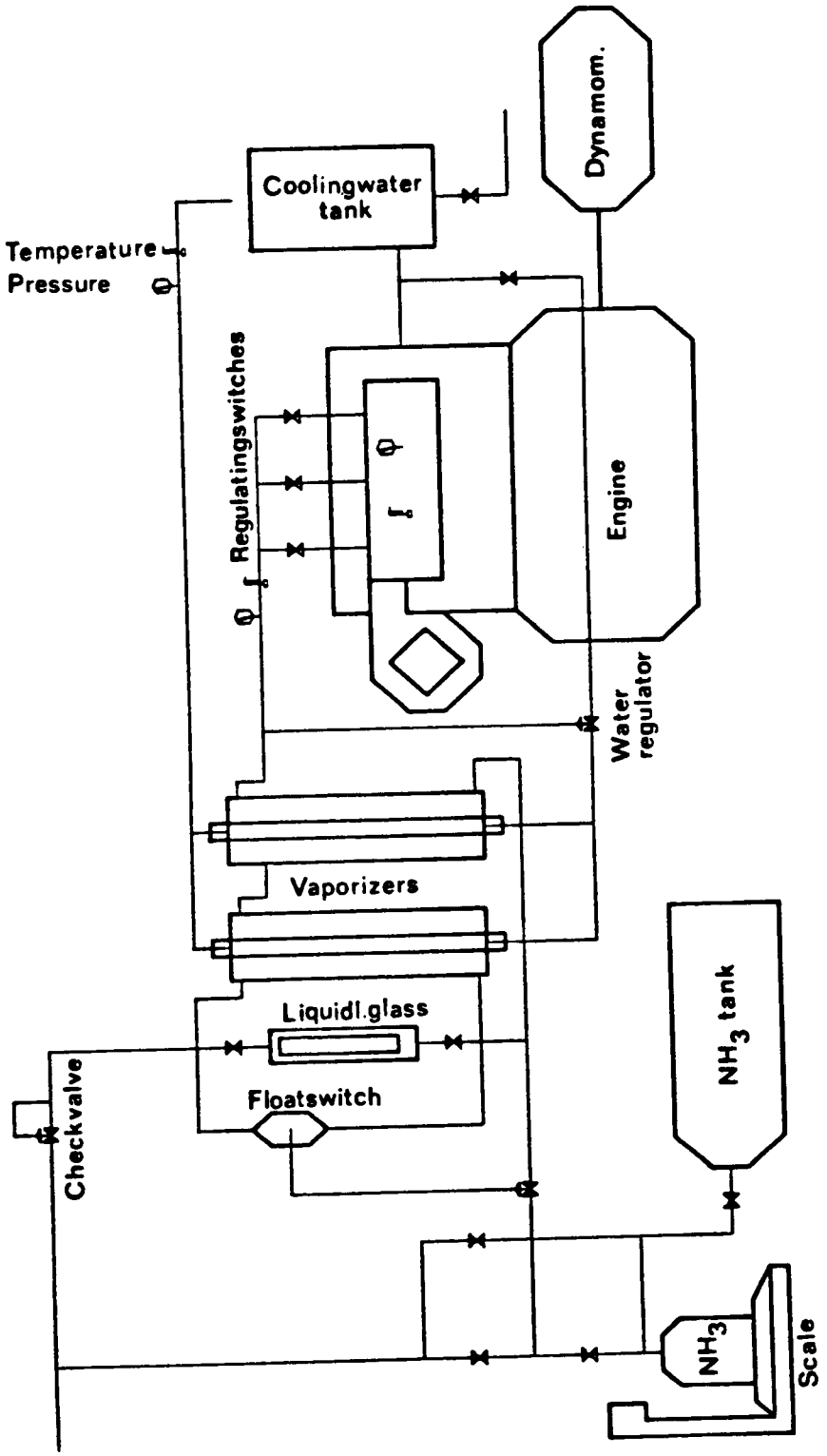


Figure IX-1. Schematic of the fuel supply system, first version.

evaporators and measuring the time it took the liquid level to drop through a specific distance. Knowledge of the geometry of the evaporators and the thermodynamic conditions of the ammonia enabled calculation of the mass flow rate. Even though this method yielded better results than the previously described method, both were judged still to be outside acceptable limits—primarily because vapor bubbles flowing through the sightglass disturbed accurate measurement of the distance that the liquid level had dropped during each measurement. The existence of the vapor bubbles in the sightglass is not fully understood, but it is known that even though the prevailing pressure of the ammonia within the evaporators is high (14.0 atm), the temperature of the cooling water is probably high enough to cause violent boiling of the ammonia (and may even cause the ammonia to flash). In addition, it is also possible that the vapor bubbles are caused by local transfer of heat to the ammonia in the piping system outside the evaporators. No attempt was made to insulate the piping system to overcome this problem.

The third method tried proved to be successful and provided values well within acceptable accuracy limits. The method consisted of a flowmeter (rotameter), placed on the ammonia vapor line immediately before the engine manifold. The main advantage of this method is that all the ammonia that flows through the device over a given time interval is consumed by the engine. Furthermore, given that the inlet conditions to the meter can be accurately determined and that they can be assumed constant over the measuring period, the

accuracy and repeatability of this flowmeter further assures accurate measurements [20].

Since flowmeters of this type measure volumetric flow, the accuracy with which the mass flow rate can be determined is directly related to the accuracy with which the density of the flowing gas can be determined. In order to evaluate the density of the inflowing ammonia, knowledge of the temperature and pressure at the inlet to the meter is sufficient. In order to assure accurate and constant inlet conditions the ammonia was led through a pressure regulator, before flowing to the meter. A pressure gauge and thermocouple were installed in the vapor line to the flowmeter, to permit measurement of the pressure and the temperature during the test. Adjustment of the flow rate to the engine was carried out by a regulating valve located on the vapor line after the flowmeter.

Calibration of this meter would ideally be done at some predetermined values of the pressure and the temperature, but it was not possible to vary the pressure and the temperature independently. The temperature was found to be related to the condition of the ammonia in the evaporators and the opening of the regulating valve. A constant value of the pressure, however, was secured by the pressure regulator.

The rotameter used for this test was calibrated by the manufacturer for air at 10 atm and 70 F, but according to the manufacturer's manual [20] conversion to different gases and conditions can be accomplished in a systematic way using the formula:

$$\dot{m}_a = \rho(10,460)SCFM, \text{ where } SCFM = RD\left(\frac{P_i + 10}{10}\right)^{1/2}\left(\frac{460}{T_i + 460}\right)^{1/2}(Sp.Gr)^{-1/2} \quad \text{(IX-1)}$$

where

RD: is the actual reading of the meter;

SCFM: is the volumetric flow rate of ammonia at the standard conditions of the meter, @ 10.0 psia; 70 F);

$\rho(10,460)$: is the density of ammonia at the standard conditions of the meter;

SP.Gr: is the specific gravity of the ammonia;

P_i: is the inlet pressure of the ammonia;

T_i: is the inlet temperature of the ammonia.

This equation provides a means by which the mass flow rate of a substance with specific gravity Sp.Gr can be related to the reading of the meter.

In order to establish the validity of these formulas, the meter was calibrated for different values of pressure and mass flow. The flowmeter, pressure regulator, pressure gauge, thermocouple, and the needle valve were disconnected from the engine and connected to a small tank of ammonia placed on a scale. The tank supplied gaseous ammonia to the system.

The calibration consisted of correlating the calculated mass flow rate (using Eq. IX-1) and the measured flow rates, for volumetric flow rates, ranging from 10% to 100% of full scale at three different pressure values.

Each test was started by adjusting the pressure to a desired value by adjusting the pressure regulator. The adjustment valve on the flowmeter was then opened until the meter float showed a specific reading. The mass flow rate of ammonia was measured using the same method as described in Chapter X for the fuel-oil flow rate. This method yielded consistent values for all adjustments with a maximum error of 5% within 95% confidence interval for each adjustment. The prevailing temperature and pressure were also recorded for each test run, thus allowing the density of the ammonia to be determined. The calculated and the measured mass flow rates were then compared. Figure IX-2 represents the result of this experiment.

From Figure IX-2 it can be observed that good correlation exists between the calculated and the measured mass flow rates. Note, however, that for higher volumetric flow rates the correlation is not as good. This discrepancy stems from the fact that in practice this particular meter type does not have a perfectly linear relationship between volumetric and mass flow rate, as it should theoretically have. However, the difference between the calculated and the measured mass flow rates never exceeded 3%. This allowed the assumption to be made that the mass flow rate of the ammonia could be derived from knowledge of the temperature, pressure and the volumetric flow rate of the ammonia through the meter.

Initially, baseline tests with oil were run from which the brake specific fuel consumption (BSFC) versus brake mean effective pressure (BMEP) were measured for one speed setting (1500 rpm). At

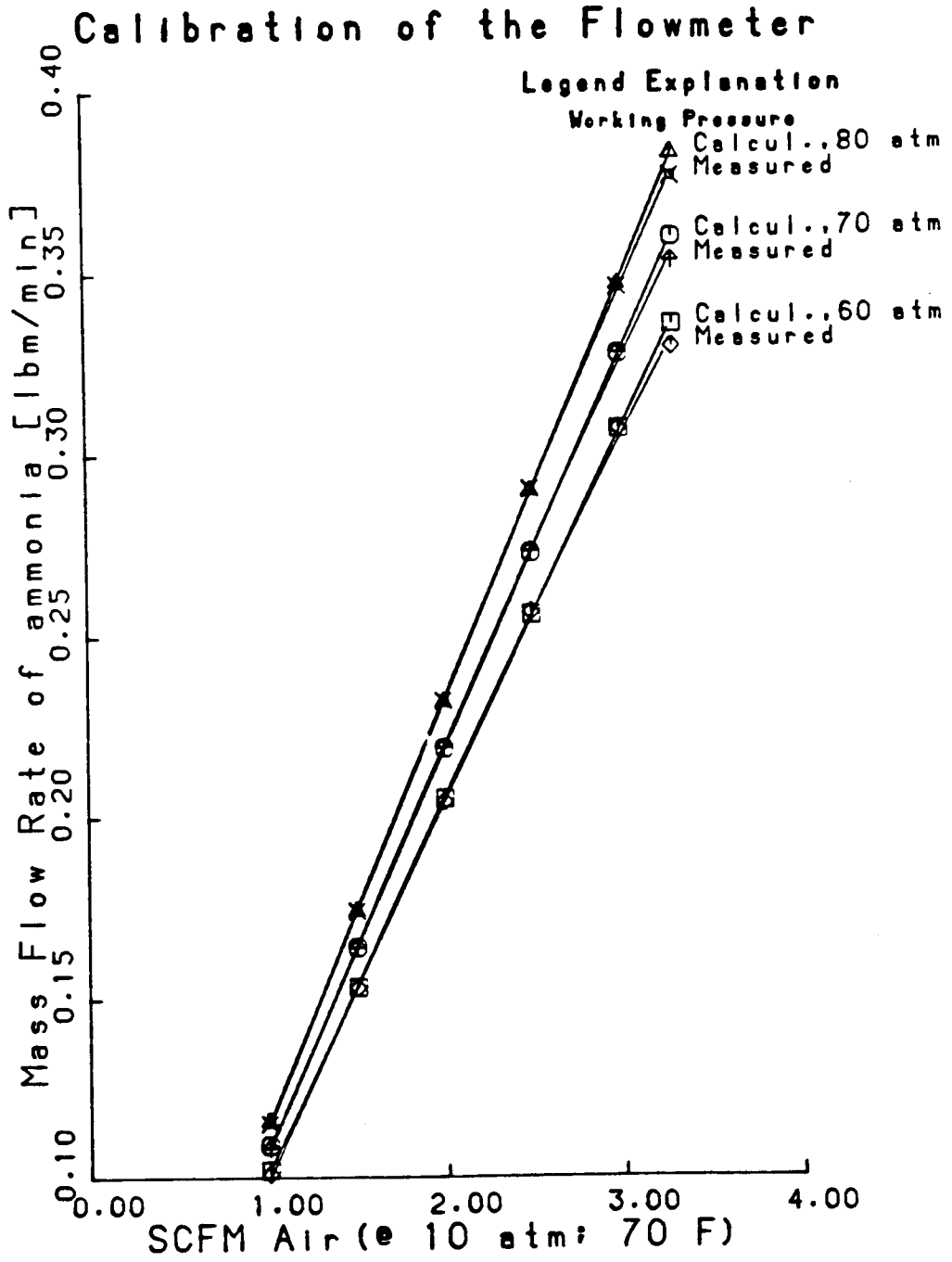


Figure IX-2. Comparison of the calculated and measured mass flow rate of ammonia.

this specified speed value the load was varied in steps from no load to maximum, and the fuel flow rate at each step measured with the method described above. No emission tests were taken during these particular tests.

The relationship between the reduction in mass flow rate of fuel-oil with increasing ammonia flow into the engine manifold was measured, for four different load conditions (100, 200, 300 and 376 [Ft-lbf]); and, with the engine running at constant speed 1500 rpm. Within each test run the mass flow rate of ammonia was increased from zero to the point where the engine was judged to be running under unacceptable conditions, determined by irregular combustion and autoignition.

Adjustment of the ammonia mass flow rate to the engine was accomplished by adjusting the pressure to the flowmeter to a predetermined value and opening the adjustment valve to the engine, thus allowing the meter float to reach some determined height. The height of the float, pressure and temperature were then recorded; thus allowing calculation of the mass flow rate of the ammonia according to Eq. IX-1. Note, however, that this method does not predetermine the mass flow of ammonia since the temperature is not an independent variable. This was repeated for torques of 100, 200, 300 and 376 [Ft-lbf], or 27%, 53%, 80%, and 100% of full load and with the engine running at 1500 rpm. As mentioned, the injection of ammonia was stopped when the engine was judged to be running at unacceptable conditions. "Unacceptable conditions," however, in this context is highly subjective (see Chapter X, p. 107, for discussions).

The relationship between the volumetric flow rates of ammonia and air to the engine were of interest. Since the ammonia is injected to the engine manifold in vapor form, it was expected that its presence might reduce the amount of air flowing to the engine and consequently reduce the engine's maximum power. Records of the air flow were, therefore, obtained for each setting of the ammonia flow rate.

Pressure-Time Trace

In order to obtain information about the pressure within the combustion chamber, the engine was modified to accept a Kistler Model 603-A pressure pickup. To gain access to the combustion chamber one of the glow plugs was removed and replaced with the pressure pickup mounted in a water cooled jacked especially designed for this project.

With this setup three tests were conducted. In the first test the engine was run under constant load, 100 [Ft-lbf], 1500 rpm and four different ammonia/fuel-oil ratios. The second test was conducted with the engine running at maximum load, 376 [Ft-lbf], 1500 rpm, and four different ammonia fuel-oil ratios.

Before any records were taken the engine was allowed to stabilize as indicated by the conditions of the cooling water and the temperature of the inlet air in the manifold. Records of the mass flow rates of ammonia and fuel-oil were obtained in the same fashion as described above.

It was noted during the test that the pressure-time trace as seen on the oscilloscope screen was consistently repeatable; and, therefore, the figures shown can be regarded as being representative of the figures seen on the oscilloscope.

The results of these tests are presented in Chapter X.

CHAPTER X

EXPERIMENTAL RESULTS

Performance Test

The brake specific fuel consumption (BSFC) versus brake mean effective pressure (BMEP) of the engine was measured for oil only at a speed of 1500 rpm. Figure X-1 presents results of this experiment.

Reduction in Fuel-Oil Consumption

One of the main concerns of this project was the relationship between the fuel flow rates of ammonia and fuel-oil. In order to establish this relationship the engine was run under different load conditions and the ammonia flow rate to the engine increased until the engine was judged to be running under unacceptable conditions. Unacceptable conditions, however, in this context, as said before, is highly subjective and no completely satisfactory definition for knock can be given. However, in general, when autoignition occurs two different types of vibration may be present. In one case, a large amount of the fuel-air mixture may autoignite and as a result a very rapid increase in pressure throughout the combustion chamber is experienced, and the engine structure as a whole will suffer. This will typically be detected by the ear as a thudding sound. In the other case, a large pressure difference may exist in the combustion chamber, and the resulting gas vibration can force the walls

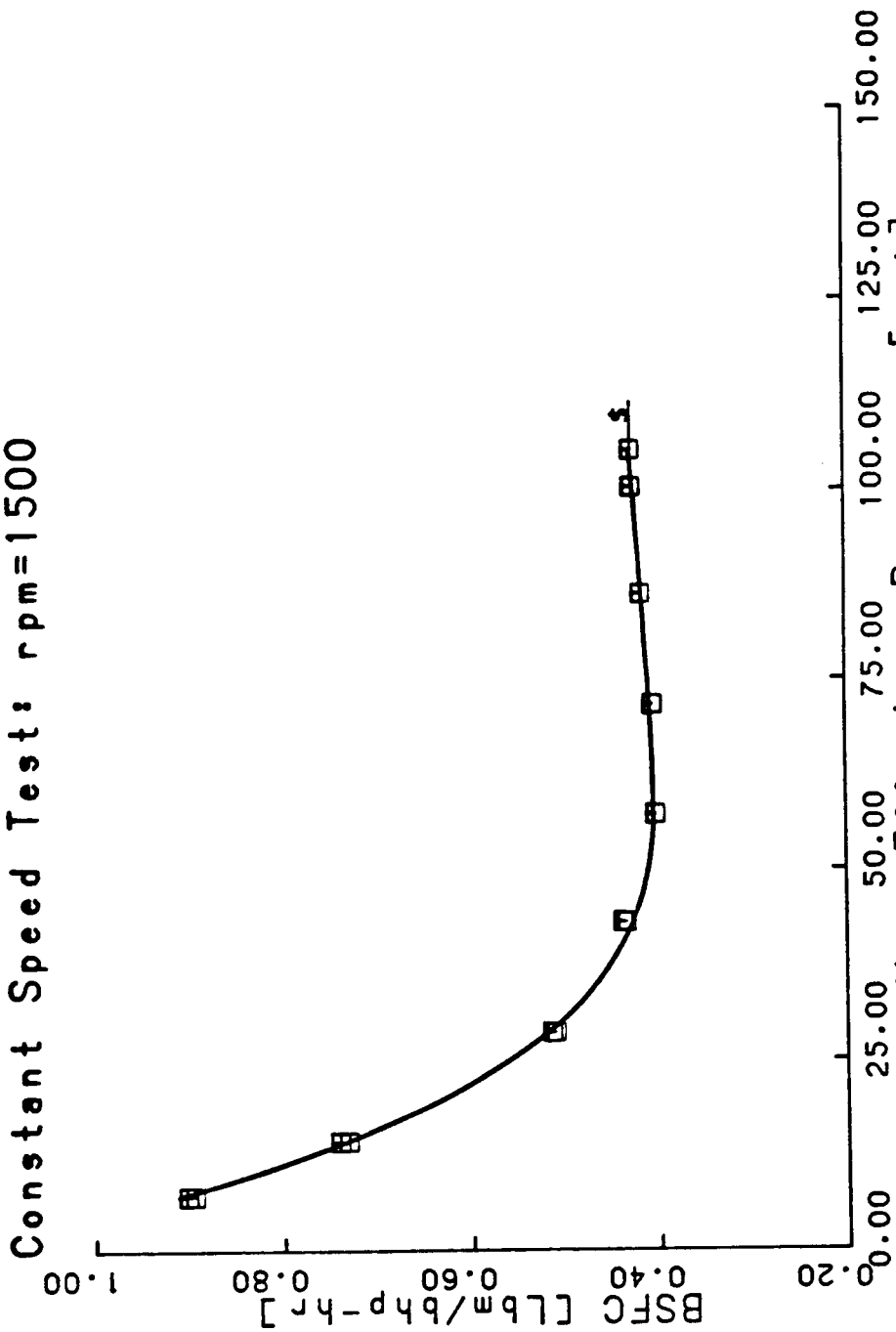


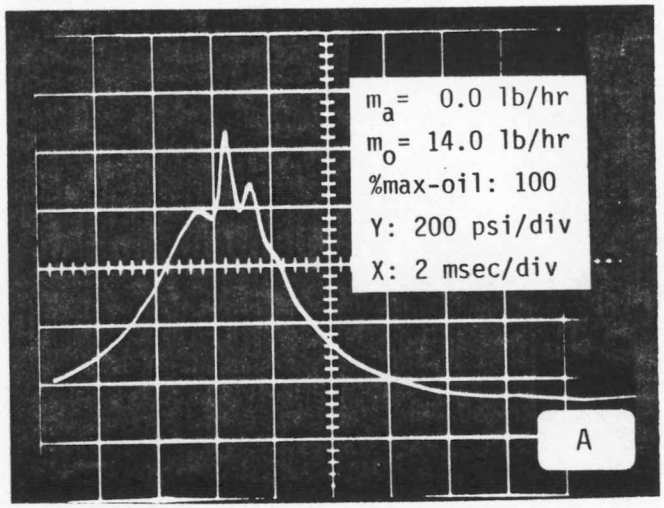
Figure X-1. Constant-speed, variable fuel injection test for CAT D330 (4 cyl., 4.75x6.0, 425 cu. in.).

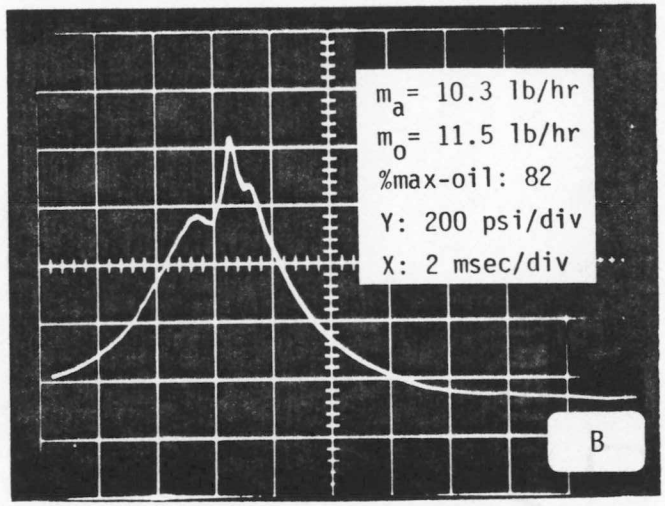
of the combustion chamber to vibrate with the same frequency as the gas. The ear will detect this sound as a pinging sound. Both of these effects are usually present in the engine when it knocks. Thus, in this test the engine was determined to be running under unacceptable conditions, when both of these sounds were clearly audible. Plates X-1 and X-2 are of photographs obtained of the pressure-time trace of the engine when run under the two different load conditions (100 and 376 Ft-lbf) and with different ammonia to fuel-oil ratios. From these figures it can be concluded that in the case of maximum ammonia injection the engine is knocking heavily, and that the shape of the graph represents unacceptable performance.

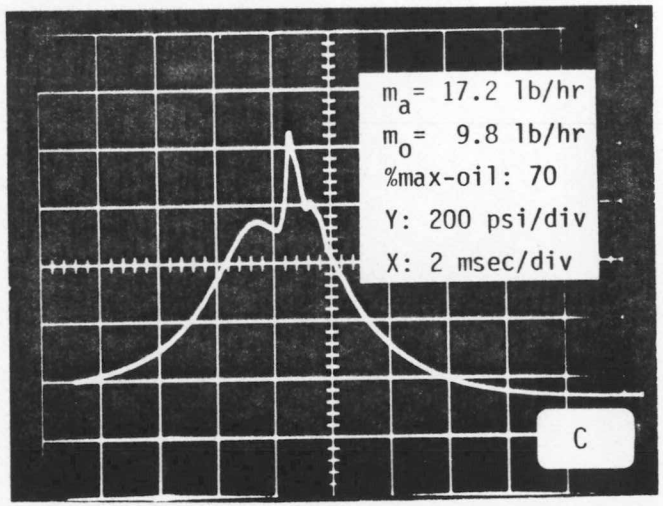
Figure X-2 shows the fuel-oil flow rate as a function of the ammonia flow rate. From the figure it can be seen that the amount of fuel-oil that can be replaced by ammonia is about the same for all load cases. Numerical analysis of the curves shows that the fuel-oil flow rate decreases by 0.25 units for each unit increase of ammonia flow rate. A number of conclusions can be drawn from this information. The following equation defines the thermal efficiency of the engine:

$$\eta_t = \left(\frac{2545\ P_b}{\dot{m}_a U_{rp_a} + \dot{m}_o U_{rp_o}}\right) \qquad (X\text{-}1)$$

where P_b is the brake horsepower of the engine, U_{rp_a} and U_{rp_o} are the lower internal energies of reaction values for ammonia and fuel-oil, respectively, and m_a and m_o are the mass flow rates of the fuels.







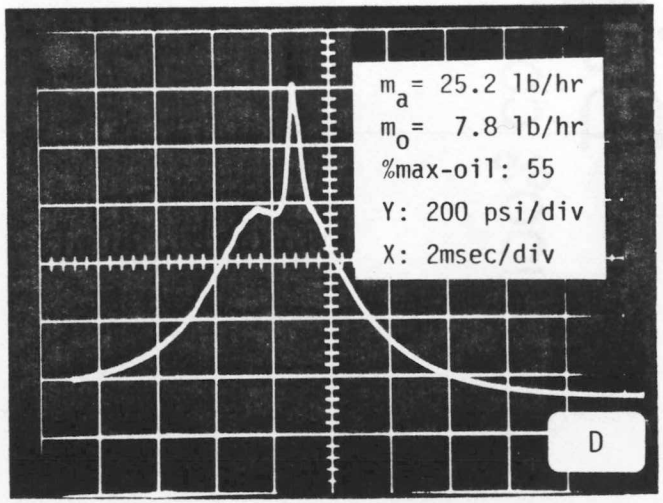
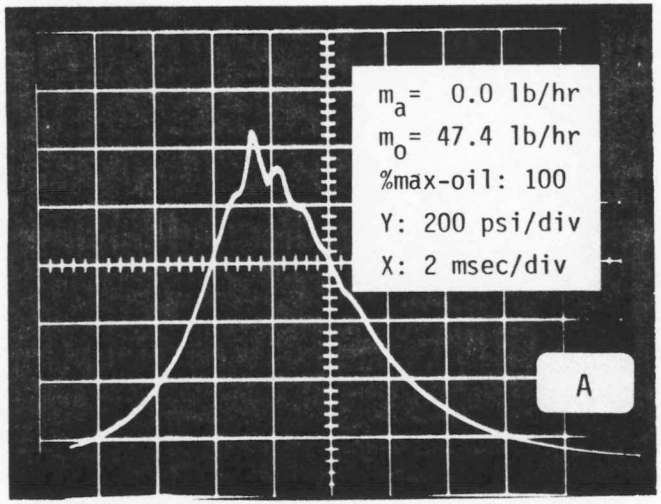
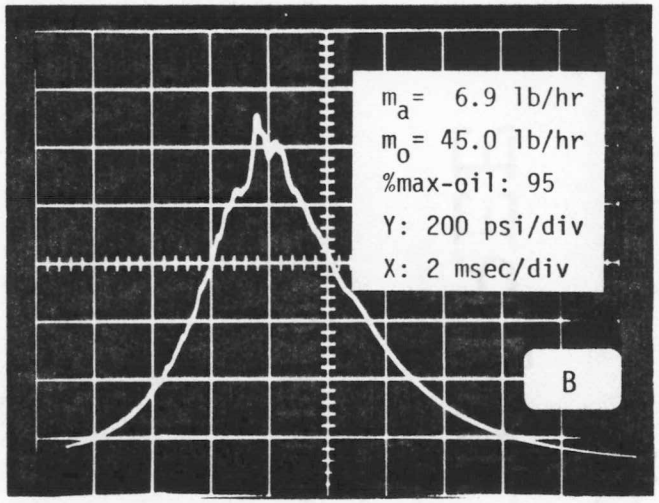
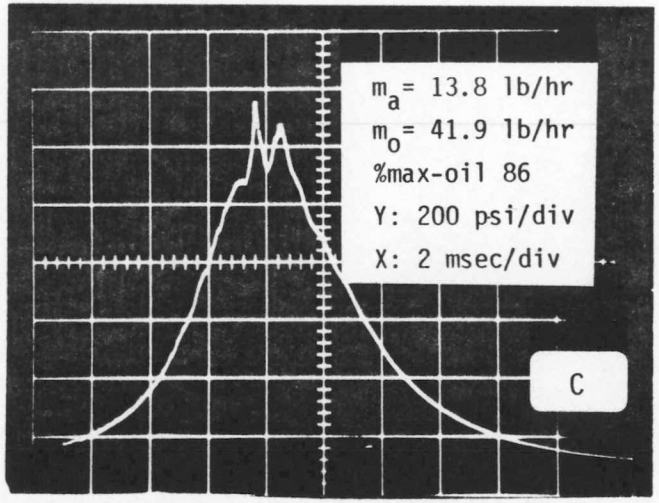


Plate X-1. Pressure-time trace for the engine, running on ammonia and fuel oil, @ 100 [Ft-lbf]; 1500 rpm.







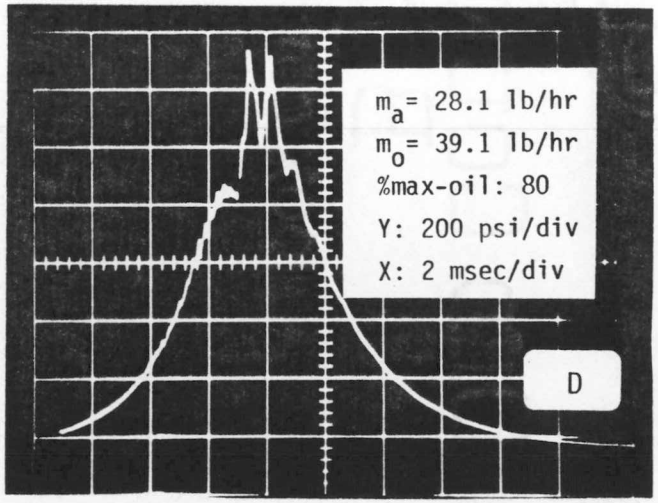


Plate A-2. Pressure-time trace for the engine, running on ammonia and fuel oil, @ max load, 376 [Ft-lbf]; 1500 rpm.

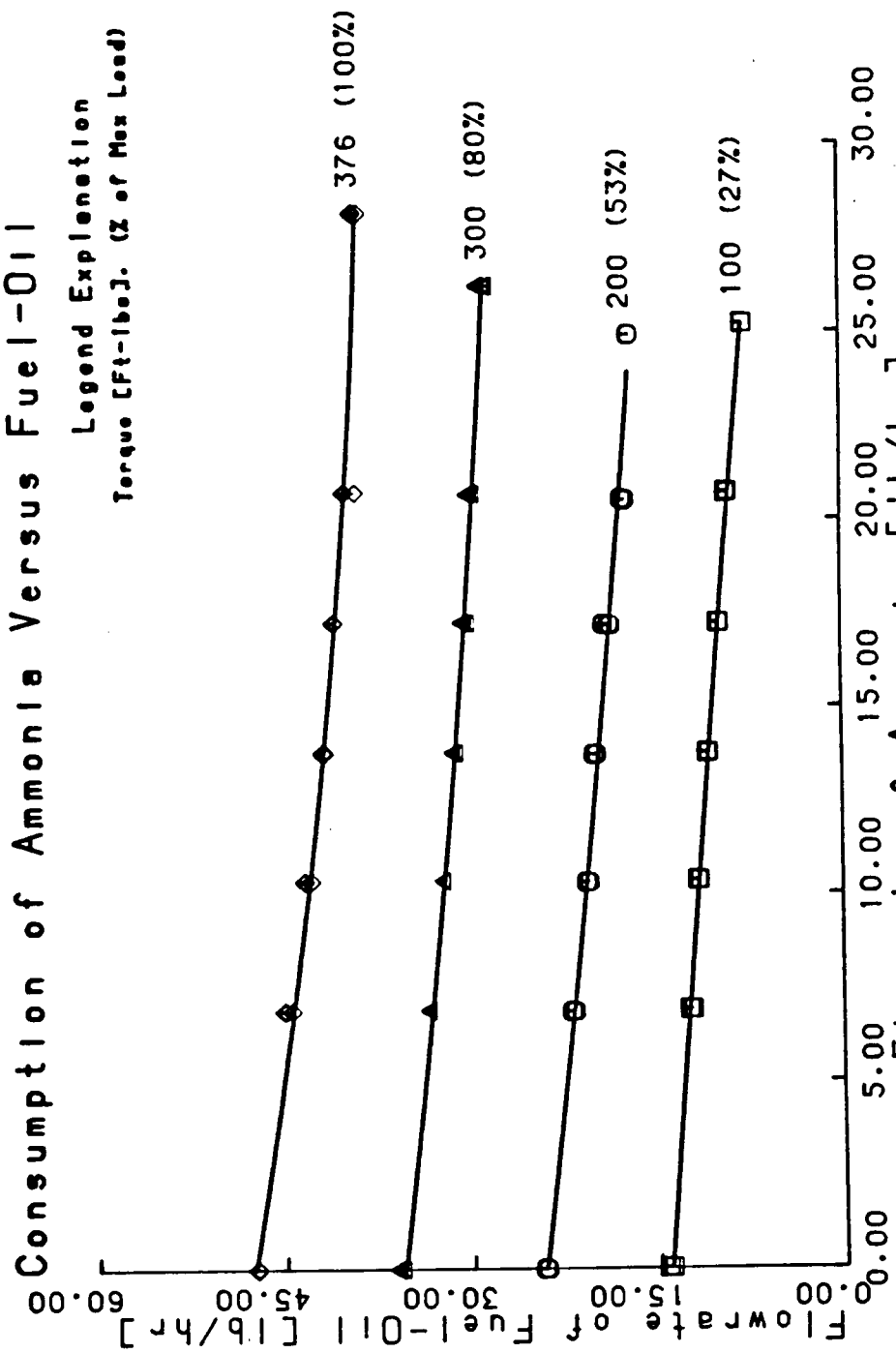


Figure X-2. Comparison of flow rate of ammonia and fuel-oil.

References [10,17] give numerical values for U_{rp_o} (17500 [Btu/lbm]) and U_{rp_a} (8080 [Btu/lbm]).

If it is assumed that for the constant load case the thermal efficiency of the engine is unaltered when the ammonia is being injected into the engine, the following relationship exists between the ammonia fuel flow rate and the fuel-oil flow rate:

$$\dot{m}_o = \frac{2545\ P_b}{U_{rp_o}} - \dot{m}_a\left(\frac{U_{rp_a}}{U_{rp_o}}\right) \qquad \text{(X-2)}$$

This equation when differentiated with respect to the ammonia flow rate reveals the relationship between change in fuel-oil rate with change in ammonia flow rate as follows:

$$d\dot{m}_o/d\dot{m}_a = -\left(\frac{U_{rp_a}}{U_{rp_o}}\right) = -\left(\frac{8080}{17500}\right) = -0.46 \qquad \text{(X-3)}$$

Therefore, when the numerical value of this last equation is compared to a much lower ratio, 0.25, obtained during the tests, the conclusion can be drawn that in the present case about 46% of the ammonia consumed by the engine is not burned, and should, therefore, be detected in the exhaust from the engine. This was partially substantiated by the presence of ammonia odor from the exhaust during testing of the engine.

This analysis is, of course, only accurate within the limits of the assumptions on which it is based; namely, that the thermal

efficiency (3%) should be expected (see Plate V-6, Figure C, p. 56). The results of the experimental part, further, substantiate this. Based on these arguments, it can be seen that the slopes of the curves normalized by the ratio (U_{rp_a}/U_{rp_o}) indicate how effectively the ammonia is burned by the engine. Figure X-3 shows the relationship between specific fuel consumptions for fuel-oil versus ammonia. The same, basically, linear relationship is preserved here as in Figure X-2.

Thermal Efficiency

The thermal efficiency of the engine indicates how well the engine utilizes the fuel fed to it. Figure X-4 shows the thermal efficiency of the engine, defined by Eq. X-1, as a function of the ammonia flow rate. The figure reveals that for low loads the thermal efficiency of the engine decreases with increases in ammonia flow rate, by as much as 35%. At higher loads it can be seen that the thermal efficiency is affected less by the increased ammonia flow rate and that the maximum increase is only about 3%. It is interesting to note that for high loads these results agree with what was projected by the mathematical model in Chapter V.

Volumetric Flow of Air

The effect of ammonia flow rate on the volumetric flow of air is of interest. Since the ammonia was injected to the engine manifold in vapor form it was expected that its presence in the manifold might

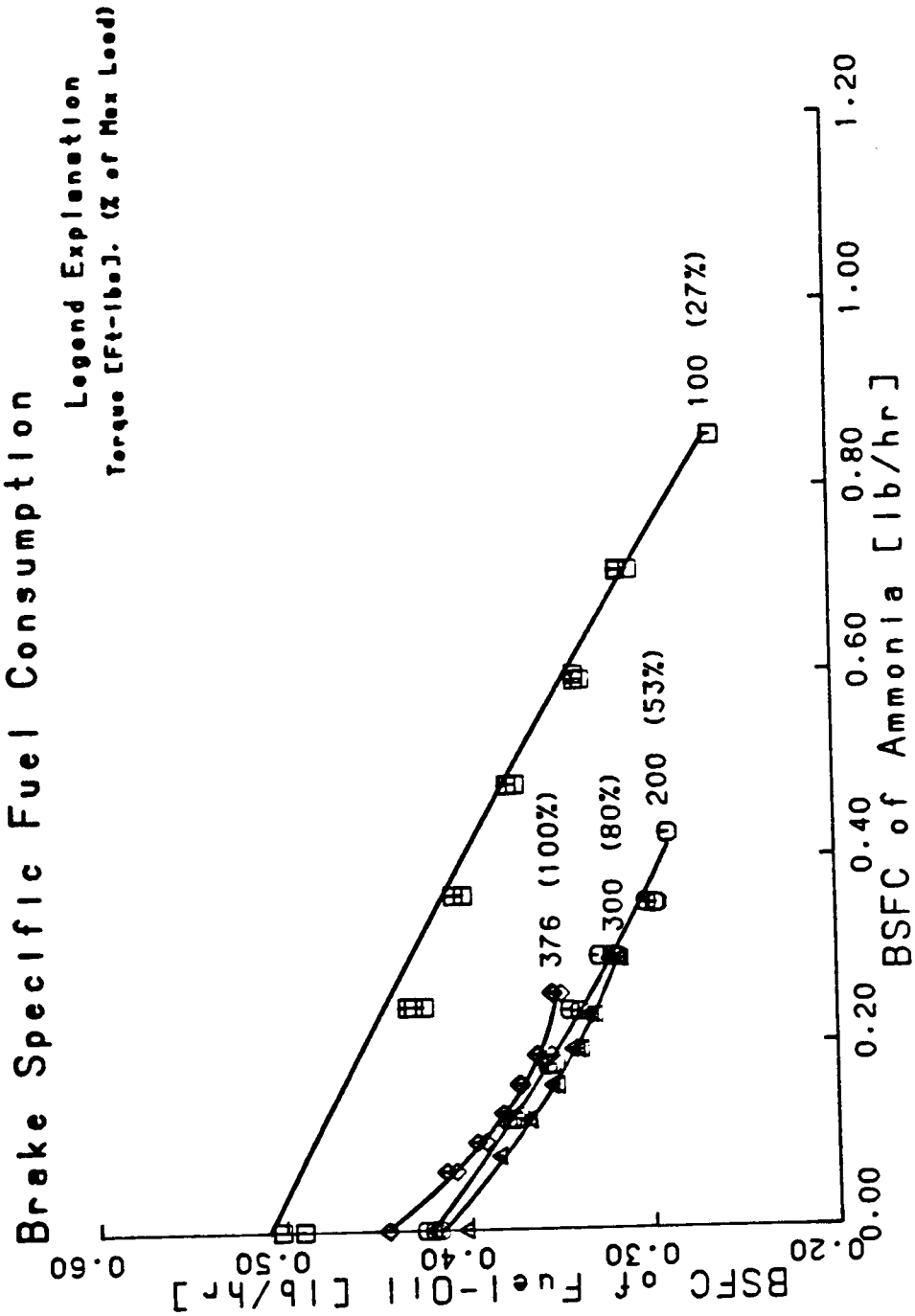


Figure X-3. Comparison of BSFC of ammonia and fuel-oil.

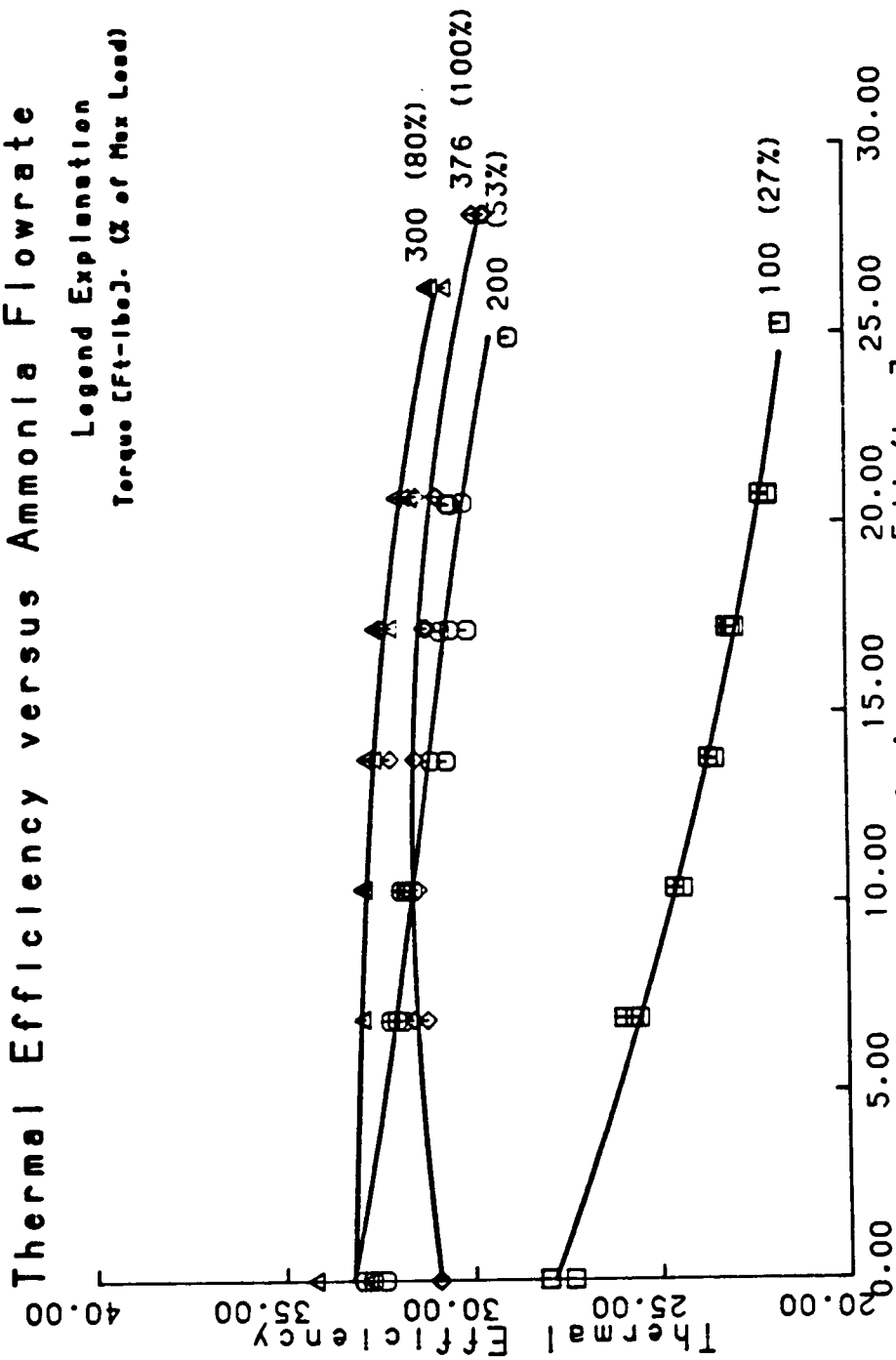


Figure X-4. Thermal efficiency of the engine as a function of flow rate of ammonia.

reduce the volumetric flow of air to the engine and thus reduce the maximum amount of power that the engine could be expected to deliver. Measurement of the air flow was accomplished by a Meriam Laminar Flow Element connected to the turbocharger intake. Figure X-5 shows the volumetric flow rate of air to the engine as a function of ammonia flow rate. The figure reveals that for all loads no appreciable change of air flow to the engine was experienced, despite the injection of ammonia to the engine. However, when the ammonia flow rate was increased the boost pressure increased slightly. The fact that the flowrate of air is not reduced by the presence of ammonia in the induction air is probably due to a conservative choice of compressor by the manufacturer. However, it should be noted that when the engine was run at full load and the ammonia flow rate adjusted to the maximum possible, minor turbine surge occurred which resulted in fluctuations of the manifold pressure. The explanation of this rests in the properties of centrifugal compressors [21,9]. Consequently, when a turbocharged engine is to be fueled with ammonia, allowance may have to be made for the increased pressure that the presence of ammonia creates in the manifold, otherwise surge and erratic operation may result.

Pressure-Time Trace

In order to obtain insight into the possible cause for the tendency of the engine to knock or rumble, a pressure transducer was adapted to the engine. During this test the engine was subjected to

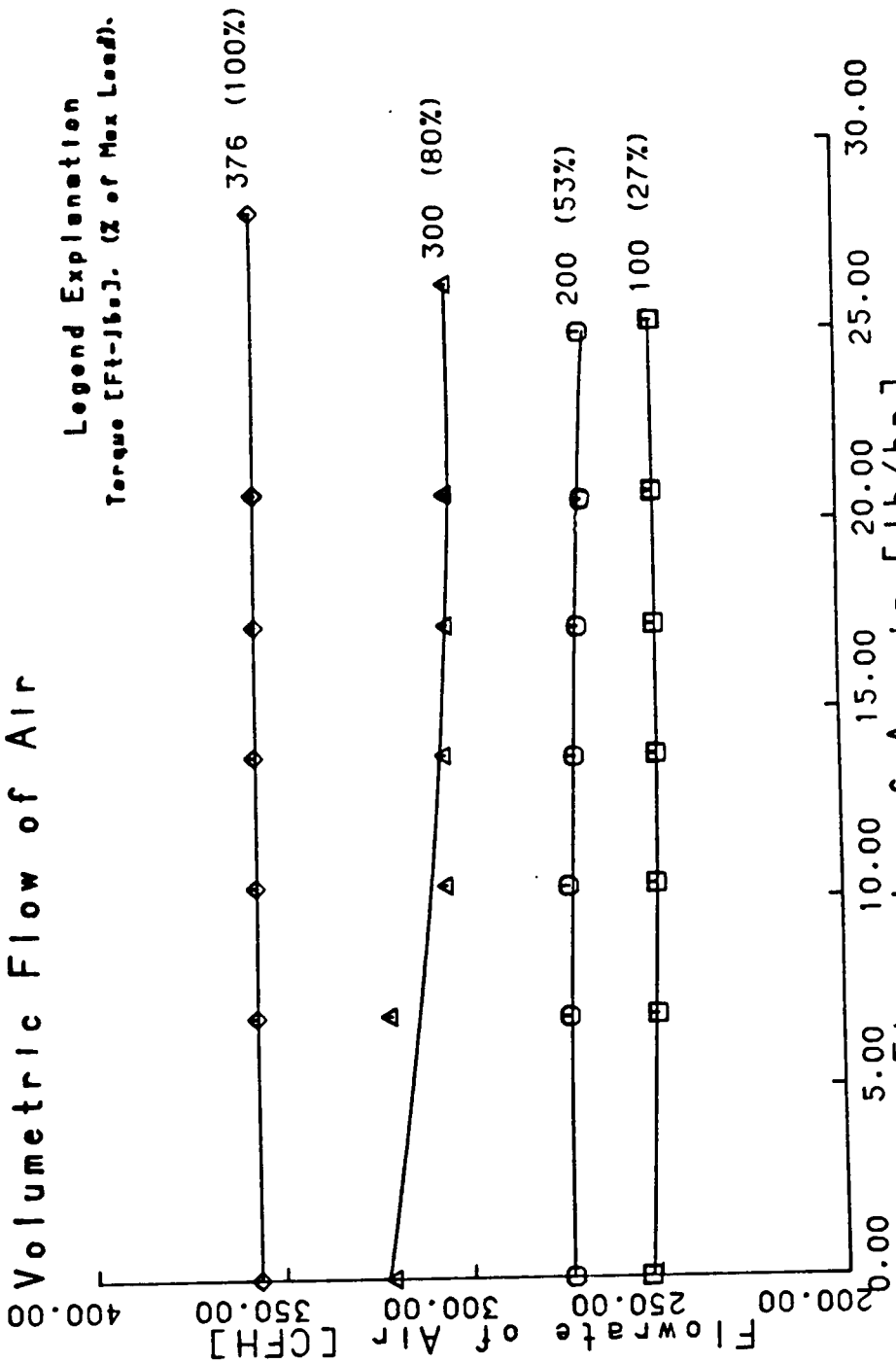


Figure X-5. Volumetric flow rate of air to the engine as a function of flow rate of ammonia.

two load conditions (100 [Ft-lbf] and full load 376 [Ft-lbf] @ 1500 rpm). Plate X-1 (p. 111) depicts the result of the 100 [Ft-lbf] test. From these photographs a number of conclusions can be drawn. First, it can be seen that all the graphs possess two maximum tips. It is believed that this shape is a consequence of the fact that the pressure transducer probed the pressure in the precombustion chamber, rather than the cylinder. However, it is believed that these graphs do convey usable information regarding the pressure in the cylinder.

Second, it can be seen that when the engine is subjected to increasingly more ammonia the average slope changes after combustion starts. For example, the 100 [Ft-lbf] case (photograph A) shows that the average slope on fuel-oil alone is about 94 [psi/deg]. Photograph B, which was obtained with the engine running on an ammonia flow rate of 6.0 lb/hr and fuel-oil flow rate of 11.5 lb/hr shows that the slope is 80 [psi/deg]. It is interesting that with this adjustment of the ammonia and fuel-oil rate the sound of the engine, as observed by the author, was smoother than when running on fuel-oil only. On the other hand, for larger ammonia flow rates the engine exhibited knock and the slope of the graphs, accordingly, exceed those of A and B (and are, respectively, for photographs C and D 200 [psi/deg] and 177 [psi/deg]).

The same is true for the full load case. Plate X-2 (p. 112), photograph A, reveals the no-ammonia case. The average slope of this graph can be measured to be about 66 [psi/deg]. Photograph B which shows an average slope of 88 [psi/deg] also indicates that the engine

is knocking at the beginning of the cycle. No comparable improvement could be detected, as for the 100 [Ft-lbf] case, with this small amount of ammonia injected into the manifold. Photograph C shows still larger average slopes of 114 [psi/deg] and photograph D, which is obtained of the engine while knocking very heavily, shows an average slope of 200 [psi/deg].

Third, it can be observed that with increasing ammonia flow to the engine the maximum pressure in the cylinder increases. This applies particularly for loads higher than 100 [Ft-lbf]. For example, for full load the maximum pressure for no ammonia is about 1040 [psi] while for the maximum ammonia injection it is 1360 [psi], an increase of about 35%. It is believed, as will be shown below, that this is caused by the high rate of release of chemical energy.

From these photographs it seems reasonable to conclude that the tendency of the engine to knock may partly be explained by the abnormally large rate of change of pressure, rather than due to auto-ignition, of fuel mixture. This is further substantiated by the fact that ammonia has been reported to exhibit a high resistance against knocking [22]. Gray et al. have reported results of a test done with a CFR cetane engine running on a mixture of ammonia and fuel-oil. Their results are comparable to the ones obtained in this study regarding the influence of the high rate of pressure increase on the tendency of the engine to knock. In their study they specify 90 [psi/deg] as the limit where the engine started to exhibit knocking. It seems from this study that this may in fact be close to the limit where the engine starts to exhibit abnormal combustion.

It is believed that this abnormal rate of pressure increase is caused by the exothermic reaction rate between the fuel and the oxygen, or the rate of change of chemical internal energy within the cylinder. The following argument is used to substantiate this.

During the period of ignition delay, the fuel is injected into the combustion chamber and an amount of fuel, dm, is transferred across the boundary of the system (which in this case is the combustion volume at each instant of time). According to the first law of thermodynamics written for an open system:

$$\delta Q + dm(u_o + p_o v_o) = \delta W + dU \qquad (X\text{-}4)$$

or

$$\frac{\delta Q}{d\theta} + \frac{dm}{d\theta} h_o = \frac{Pdv}{d\theta} + mc_v \frac{dT}{d\theta} \qquad (X\text{-}5)$$

where hf is the enthalpy of the injected fuel-oil at injected pressure; $m = m_f + m_a + m_{NH_3}$, of which the mass $m_a + m_{NH_3}$ remains constant; c_v is the specific heat of the air or the ammonia-air mixture (depending on whether ammonia is present in the induction air) at constant volume; and Q denotes the equivalent of heat obtained by the volume, due to both chemical reactions and heat transfer from the combustion volume. Now applying the ideal gas law

$$d(PV) = d(m\bar{R}\,T) \qquad (X\text{-}6)$$

or

$$PdV + VdP = mRdT + RTdm \qquad (X\text{-}7)$$

Combining Eqs. X-5 and X-7 gives

$$\frac{dP}{d\theta} = \frac{R}{c_v V}\left(\frac{\delta Q}{d\theta} - P\frac{dV}{d\theta}\left(\frac{c_v}{R} + 1\right) + (h_o + c_v T)\frac{dm}{d\theta}\right) \qquad (X\text{-}8)$$

This equation, which gives the contributing factors to the rate of pressure rise, depends upon the following factors:

1. The volume of the mixture, V. The bigger the volume of the system, with all other parameters constant, the smaller $dP/d\theta$ will be.

2. The term $dV/d\theta$, which comes about because of the movement of the piston, changes sign as the piston moves through TDC. Note, however, that this term of the equation is not likely to be affected by the addition of ammonia to the induction air.

3. The term $(h_f + c_v T)\ dm/d\theta$ comes about because there exists a change of mass due to the injection of fuel crossing the boundary of the cylinder. The contribution of h_f to this term can be neglected at the high temperature experienced in the engine during combustion. The contribution of $c_v T(dm/d\theta)$ on the other hand may be significant compared to the other terms, but as before it is assumed that the size of this term is not significantly altered when ammonia is present in the induction air.

4. The term $\delta Q/d\theta$ is the heat addition to the mixture. This term represents the net heat added to the mixture; and, it consists of the following two terms:

$$\frac{\delta Q}{d\theta} = \left(\frac{\delta Q_{ch}}{d\theta} - \frac{\delta Q_c}{d\theta}\right) \qquad (X\text{-}9)$$

The term $\delta Q_c/d\theta$ denotes the heat transfer losses to the cylinder walls. It is anticipated that this term will not change significantly when ammonia is present in the induction air. The term $Q_{ch}/d\theta$, on the other hand, denotes the heat addition to the mixture as a result of the heat of reaction. This term is a function of, among other variables, the velocity of the chemical reaction, the volume of the reactants, and their concentration. This term, contrary to the others in Eq. X-8, is affected by the presence of ammonia in the combustion chamber. As has been shown in the introduction to this work, most properties of ammonia pertinent to combustion indicate that the chemical reaction of ammonia within the cylinder should be slower when compared to hydrocarbon fuels. Therefore, in order to explain the high rate of pressure rise, it can be concluded that the combustion mechanism in the cylinder is in some way altered by presence of ammonia. The most probable alteration is that the ammonia experiences heterogeneous combustion within the combustion volume. That is, when the mixture of fuel-oil and ammonia-air mixture is expelled from the precombustion chamber and into the main combustion volume, droplets of unburned fuel-oil, now traveling through a combustible mixture of ammonia and air, sets off conical flame fronts that in turn release energy. The results are that heterogeneous combustion of ammonia is experienced at locations throughout the volume. This results in abnormally high rates of release of chemical energy, which in turn manifests itself in high rates of pressure change. Also, it is likely, based on the high temperature, that partial dissociation of

the ammonia is experienced in the cylinder during compression [24]. If true, this would cause a release of hydrogen, which could initiate combustion at locations throughout the combustion volume, even before injection of the fuel-oil.

CHAPTER XI

CONCLUSIONS AND RECOMMENDATIONS

In this second part of this study a Catepillar D330 compression ignition engine was converted to run on mixture of ammonia and fuel-oil. In order to accomplish this a separate fuel system had to be designed and built to prepare the ammonia before going to the engine.

The main findings of the engine tests, which used a total of 52 engine hours, a total of 500 lbm of ammonia, and 110 U.S. gal. of fuel-oil are:

1. The amount of ammonia that can be substituted for the fuel-oil depends on the load the engine is delivering. Thus, for example, for engine load of 100 [Ft-lbf], or 27% of full load, 50% of the fuel-oil by mass could be substituted by the ammonia; for full load the percentage was 25%.

2. When the ammonia flow rate is increased beyond specific limits, determined by the engine load, the engine starts to knock or rumble. It is believed that this is due to a heterogeneous combustion of the fuel mixture in the cylinders.

3. Contrary to predictions in the first part of this work, it is shown that the thermal efficiency of the engine is not significantly improved by increased ammonia flow.

4. With increasing ammonia injected to the cylinders, the rate of pressure rise in the cylinders increases and in some cases becomes three times that for pure fuel-oil.

5. It is estimated that the emission of unburned ammonia is close to 45% of the total ammonia exposed to the engine.

6. Due to the characteristics of the engine's turbocharger the volumetric efficiency of the engine is not decreased due to the presence of ammonia in the induction air.

The main conclusions of this study show that the amount of ammonia that can be substituted for fuel-oil is limited by the high rate of pressure increase within the engine's cylinders, caused by heterogeneous combustion of the ammonia air mixture throughout the combustion volume. In order to address this problem it is proposed that an effort should be directed towards modification of the engine and the fueling system to secure more controlled combustion of the fuel mixture.

It is believed that a conventional spark ignition system would accomplish this because with such a system the initiation of the combustion is confined to a single point in the combustion volume, and also because it is possible to more closely control the time when combustion begins (through spark advance adjustments).

A number of sources [3,5,6,7,8,23] have shown that by dissociating a small fraction of the ammonia, combustion properties (such as minimum ignition energy and flammability limits) of the resulting mixture are greatly improved. Therefore, it is proposed that an investigation of the performance of a system which would partially dissociate the ammonia outside the engine should be performed.

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APPENDICES

APPENDIX A

EXPERIMENTAL DATA

Table A-1. Test data.

Test number: 9, Date: 07:09:84 RUNTIME: 2.20 hr Fuel-Oil Usage: 10 gal Ammonia Usage: 35
Twet: 65.0 Deg F Tdry: 78.0 Deg F %Humitity: 49.7 Bar press: 712.0 mbar
Fuel-Oil: Sp.Gr = 0.8565 @ 78 F; API = 33.5 @ 79.0 F Ammonia: Grade-A 99.9995 % NH3

Torque Ft-lb	RPM	Boost psig	Tmanif. Deg F	Weight oz	Time sec	Read SCFM	TNH3 Deg F	PNH3 psig	DP Meriam in-H2O	Tair Deg F	Note
[		Engine	]	[	Fuel-Oil]	[		Ammonia	] [	Air]	
100	1505	0.00	130	2	32	0.0	0	0	1.64	86	oil-ref
100	1505	0.00	130	4	64	0.0	0	0	1.64	86	oil-ref
100	1505	0.00	130	8	125	0.0	0	0	1.64	86	oil-ref
100	1506	0.00	130	2	37	1.0	81	80	1.62	86	
100	1506	0.00	130	4	73	1.0	81	80	1.62	86	
100	1505	0.00	130	8	145	1.0	81	80	1.62	86	
100	1507	0.50	130	2	39	1.5	82	80	1.62	86	
100	1507	0.50	130	4	78	1.5	82	80	1.62	86	
100	1507	0.50	130	8	154	1.5	83	80	1.62	86	
100	1511	0.60	130	2	42	2.0	83	80	1.62	87	
100	1511	0.60	130	4	83	2.0	85	80	1.62	87	
100	1511	0.60	130	8	166	2.0	85	80	1.62	87	
100	1514	0.80	130	2	46	2.5	84	80	1.62	87	
101	1515	0.80	130	4	91	2.5	84	80	1.62	87	
101	1514	0.80	130	8	184	2.5	83	80	1.62	87	
101	1517	0.90	130	2	49	3.0	82	80	1.62	87	
101	1517	0.90	130	4	98	3.0	80	80	1.62	87	
101	1517	0.90	130	8	200	3.0	80	80	1.62	87	
102	1520	1.10	130	2	58	3.3	80	100	1.62	87	knock limit
102	1520	1.10	130	4	116	3.3	80	100	1.62	87	
102	1520	1.10	130	8	232	3.3	80	100	1.62	88	

Table A-1 (continued)

Test number: 10 Date: 07:09:84 RUNTIME: 3.15 hr Fuel-Oil Usage: 12 gal Ammonia Usage: 40 lb.
Twet: 65.0 Deg F Tdry: 78.0 Deg F %Humitity: 49.7 Bar press: 712.0 mbar
Fuel-Oil: Sp.Gr = 0.8565 @ 78 F; API = 33.5 @ 79.0 F Ammonia: Grade-A 99.9995 % NH3

Torque Ft-lb	RPM	Boost psig	Tmanif. Deg F	Weight oz	Time sec	Read SCFM	TNH3 Deg F	PNH3 psig	DP Meriam in-H2O	Tair Deg F	Note
[		Engine	]	[	Fuel-Oil	]	[	Ammonia	]	[Air]	
200	1504	1.60	150	4	37	0.0	0	0	1.80	94	oil-ref
202	1505	1.60	150	8	74	0.0	0	0	1.80	94	oil-ref
202	1505	1.60	150	16	149	0.0	0	0	1.80	94	oil-ref
201	1510	1.70	150	4	41	1.0	89	80	1.80	94	
201	1510	1.70	150	8	83	1.0	88	80	1.80	94	
201	1510	1.70	150	16	165	1.0	87	80	1.80	94	
201	1512	1.75	150	4	44	1.5	87	80	1.80	94	
202	1512	1.75	150	8	87	1.5	87	80	1.80	94	
201	1511	1.75	150	16	174	1.5	88	80	1.80	94	
201	1514	1.80	150	4	45	2.0	88	80	1.79	95	
201	1514	1.80	150	8	90	2.0	88	80	1.79	95	
202	1514	1.80	150	16	182	2.0	88	80	1.79	95	
202	1515	1.80	150	4	47	2.5	86	80	1.78	95	
202	1516	1.80	150	8	96	2.5	86	80	1.78	95	
202	1516	1.80	150	16	194	2.5	88	80	1.78	95	
202	1518	1.90	150	4	51	3.0	90	80	1.77	95	
202	1519	1.90	150	8	104	3.0	91	80	1.77	95	
202	1519	1.90	150	16	207	3.0	93	80	1.77	95	
202	1522	2.00	150	4	53	3.3	93	100	1.77	95	Knock limit
202	1522	2.00	150	8	106	3.3	93	100	1.77	95	
202	1522	2.00	150	16	212	3.3	93	100	1.77	95	

Table A-1 (continued)

Test number: 11, Date: 07:09:84 RUNTIME: 2.48 hr Fuel-Oil Usage: 16 gal Ammonia Usage: 36 lb.
Twet: 65.0 Deg F Tdry: 78.0 Deg F %Humitity: 49.7 Bar press: 712.0 mbar
Fuel-Oil: Sp.Gr = 0.8565 @ 78 F; API = 33.5 @ 79.0 F Ammonia: Grade-A 99.9995 % NH3

Torque Ft-lb	RPM	Boost psig	Tmanif. Deg F	Weight oz	Time sec	Read SCFM	TNH3 Deg F	PNH3 psig	DP Meriam in-H2O	Tair Deg F	Note
[		Engine	]	[	Fuel-Oil]	[	Ammonia	]	[Air	]	
300	1506	3.25	177	2	13	0.0	0	0	2.10	90	oil-ref
299	1506	3.25	177	4	25	0.0	0	0	2.10	90	oil-ref
299	1506	3.25	177	8	50	0.0	0	0	2.10	90	oil-ref
300	1521	4.00	177	4	27	1.0	82	80	2.10	90	
300	1521	4.00	177	8	54	1.0	82	80	2.10	90	
300	1521	4.00	177	16	108	1.0	82	80	2.10	90	
301	1526	4.10	177	4	28	1.5	83	80	2.00	90	
301	1526	4.10	177	8	56	1.5	83	80	2.00	90	
301	1530	4.10	177	16	112	1.5	83	80	2.00	90	
302	1535	4.20	177	4	29	2.0	84	80	2.00	90	
302	1535	4.20	177	8	58	2.0	84	80	2.00	90	
302	1535	4.20	177	16	115	2.0	84	80	2.00	90	
302	1543	4.30	177	4	30	2.5	84	80	2.00	92	
302	1543	4.30	177	8	59	2.5	83	80	2.00	92	
302	1546	4.30	177	16	119	2.5	83	80	2.00	92	
303	1550	4.40	177	4	30	3.0	84	80	2.00	92	
303	1550	4.40	177	8	61	3.0	83	80	2.00	92	
303	1550	4.40	177	16	121	3.0	82	80	2.00	93	
303	1559	4.60	177	4	31	3.3	85	110	2.00	94	Knock limit
303	1559	4.60	177	8	63	3.3	85	110	2.00	94	
303	1557	4.60	177	16	127	3.3	85	110	2.00	94	

Table A-1 (continued)

Test number: 12 Date: 07:09:84 RUNTIME: 3.05 hr Fuel-Oil Usage: 22 gal Ammonia Usage: 37 lb.
Twet: 65.0 Deg F Tdry: 78.0 Deg F %Humitity: 49.7 Bar press: 712.0 mbar
Fuel-Oil: Sp.Gr = 0.8565 @ 78 F; API = 33.5 @ 79.0 F Ammonia: Grade-A 99.9995 % NH3

Torque Ft-lb	RPM	Boost psig	Tmanif. Deg F	Weight oz	Time sec	Read SCFM	TNH3 Deg F	PNH3 psig	DP Meriam in-H2O	Tair Deg F	Note
[Engine]				[Fuel-Oil]		[Ammonia]			[Air]		
373	1499	6.60	220	4	19	0.0	0	0	2.35	94	oil-ref
373	1500	6.60	220	8	38	0.0	0	0	2.35	94	oil-ref
373	1500	6.60	220	16	76	0.0	0	0	2.35	94	oil-ref
375	1526	6.80	220	4	20	1.0	85	80	2.35	94	
375	1526	6.80	220	8	40	1.0	85	80	2.35	94	Max Load
375	1526	6.80	220	16	81	1.0	85	80	2.35	94	
376	1529	6.80	220	4	21	1.5	84	80	2.35	94	
376	1529	6.80	220	8	42	1.5	84	80	2.35	94	
376	1529	6.80	220	16	83	1.5	84	80	2.35	94	
376	1533	6.80	220	4	22	2.0	84	80	2.35	94	
376	1532	6.80	220	8	43	2.0	84	80	2.35	94	
376	1532	6.80	220	16	86	2.0	84	80	2.35	94	
376	1536	6.80	218	4	22	2.5	83	80	2.35	95	
375	1536	6.80	218	8	44	2.5	83	80	2.35	95	
376	1536	6.80	218	16	88	2.5	83	80	2.35	95	
376	1537	6.80	218	4	23	3.0	81	80	2.35	95	
376	1537	6.80	218	8	45	3.0	81	80	2.35	95	
377	1535	6.80	218	16	90	3.0	81	80	2.35	96	
377	1537	6.80	220	4	23	3.4	84	120	2.35	96	Knock limit
378	1537	6.50	220	8	46	3.4	84	120	2.35	96	
378	1537	6.50	220	16	93	3.4	84	120	2.35	96	Turbine Surge

Table A-2. Derived results from Table A-1.

Torque Ft-lbs	lb/hr Fuel-Oil	lb/hphr	lb/hr Ammonia	lb/hphr	hp Hp	Thermal Efficie.	Volum. Efficie.	Max-FI Reduct.	Max-BSCF Reduct.	Air FI CFM.
100	14.1	0.491	0.0	0.000	28.7	28.0	54.1	1.00	1.00	252.6
100	14.1	0.491	0.0	0.000	28.7	28.0	54.1	1.00	1.00	252.6
100	14.4	0.503	0.0	0.000	28.7	27.4	54.1	1.02	1.02	252.6
100	12.2	0.424	6.9	0.241	28.7	26.0	53.4	0.86	0.86	249.5
100	12.3	0.430	6.9	0.241	28.7	25.7	53.4	0.88	0.88	249.5
100	12.4	0.433	6.9	0.241	28.7	25.6	53.5	0.88	0.88	249.5
100	11.5	0.402	10.3	0.361	28.7	24.6	53.4	0.82	0.82	249.5
100	11.5	0.402	10.3	0.361	28.7	24.6	53.4	0.82	0.82	249.5
100	11.7	0.407	10.3	0.360	28.7	24.4	53.4	0.83	0.83	249.5
100	10.7	0.372	13.8	0.479	28.8	23.7	53.3	0.76	0.76	249.1
100	10.8	0.377	13.8	0.478	28.8	23.5	53.3	0.77	0.77	249.1
100	10.8	0.377	13.8	0.478	28.8	23.5	53.3	0.77	0.77	249.1
100	9.8	0.339	17.2	0.597	28.8	22.9	53.1	0.70	0.69	249.1
101	9.9	0.339	17.2	0.591	29.1	23.0	53.1	0.70	0.69	249.1
101	9.8	0.336	17.2	0.592	29.1	23.2	53.1	0.70	0.68	249.1
101	9.2	0.315	20.7	0.710	29.2	22.0	53.0	0.65	0.64	249.1
101	9.2	0.315	20.7	0.711	29.2	22.0	53.0	0.65	0.64	249.1
101	9.0	0.309	20.7	0.711	29.2	22.3	53.0	0.64	0.63	249.1
102	7.8	0.263	25.2	0.854	29.5	21.7	52.9	0.55	0.54	249.1
102	7.8	0.263	25.2	0.854	29.5	21.7	52.9	0.55	0.54	249.1
102	7.8	0.263	25.2	0.854	29.5	21.7	52.9	0.55	0.54	248.6

Table A-2 (continued)

Torque Ft-lbs	lb/hr Fuel-Oil	lb/hphr	lb/hr Ammonia	lb/hphr	hp Hp	Thermal Efficie.	Volum. Efficie.	Max-Fl Reduct.	Max-BSCF Reduct.	Air Fl CFM.
200	24.3	0.425	0.0	0.000	57.3	32.4	59.4	1.00	1.00	273.3
202	24.3	0.420	0.0	0.000	57.9	32.7	59.4	1.00	0.99	273.3
202	24.2	0.417	0.0	0.000	57.9	33.0	59.4	0.99	0.98	273.3
201	22.0	0.380	6.9	0.119	57.8	31.9	59.2	0.90	0.89	273.3
201	21.7	0.375	6.9	0.119	57.8	32.2	59.2	0.89	0.88	273.3
201	21.8	0.378	6.9	0.119	57.8	32.0	59.2	0.90	0.89	273.3
201	20.5	0.353	10.3	0.178	57.9	31.9	59.1	0.84	0.83	273.3
202	20.7	0.356	10.3	0.177	58.2	31.8	59.1	0.85	0.84	273.3
201	20.7	0.358	10.3	0.178	57.8	31.6	59.2	0.85	0.84	273.3
201	20.0	0.345	13.7	0.237	57.9	30.7	58.7	0.82	0.81	271.3
201	20.0	0.345	13.7	0.237	57.9	30.7	58.7	0.82	0.81	271.3
202	19.8	0.340	13.7	0.236	58.2	31.1	58.7	0.81	0.80	271.3
202	19.1	0.329	17.2	0.295	58.3	30.1	58.4	0.79	0.77	269.7
202	18.8	0.322	17.2	0.295	58.3	30.6	58.3	0.77	0.76	269.7
202	18.6	0.318	17.2	0.294	58.3	30.8	58.3	0.76	0.75	269.7
202	17.6	0.302	20.5	0.352	58.4	30.2	57.9	0.73	0.71	268.2
202	17.3	0.296	20.5	0.351	58.4	30.6	57.9	0.71	0.70	268.2
202	17.4	0.298	20.5	0.351	58.4	30.5	57.9	0.71	0.70	268.2
202	17.0	0.290	24.9	0.426	58.5	28.9	57.8	0.70	0.68	268.2
202	17.0	0.290	24.9	0.426	58.5	28.9	57.8	0.70	0.68	268.2
202	17.0	0.290	24.9	0.426	58.5	28.9	57.8	0.70	0.68	268.2

Table A-2 (continued)

Torque Ft-lbs	lb/hr Fuel-Oil	lb/hphr	lb/hr Ammonia	lb/hphr	hp Hp	Thermal Efficie.	Volum. Efficie.	Max-Fl Reduct.	Max-BSCF Reduct.	Air Fl CFM.
300	34.6	0.402	0.0	0.000	86.0	34.2	69.3	1.00	1.00	321.1
299	36.0	0.420	0.0	0.000	85.7	32.8	69.3	1.04	1.04	321.1
299	36.0	0.420	0.0	0.000	85.7	32.8	69.3	1.04	1.04	321.1
300	33.3	0.384	6.9	0.079	86.9	32.9	68.6	0.96	0.95	321.1
300	33.3	0.384	6.9	0.079	86.9	32.9	68.6	0.96	0.95	321.1
300	33.3	0.384	6.9	0.079	86.9	32.9	68.6	0.96	0.95	321.1
301	32.1	0.368	10.3	0.118	87.5	32.8	65.1	0.93	0.91	305.8
301	32.1	0.368	10.3	0.118	87.5	32.8	65.1	0.93	0.91	305.8
301	32.1	0.367	10.3	0.118	87.7	32.9	64.9	0.93	0.91	305.8
302	31.0	0.352	13.8	0.156	88.3	32.8	64.7	0.90	0.87	305.8
302	31.0	0.352	13.8	0.156	88.3	32.8	64.7	0.90	0.87	305.8
302	31.3	0.355	13.8	0.156	88.3	32.6	64.7	0.90	0.88	305.8
302	30.0	0.338	17.2	0.194	88.7	32.5	64.4	0.87	0.84	304.7
302	30.5	0.344	17.2	0.194	88.7	32.1	64.4	0.88	0.85	304.7
302	30.3	0.340	17.2	0.194	88.9	32.4	64.3	0.87	0.85	304.7
303	30.0	0.335	20.7	0.231	89.4	31.5	64.1	0.87	0.83	304.7
303	29.5	0.330	20.7	0.231	89.4	31.9	64.1	0.85	0.82	304.7
303	29.8	0.333	20.7	0.231	89.4	31.7	64.1	0.86	0.83	304.2
303	29.0	0.323	26.2	0.292	89.9	30.6	63.7	0.84	0.80	303.6
303	28.6	0.318	26.2	0.292	89.9	30.9	63.7	0.83	0.79	303.6
303	28.3	0.316	26.2	0.292	89.8	31.1	63.8	0.82	0.78	303.6

Table A-2 (continued)

Torque Ft-lbs	lb/hr Fuel-Oil	lb/hphr	lb/hr Ammonia	lb/hphr	hp Hp	Thermal Efficie.	Volum. Efficie.	Max-FI Reduct.	Max-BSCF Reduct.	Air FI CFM.
373	47.4	0.445	0.0	0.000	106.5	30.9	77.9	1.00	1.00	356.8
373	47.4	0.445	0.0	0.000	106.5	30.9	77.8	1.00	1.00	356.8
373	47.4	0.445	0.0	0.000	106.5	30.9	77.8	1.00	1.00	356.8
375	45.0	0.413	6.9	0.063	109.0	31.2	76.5	0.95	0.93	356.8
375	45.0	0.413	6.9	0.063	109.0	31.2	76.5	0.95	0.93	356.8
375	44.4	0.408	6.9	0.063	109.0	31.6	76.5	0.94	0.92	356.8
376	42.9	0.392	10.3	0.094	109.5	31.8	76.3	0.90	0.88	356.8
376	42.9	0.392	10.3	0.094	109.5	31.8	76.3	0.90	0.88	356.8
376	43.4	0.396	10.3	0.094	109.5	31.5	76.3	0.92	0.89	356.8
376	40.9	0.373	13.8	0.126	109.7	32.2	76.1	0.86	0.84	356.8
376	41.9	0.382	13.8	0.126	109.7	31.5	76.2	0.88	0.86	356.8
376	41.9	0.382	13.8	0.126	109.7	31.5	76.2	0.88	0.86	356.8
376	40.9	0.372	17.2	0.157	110.0	31.2	76.0	0.86	0.84	356.1
375	40.9	0.373	17.2	0.157	109.7	31.2	76.0	0.86	0.84	356.1
376	40.9	0.372	17.2	0.157	110.0	31.2	76.0	0.86	0.84	356.1
376	39.1	0.356	20.7	0.188	110.0	31.4	75.9	0.83	0.80	356.1
376	40.0	0.364	20.7	0.188	110.0	30.9	75.9	0.84	0.82	356.1
377	40.0	0.363	20.7	0.188	110.2	30.9	76.0	0.84	0.82	355.5
377	39.1	0.355	28.1	0.255	110.3	29.5	75.9	0.83	0.80	355.5
378	39.1	0.354	28.1	0.254	110.6	29.6	75.9	0.83	0.80	355.5
378	38.7	0.350	28.1	0.254	110.6	29.9	75.9	0.82	0.79	355.5

APPENDIX B

PROGRAM CODES, TEXT

In this section the algorithm developed to generate solution to the analytical model are described. The program codes consist of a main program, called KJUPPI, subroutine, DISSOC, which calculates equilibrium composition of the product gases, and a subroutine, PROPER, which enables calculations of necessary thermodynamic properties for the gases involved. In order to use the codes, all three of them have to be "linked" together before running. Otherwise, there are no restrictions for the use of the codes.

Main Program KJUPPI

Figure B-1 shows a flowchart of the main program. When invoked, the program prompts the user, in an interactive mode, for pertinent data. Table B-1 shows a typical input respond to the program and Table B-2 is an explanation of the input data. Table B-3 contains a listing of the relationship between the notation used in the program codes and the analytical derivation.

Subroutine DISSOC

In order to solve the equation system VI-7 the program DISSOC was generated. The program, which is in the form of a subroutine, accepts thermodynamic properties and constraints of the fuel-air mixture as input data. The returned data is the composition of the product gases. A flowchart of the routine is presented in Figure B-2.

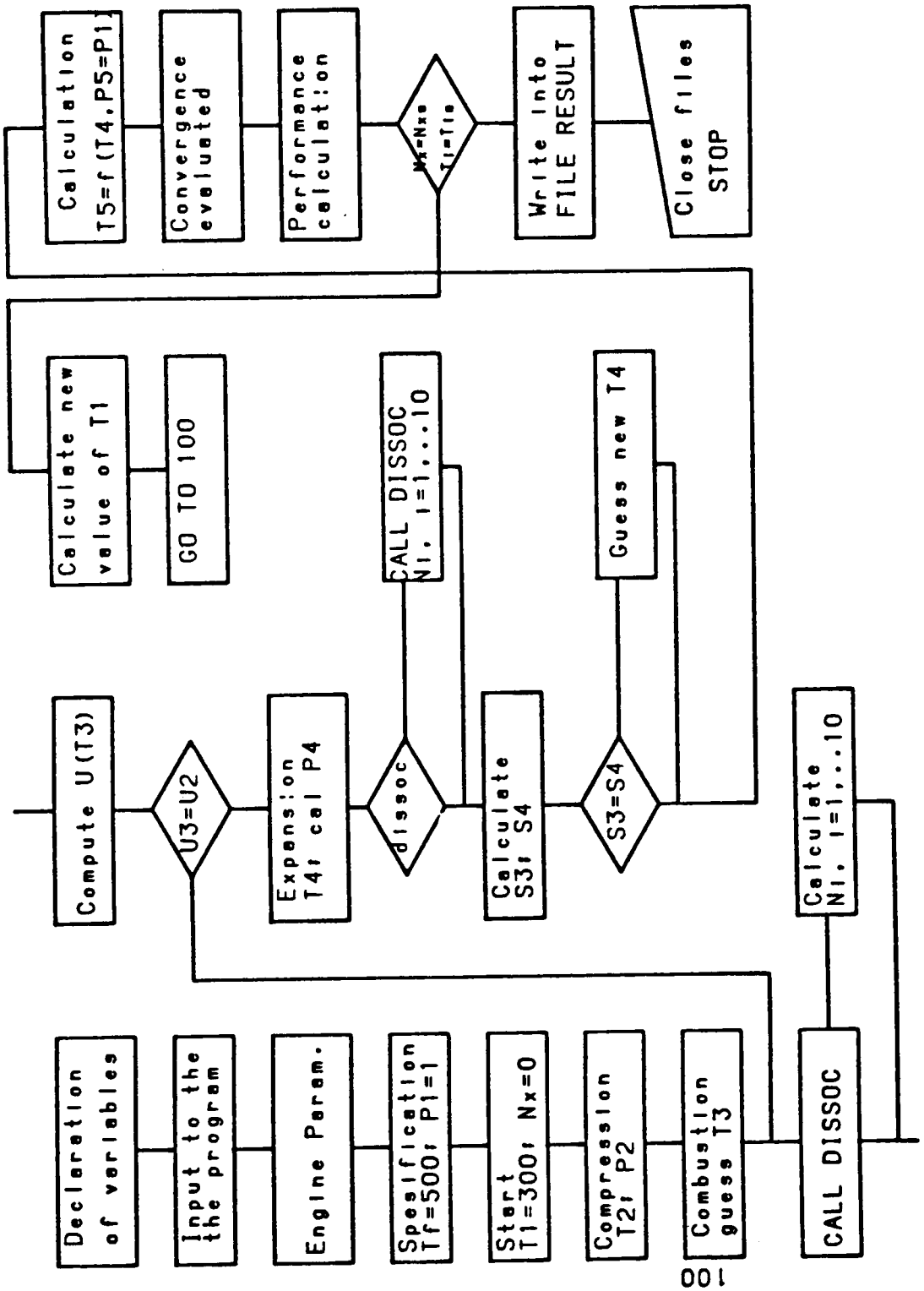


Figure B-1. Flowchart for KJUPPI.FOR.

Table B-1. Typical Input to the Main Program.

Name of the output file	=<NAME>	<--(Char/Numer)
Read in MEMO if here	=<MEMO>	<--(Char/Numer)
Read in the mole fraction of AMMONIA	=<Mole>	<--(Numer)
Read in the mole fraction of n-DECANE	=<Mole>	<--(Numer)
Dissociation during combustion	=<Y/N>	<--(Char)
Dissociation during expansion	=<Y/N>	<--(Char)
Compression ratio	=<CR>	<--(Numer)
Min value of Eq	=<Min Eq>	<--(Numer)
Max value of Eq	=<Max Eq>	<--(Numer)

where: (Char) = Character Variable; (Numer) = Numerical Variable.

Table B-2. Explanation of Input Data to the Main Program.

Prompt	Data
Name of output file	Desired name of the file to store the output.
Write memo	Enables the user to write memo to the solution file.
Moles of ammonia	Number of moles of ammonia in the chemical equation describing the combustion. See Eq. II-1.
Moles of n-Decane	Number of moles of n-Decane in the chemical equation describing the combustion. See Eq. II-1.
Dissociation during combustion	Question. Options are: Yes or No.
Dissociation during expansion	Question. Options are: Yes or No.
Compression ratio	The compression ratio of the engine at hand.
Min value of Eq	Eq is the actual air-fuel ratio divided by the stoichio. air-fuel ratio.
Max value of Eq	The maximum value to which Eq is to be incremented.

Table B-3. Computer Codes Nomenclature.

Symbol		Definition	Units
Comp.	Anal.		
Cr	CR	Compression ratio.	---
cm	C_m	See Eq. II-2.	---
eff		Thermal efficiency, Eq. III-3.	---
Eq	Y/Y_{cc}	The ratio of actual air-fuel ratio to the stoichiometric air-fuel ratio.	---
Ha298	h_{NH_3}	Enthalpy of ammonia at 298 K. See Eq. II-11.	kJ/kmol
Hf298	$h_{C_{10}H_{22}}$	Enthalpy of n-Decane at 298 K. See Eq. II-20.	kJ/kmol
HoCO2	h_{CO_2}	Enthalpy of CO2 at 298 K.	kJ/kmol
HoH2O	h_{H_2O}	Enthalpy of H2O at 298 K.	kJ/kmol
HoO2	h_{O_2}	Enthalpy of O2 at 298 K.	kJ/kmol
HoN2	h_{N_2}	Enthalpy of N2 at 298 K.	kJ/kmol
HrDec	$h_{C_{10}H_{22}}$	Enthalpy of n-Decane at T_f K. See Eq. II-23.	kJ/kmol
Hrpa	H_{rp_a}	Heat of reaction for gaseous ammonia, at constant pressure. See Eq. II-10.	kJ/kmol
Hrpf	H_{rp_o}	Heat of reaction for liquid n-Decane, at constant press. See Eq. II-20.	kJ/kmol
kr	k	Def: c_p/c_v, for the mixture in the cylinder during comp. See Eq. II-2.	---
kp	k	Def: c_p/c_v, at state-point (3)	---
kp4	k	Def: c_p/c_v, at state-point (4)	---

Table B-3 (continued)

Symbol Comp.	Symbol Anal.	Definition	Units
Mc	AC	Number of carbon atoms in the fuel. See Eq. VI-6.	kmol
Mep	IMEP	Indicated mean effective pressure. Eq. III-2.	atm
Mh	AH	Number of hydrogen atoms in the fuel. See Eq. VI-6.	kmol
Mo		Number of oxygen atoms in the fuel. For the present case this parameter is equal to zero.	kmol
Na	n_a	Number of moles of ammonia in the chemical equation, II-1.	mol
Nmo		Number of moles of ammonia and air in Eq. II-1.	mol
No	n_o	Number of moles of n-Decane in the chemical equation, II-1.	mol
Np(i)	N(i);n_i	The composition of product gases at state-points. See Eq. II-1.	---
Npo	N_{po}	Kilomoles of products formed from combustion of 1 kmol of fuel + 4.76Y kmol of air.	kmol
Nx	M_x	Actual number of moles of product gases remaining in the cylinder at the onset of compression. See Eq. II-48.	kmol
P1	P_1	The manifold pressure.	atm
P2	P_2	Press. at the end of compres.	atm
P3	P_3	Press. at the end of comb. Eq. II-44.	atm

Table B-3 (continued)

Symbol		Definition	Units
Comp.	Anal.		
P4	P_4	Pressure at the end of expans. See Eq. II-44.	atm
P5	P_5	Pressure at state-point (5). Note: $P_5 = P_1$.	atm
spfam	$ISFC_a$	Specific fuel consumption of ammonia. See Eq. III-5.	g/MJ
spfol	$ISFC_o$	Specific fuel consumption of oil. See Eq. III-6.	g/MJ
T1	T_1	The pressure in the cylinder at the onset of compression. See Eq. II-48.	K
T2	T_2	Temperature at the end of compr. See Eq. II-2.	K
T3	T_3	Temperature at the end of combustion. See Eq. II-5.	K
T4	T_4	Temperature at the end of expansion. See Eq. II-44.	K
T5	T_5	Temperature at state-point (5). See Eq. II-47.	K
Tm	T_m	Manifold temperature. See Eq. II-49.	K
Tf	T_f	Temperature of the n-Decane, when introduced to the cyl. See Eq. II-22.	K
Ua298	u_a	Internal energy of ammonia at 298 K. Eq. II-14.	kJ/kmol
Ur	$u_{a\text{-}air}$	Internal energy of the ammonia air mixture at T2. Eq. II-5.	kJ/kmol
UrDec	$u_{C_{10}H_{22}}$	Internal energy of n-Decane at T_f. See Eq. II-23.	kJ/mol

Table B-3 (continued)

Symbol		Definition	Units
Comp.	Anal.		
Up	u_p	Internal energy of the product gases. See Eq. II-5.	kJ/kmol
Y	Y	Number of moles of air in the chemical equation, II-1.	kmol
Ycc	Y_{cc}	Stoichiometric amount of air, according to Eq. II-1.	kmol
Voleff	η_{vol}	Volumetric efficiency. See Eq. III-4.	---
Wcomp	W_{comp}	Compression work performed by the piston on the fuel-air mixture per cycle.	kW/cycle
Wexp	W_{exp}	Expansion work of the product gases per cycle.	kW/cycle
Wnet	W_{net}	Net work output per cycle. See Eq. III-1.	kW/cycle
Work		Def: Wnet*RPM/120	kW

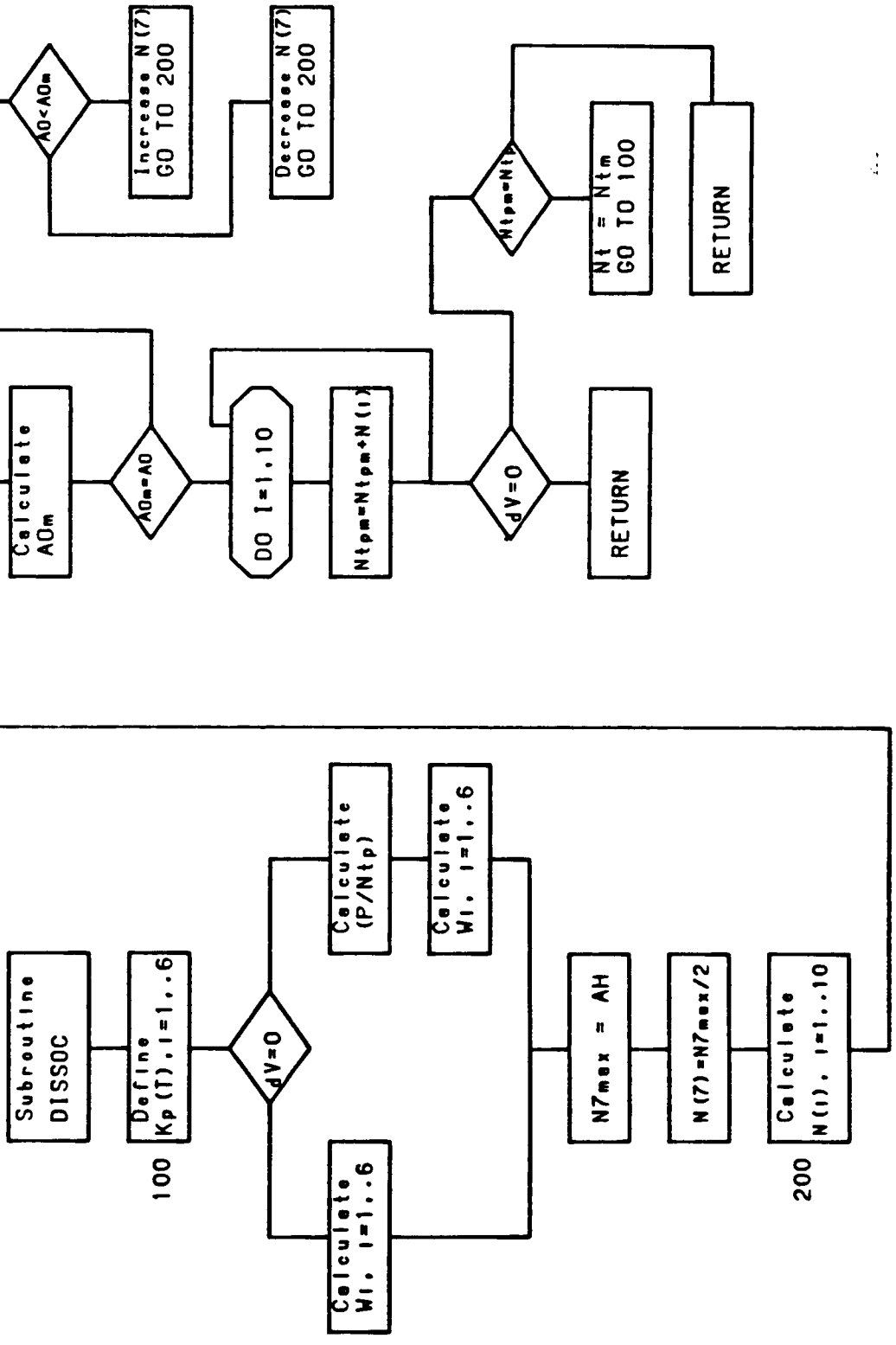


Figure B-2. Flowchart for DISSOC.FOR.

Because of the minimum effort the routine was extended to include combustion at constant pressure, as well as constant volume. Note, however, that the former capability is not used in this work.

If the reference values, and the constraint, of the air-fuel mixture is taken to be a parameter of the problem, the function of the routine is that of a vector function operating on a scalar variable—the temperature at the end of the combustion. The returning, or the function, value is a 10-dimensional vector containing the composition of the 10 product gases. Therefore, in order to make use of the routine, an algorithm has to be at hand which controls the search for the temperature which satisfies the correct energy relationship (like Eq. II-5). In the special case of constant pressure combustion, which then serves as the constraint of the problem, the pressure, temperature and the initial number of moles in the combustion chamber has to be known and has to be supplied to the routine in the call statement. On the other hand, for the case when the volumetric behavior of the combustion chamber is a known variable (which for equilibrium thermodynamics merely means that the initial and the final volume is known) the ratio of the two volumes, which in this case is numerically equal to the compression ratio of the engine, CR, has to be supplied to the routine along with the initial temperature and pressure of the air-fuel mixture, Tr and Pr. Otherwise, the routine is used as follows:

CALL DISSOC (cond,cr,Pr,Tr,AC,AH,AO,AN,P,T,n,Nt), where:

Cond: Is a character variable. Allowable values for cond are V or P. These values correspond to the physical constraint of specified volume behavior or constant pressure combustion, respectively. Note that V and P are character variables.

CR: Compression ratio of the cycle.

Tr: Reference pressure for the fuel-air mixture.

Pr: Reference pressure of the fuel-air mixture.

AC: Abundance of carbon in the fuel-air mixture. See Eq. VI-6.

AH: Abundance of hydrogen in the fuel-air mixture. See Eq. VI-6.

AO: Abundance of oxygen in the fuel-air mixture. See Eq. VI-6.

AN: Abundance of nitrogen in the fuel-air mixture. See Eq. VI-6.

P: Pressure under which constant pressure combustion takes place. Note: This parameter is not used in the case of constant volume combustion.

T: Temperature at which composition is to be evaluated. This should be thought of as the independent variable of the routine.

n: Returning value of the composition of the product gases.

Nt: Total mol number of the product gases. For the case of constant pressure combustion value of this parameter is provided in the call statement. For the constant volume combustion case value is returned by the subroutine.

It should be noted that for the special case of constant pressure combustion values of Cr, Tr, and Pr do not need to be provided, since these parameters do not enter into that particular problem.

Subroutine PROPER

The program PROPER is based on the equations derived in Chapter VII, and was generated to provide the main program KJUPPI with access to pertinent thermodynamic values. The program consists of a number of smaller routines which all resemble each other, both in function and appearance. Therefore, what follows applies equally well to each of them. The call to the routines is of this form:

CALL <PROPER>(GAS,T,PR), where:

PROPER: Is the name of the routine, which calculates the property PROPER. Allowable values for PROPER are:
- ENTHP: Enthalpy
- INTEN: Internal Energy
- CPRES: Specific Heat @ Constant Pressure
- CVOLU: Specific Heat @ Constant Volume
- ENTRO: Entropy

GAS: Is the code name for the particular gas, which property PROPER is to be calculated. Allowable values are: CO2, CO, O2, O, NO, N2, H, H2, OH and H2O.

T: Temperature at which properties are to be calculated.

Pr: The returning value, in SI units, of the property PROPER, for the gas GAS.

The function of the routine is based on the idea of a search word given in the call statement. For example, in order to calculate the entropy value of CO2 at T = Ti the correct values of the search words are as follows: <PROPER> = ENTHP, GAS = CO2 and T = Ti; the call to the routine:

CALL ENTHP('CO2', Ti, returning value of hCO2).

Listings of the program codes are to be found in Appendix C.

APPENDIX C

PROGRAM CODES, LISTINGS

```
1     ****************************************************************
c     **           <<<<<< MAIN PROGRAM KJUPPI >>>>>>                **
c     ****************************************************************
c     ** PURPOSE: Calculate solutions to the mathematical           **
c     **          model derived in chapter II.                      **
c     **                                                            **
c     ** INPUT:   The program prompts the user in an inter-         **
c     **          active form for pertinent data.                   **
c     **                                                            **
c     **          INPUT                MEANING                      **
c     **          -------              ---------                    **
c     **          NAME : Name of the data file where the            **
c     **                 output will be found.                      **
c     **          MEMO : This is a character variable, length       **
c     **                 70 characters. The value of this           **
c     **                 variable is printed in to the out-         **
c     **                 put file. NOTE: It is not necessary        **
c     **                 to respond to this prompt.                 **
c     **          Na:    Number of moles of ammonia in the          **
c     **                 chemical equation describing the           **
c     **                 combustion. Se equation II-1.              **
c     **          No:    Number of moles of n-Decane in the         **
c     **                 chemical equation describing the           **
c     **                 combustion. Se equation II-1.              **
c     **          DISOC: Question: Dissociation during comb-        **
c     **                 ustion? I.e. frozen equilibrium.           **
c     **                 NOTE: Allowable values are: (Y)es          **
c     **                 or (N)o.                                   **
c     **          DISAFT: Qestion: Dissociation during exp-         **
c     **                 ansion. I.e. Shifting equilibrium.         **
c     **                 NOTE: Allowable values are (Y)es           **
c     **                 or (N)o.                                   **
c     **          CR:    Compression ratio of the engine.           **
c     **          eq:    the equivalence ratio to be used in        **
c     **                 the computations. NOTE: eq is defined      **
c     **                 as follows.                                **
c     **                                                            **
c     **                                                            **
c     **                     Def: eq = (A/F)/(A/F) = Y/Ycc          **
c     **                                        c                   **
c     **                                                            **
c     **                  Where: (A/F) is the air-fuel ratio        **
c     **                         (A/F) is the stoichiometric        **
c     **                             c   air-fuel ratio.            **
c     **                                                            **
c     **          eqmax:  Is the max value of eq, to which          **
c     **                  eq is incremented.                        **
c     **                                                            **
c     ** OUTPUT: The program creates a output file which           **
c     **          is named the value of the variable NAME.          **
c     **                                                            **
c     ** RESTRICTIONS:  This program only works in conjunction     **
c     **                with the programs DISSOC and PROPER.        **
c     **                                                            **
c     ** LANGUAGE:      FORTRAN 7.                                  **
c     **                                                            **
c     ** HISTORY:       This code was constructed by                **
c     **                Gestur Valgardsson, in a partial            **
c     **                fulfillment of a MS thesis at the           **
c     **                University of Tennessee, 1984.              **
c     **                                                            **
```

```
c       ** CHANGES:        NONE                                          **
c       **                                                               **
c       ** DATE:           Completed [06:20:84]                          **
c       **                                                               **
c       *******************************************************************
c
c       *******************************************************************
c       **                                                               **
c       **                  THE COMBUSTION CYCLE                         **
c       **                  --------------------                         **
c       **  I                                                            **
c       **  I                                                            **
c       **  I         (3)<---P3                                          **
c       **  I         *  *                                               **
c       **  I         *   *                                              **
c       **  I         *    *                                             **
c       **P I         *      *                                           **
c       **R I         *        *                                         **
c       **E I         *          *                                       **
c       **S I         *            *                                     **
c       **S I         *              *                                   **
c       **U I        *                *                                  **
c       **R I  --->(2)<--- UR            *                              **
c       **E I C10H22  *                    *                            **
c       **  I             *                   (4)<---UP4                 **
c       **  I                *                 *   *                    **
c       **  I                    *             *       *                **
c       **  I                        *         *           *            **
c       **  I                            (1) * * * * * * (5)            **
c       **  I                      NH3+air--->                           **
c       **  I---------I----------------------I---------------------     **
c       **          Vtdc                   Vbdc                         **
c       **                                                              **
c       **                       VOLUME                                 **
c       **                                                              **
c       *******************************************************************
c
c       *******************************************************************
c       **                                                               **
c       **                DECLARATION OF VARIABLES                       **
c       **                ------------------------                       **
c       **                                                               **
c       implicit real(a-h,m-z)
c       real*4 u1(10),u2(10),u3(10),u4(10)       |Internal Energy        **
c                 at different locations on the combustion cycle        **
c                                                                       |**
c       real*4 newch(10),olch(10)                                        **
c       real*4 h1(10),h2(10),h3(10),h4(10)       |Enthalpy values        **
c                 at different locations on the combustion cycle        **
c       real*4 nr(10) |nr(1to3)=Molefractions of the NH3-air mixt       **
c                     nr(3to8)=Molefractions of the product gases       **
c       real*4 Cpr(10)          |Specific heat of the reactants          **
c       real*4 Cp(10)           |Specific heat of the products           **
c       real*4 np(10)    |No of moles of product at statepoint 3         **
c       real*4 np4(10)   |No of moles of product at statepoint 4         **
c       real*4 ntp       |Total number of moles at statepoint 3         **
c       real*4 ntp4      |Total mole number at statepoint 4             **
c       real*4 saveNp(20,11)     |Saves the compos. at statep. (3)       **
c       real*4 savNp4(20,10)     |Saves the compos. at statep. (4)       **
c       real*4 mc        |No of moles of carbon in then fuel            **
c       real*4 mh        |No of moles of hydrogen in the fuel           **
c       real*4 mo        |No of moles of oxygen in the fuel             **
```

```
      real*4 eq          |Equivalence ratio of the oxygen.          **
      real*4 kr          |kr=Cp/Cv for the mixture in the cylinder **
      real*4 kp          |kp=Cp/Cv for the prod. at statep. (3)     **
      real*4 kp4         |kp4=Cp/Cv for the prod. at statep. (4)    **
      real*4 CR          |Compression ratio                         **
      real*4 mep         |Mean effective pressure                   **
      real*4 Nmr         |No of moles of reactants in the cylinder **
      real*4 Nmo         |Mole of air an NH3 in the stoichiom. eqn.**
      real*4 Volla       |Volume ratio of NH3 to C10H22             **
      real*4 Massa       |Mass ratio of NH3 to C10H22               **
      real*4 Enrat       |Energ ratio of NH3 to C10H22              **
      real*4 eff         |Thermal efficiency of the cycle           **
      character*9 spur,name,disos,disaft      |control param.       **
      character*70 memo        |Enables  memo to be writen with     **
                                into the solution file.              **
c                                                                    **
c     **                                                             **
c     ***************************************************************
c
c     ***************************************************************
c     **                                                             **
c     **                   INPUT TO THE PROGRAM                      **
c     **                  ----------------------                     **
c     **                                                             **
      write(5,10)                                                    |**
      read(5,20) name                  |Name of the output file      |**
      open(unit=21,file=name)          |Output file is opened        |**
      open(unit=22,file='yy25',access='append')
      open(unit=23,file='comp25',access='append')
      open(unit=24,file='f25',access='append')
                                                                     **
c                                                                    |**
      write(5,30)
      read(5,40) memo                  |Memo to be printed into
      write(21,40) memo                |the output file
c
      write(5,50)
      read(5,*) Na          |Moles of ammonia in the chemical eqn.
c
      write(5,60)
      read(5,*) No          |Moles of n-Decane in the chemical eqn.
c
      write(5,70)
      read(5,20) disos          |Question dissociation during
                                 combustion, Yes or No?
c
c
      write(5,80)
      read(5,20) disaft         |Question Dissociation during
                                 expansion, Yes of No?
c
c
      write(5,90)
      read(5,*) CR          |Compression ratio of the cycle
c
      write(5,100)                    |Min and Max value of Y/Ycc
      read(5,*) Eq,eqmax              |Kmol of Oxigen per (Na+No)
                                       kmol of fuel
c
c     ***************************************************************
c     **                                                             **
c     **              ENGINE/PARAMETER SPECIFICATIONS                **
c     **             --------------------------------                **
      Rpm = 1500.0          |Rpm of the engine                       **
      Vdisp = 0.000823      |Dispalacement cylinder     (m**3)       **
```

```
      Vtdc = Vdisp/(CR-1.0)    |Volume at top dead center (m**3) **
      Vbdc = CR*Vdisp/(CR-1.0)  |Volume at botom dead c. (m**3) **
      Bo = 0.1016              |Bore of the cyclinder [m]        **
      S = 0.1016               |Stroke of the cylinder [m]       **
      L = 2.0*0.1016           |The conecting rod length [m]     **
      R = 8.314                    |The gas constant (kJ/kmol K) **
      **                                                         **
c     ** NOTE: It is not necessary to provide accurate numbers **
c     **       for these parameters, since the output data is  **
c     **       intensive in nature, and does not depend on the **
c     **       actual size of the engine. On the oter hand, it **
c     **       is possible to probe the program for values     **
c     **       such as power.                                  **
c     ************************************************************
c
c     ************************************************************
c     **                                                         **
c     **          PARAMETERS IN THE CHEMICAL EQN.                **
c     **          -------------------------------                **
c     **                                                         **
      Mc = 10.*No       |Moles of carbon in the chemic.          **
c                       |eqn. describing the combustion          **
      Mh = 22.0*No + 3.0*Na |Moles of hydrogen in the chem       **
c                           |eqn. describing the combustion      **
      Mo = 0.0              |Moles of oxygen in the chemic       **
c                           |eqn describing the combustion       **
c     **     Mo is variable is allways zero for C10H22 and NH3   **
c     **                                                         **
c     ************************************************************
c
      K1 = 0          |Control Parameter, counts the no of iterations
c
c     ************************************************************
c     **                                                         **
c     **    Heat of reaction (kJ/kmol).....Gaseous products      **
c     **    ------------------------------------------------     **
      Hrpa = -318612.0     |Enthalpy of react. for NH3 (gas)     **
      Hrpf = -6261300.0    |Enthalpy of react. for C10H22 (liq)  **
c     **        298.16 K                                         **
c     ************************************************************
c
c
      Ycc = Mc + Mh/4.0 + Mo/2.0    |Chemically correct amount of
c     oxygen neaded to burn the fuel mixture with out exes air
c
      Ymin = Ycc - Mc/2.0    |Minimum amount of air required to
                              compleatily burn all the fuel
c
c
10000 write(5,110),eq,CR
      Y = Eq*Ycc
c     write(5,*)'value of Y',Y                                   **
c     **                                                         **
c     ** The number of moles of product depends on the number   **
c     ** of moles of oxygen present in the cylinder             **
c     **                                                         **
      if(Y.ge.Ycc) then          |condition of Y being checed    **
      Npo = mc + (Y-Ycc) + mh/2 + Y*3.76 + Na/2.0 |kilomoles of **
c           product formed from combustion of 1 kmole of fuel + **
c           4.76Y Kmol of                                        **
      else if(y.lt.Ycc) then
      Npo = 2.0*(Y-Ymin)+2.0*(Ycc-Y)+mh/2.0+Y*3.76+Na/2.0
c           Kmol of prod. formed from comb. of 1 kmol of fuel + **
```

```
c            4.76Y of air                                              **
      end if
c                                                                      **
      if(Y.lt.Ymin) write(5,*)'Warning walue of Y is too low'
c     **                                                               **
c     ********************************************************************
c
c     ********************************************************************
c     **        Spesification of thermodynamic properties               **
c     **        at the inlet to the engine                              **
c     **                                                                **
c     **                                                                **
10010 Tm = 300.0    |Assumed manifold temperature                       **
      Tf = 500.0    |Assumed inlet temp. of the pilot fuel              **
      P1 = 1.0      |Assumed manifold pressure (atm)                     **
      T1 = Tm       |Initial assumption                                 **
c     **                                                                **
c     ********************************************************************

c     ********************************************************************
c     **                                                                **
c     **                BEGINING OF CALCULATIONS                        **
c     **                ------------------------                        **
c     **                                                                **
      Nx = 0.0         |Initialli there is no product remainings        **
c     **                left in the cylinder                            **
c     **                                                                **
      Nm = ((P1*Vbdc)/(R*Tm))*1.01316*10.0**2.0          |Kmoles
c     of air in the cylinder during the first comp. stroke
c     this value is then modified after injection of pilot fuel.
c
      K1 = K1 + 1          |Cycle counter i.e. counts the cycles
c
10020      Nmo = Na + 4.76*Y          |kmoles of air and NH3 in the
c                            ||Berical equation
c
c     ********************************************************************
c     **                                                                **
c     **                    COMPRESSION STROKE                          **
c     **                    ------------------                          **
c     ** ---------------------------------------------------            **
c     ** Evaluation of Specific heat values of the air and NH3          **
c     **                                                                **
c     **                                                                **
c     **                          Specific heat,const press:            **
c     **                         ---------------------------            **
      Cpr(1) = 29.1 + 0.0248*T1          |for NH3                       **
      Cpr(2) = 27.0 + 0.0079*T1          |for O2                        **
      Cpr(3) = 27.6 + 0.0051*T1          |for N2                        **
c     **                                                               **
c     **   ---------------------------------------------               **
c     **   Mole fractions of pertinent gases present in the            **
c     **   cylinder during compression                                 **
c     **                                                               **
c     **                                Mole fractions:                **
c     **                               ------------------              **
      nr(1) = Na/nmo                       |of NH3                  **
      nr(2) = Y/nmo                        |of O2                    **
      nr(3) = Y*3.76/nmo                   |of N2                        **
c     **                                                                **
c     **                                                                **
```

```
      Cprt = nr(1)*cpr(1) + nr(2)*cpr(2) + nr(3)*cpr(3)          |**
      **                                                          **
c     **--------------------------------------------------------**
c     ** Evaluation of Specific heat value of the product gases **
c     ** st T1.                                                  **
c     **                                                        |**
      if(Y.ge.Ycc) then                                         **
c     **                                                        **
c     **                              Mole fractions:           **
c     **                            ------------------          **
      nr(4) = mc/Npo                        |for CO2              **
      nr(5) = (Y-Ycc)/Npo                   |for O2               **
      nr(7) = mh/(2.0*Npo)                  |for H2O              **
      nr(8) = (Y*3.76 + Na/2.0)/Npo         |for N2               **
c     **                                                        **
c     **                           Specific heat,const press:   **
c     **                          ----------------------------  **
      cpr(4) = 28.8 + 0.0280*T1             |for CO2              **
      cpr(5) = 27.0 + 0.0079*T1             |for O2               **
      cpr(7) = 30.5 + 0.0103*T1             |for H2O              **
      cpr(8) = 27.6 + 0.0051*T1             |for N2               **
c     **                                                        **
      Cppt=nr(4)*cpr(4)+nr(5)*cpr(5)+nr(7)*cpr(7)+nr(8)*cpr(8)  |**
c     **                                                        **
      else if(Y.lt.Ycc) then                                    **
c     **                                                        **
c     **                              Mole fractions:           **
c     **                            ------------------          **
      nr(4) = 2.0*(Y-Ymin)/Npo              |for CO2              **
      nr(6) = 2.0*(Ycc-Y)/Npo               |for CO               **
      nr(7) = mh/(2.0*Npo)                  |for H2O              **
      nr(8) = (Y*3.76 + Na/2.0)/Npo         |for N2               **
c     **                                                        **
c     **                           Specific heat,const press:   **
c     **                          ----------------------------  **
      cpr(4) = 28.8 + 0.0280*T1             |for CO2              **
      cpr(6) = 27.4 + 0.0058*T1             |for CO               **
      cpr(7) = 30.5 + 0.0103*T1             |for H2O              **
      cpr(8) = 27.6 + 0.0051*T1             |for N2               **
c     **                                                        **
      Cppt=nr(4)*cpr(4)+nr(6)*cpr(6)+nr(7)*cpr(7)+nr(8)*cpr(8)  |**
c     **                                                        **
      end if
c
      Cprt = (nm*Cprt + nx*Cppt)/(nm+nx)  |Specific heat of the
c                                         |mixture in the cyl.
c                                         |during compression
      Kr = Cprt/(Cprt-R)                  |  K = cp/cv for the mixture
c     **                                                        **
c     **                                                        **
c     **            PROPERTIES AT END OF COMPRESSION            **
c     **            --------------------------------            **
c     **                                                        **
      T2 = T1*(CR**(kr-1.0))              |Temperature after compression **
      P2 = P1*CR**Kr                      |Pressure after compression    **
      Write(5,*)'Step.....(2)....finished',T2,P2
      Wcomp = (nm + Nx)*(cprt - R)*(T2-T1)   |Compression work
      performed by the engine on the fuel air mixture           **
c     **                                                        **
c     ************************************************************
c     **
```

```
c     **              BEGINING OF COMBUSTION                          **
c     **              ----------------------                          **
c     **                                                              **
c     **    Enthalpy values of gases at temperature 298.16            **
c     **    ----------------------------------------------            **
c     **                                                              **
c     **                          Enthalpy of:                        **
c     **                          ------------                        **
      HoCO2 =   9364.0            |off CO2                            **
      HoCO  = 283754.0            |of CO                              **
      HoH2O =  57316.0            |of H2O                             **
      HoO2  =  17200.0            |of O2                              **
      HoN2  =  15780.0            |of N2                              **
c     **                                                              **
c     **                                                              **
c     ** Enthalpy of C10H22  cal. from the heat of react. eqn.        **
c     ** ------------------------------------------------------       **
c     **                                                              **
      Hf298 = -Hrpf + 10.0*HoCO2 + 11.0*HoH2O - 15.5*HoO2

      Uf298=Hf298+(21.0-16.5)*298.16*R-(10+22./2.0-Ycc)*298.16*R
                                                                      **
c     **                                                              **
c     ** Enthalpy of NH3 cal. from the heat of reaction eqn.          **
c     ** ------------------------------------------------------       **
      Ha298 = -Hrpa + 1.5*HoH2O + 0.5*HoN2 - 0.75*HoO2                |**
      Ua298 =Ha298+(2.0-1.75)*298.16*R-(1.5+0.5-0.75)*298.16*R        |**
c     **                                                              **
c     **                                                              **
c     ** Internal energy of air and NH3 mixt. per kmol of mixt.      **
c     ** ------------------------------------------------------       **
c     **                                                              **
      Ur = nr(1)*Ua298 + nr(2)*HoO2 + nr(3)*HoN2        |[kj/kmol]
      1-(nr(2)+nr(3))*298.16*R          |Internal energy of the
c     **                                 mixture of NH3; air per kmol **
c     **                                                              **
c     **                                                              **
c     ** Internal energy, per mol of the product remainings           **
c     ** ------------------------------------------------------       **
c     **                                                              **
      if(Y.ge.Ycc) then                                               |**
c     **                                                              **
c     **                            Mole fractions:                   **
c     **                           ------------------                 **
      nr(4) = mc/Npo                      |for CO2                    **
      nr(5) = (Y-Ycc)/Npo                 |for O2                     **
      nr(7) = mh/(2.0*Npo)                |for H2O                    **
      nr(8) = (Y*3.76 + Na/2.0)/Npo       |for N2                     **
c     **
      Up = nr(4)*HoCO2+nr(5)*HoO2+nr(7)*HoH2O+nr(8)*HoN2
      1-(nr(4)+nr(6)+nr(7)+nr(8))*298.16*R
c     ** Internal energy of the product gases per kmol.               **
c     **                                                              **
      else if(Y.lt.Ycc) then                                          **
c     **                                                              **
c     **                            Mole fractions:                   **
c     **                           ----------------                   **
      nr(4) = 2.0*(Y-Ymin)/Npo            |for CO2                    **
      nr(6) = 2.0*(Ycc-Y)/Npo             |for CO                     **
      nr(7) = mh/(2.0*Npo)                |for H2O                    **
      nr(8) = (Y*3.76 + Na/2.0)/Npo       |for N2                     **
c     **
```

```
      Up = nr(4)*HoCO2+nr(6)*HoCO+nr(7)*HoH2O+nr(8)*HoN2
      1-(nr(4)+nr(6)+nr(7)+nr(8))*298.16*R
c     ** Internal energy of the product gases per kmol.          **
c     **                                                         **
      end if
c     **                                                         **
c     ** To calculate the energy values at T2 integration has    **
c     ** to be performed. Here Cp(T) = Ai + Bi*T. and the        **
c     **                                                         **
c     **                2                                2   2   **
c     **       H(t) = S cp(t) dt = Ai(T - T ) + Bi(T - T )/2     **
c     **              1                  2   1         2   1     **
c     **                                                         **
c     ** ------------------------------------------------------  **
c     **                                                         **
      Ar = nr(1)*29.1 + nr(2)*27.0 + nr(3)*27.6
      Br = nr(1)*0.0248 + nr(2)*0.0079 + nr(3)*0.0051
c     **                                                         **
      if(Y.ge.Ycc) then
c     **                                                         **
      Ap = nr(4)*28.8 + nr(5)*27.0 + nr(7)*30.5 + nr(8)*27.6
      Bp = nr(4)*0.028 +nr(5)*0.0079+nr(7)*0.0103+nr(8)*0.0051
c     **                                                         **
      else if(Y.lt.Ycc) then
c     **                                                         **
      Ap = nr(4)*28.8 + nr(6)*27.4 + nr(7)*30.5 + nr(8)*27.6
      Bp = nr(4)*0.028 +nr(6)*0.0058+nr(7)*0.0103+nr(8)*0.0051
c     **                                                         **
      end if
c     **                                                         **
c     Integration performed                                      **
c     **
      Cpr2 = Ar*(T2-298.16) + Br*(T2**2.0 - 298.16**2.0)/2.0
      Cpp2 = Ap*(T2-298.16) + Bp*(T2**2.0 - 298.16**2.0)/2.0
      Cvr2 = Cpr2 - R*(T2-298.16)
      Cvp2 = Cpp2 - R*(T2-298.16)
      Ur = Ur + cvr2  |Internal energry of the air; NH3 mixture
                      |per kmol mixture fuel-air [kj/kmol]
      Up = Up + Cvp2  |Internal energy, per kmol of the
c     **                product gases                            **
c     **                                                         **
c     **                                                         **
c     **    Energy value of the fuel at temperature Tf           **
c     **    ------------------------------------------           **
c     **                                                         **
      HrDec = Hf298+313.82*(Tf-298.16)                           |**
      UrDec = Hrdec |Incompressible fluid                        |**
c     **                                                         **
c     **                                                         **
c     **    The internal energy of the charge at statepoint 2    **
c     **   ---------------------------------------------------   **
c     ** At this point the pilot oil is injected into the cyl.   **
c     ** and therefore the total number of kmoles of fuel-air    **
c     ** Given by Nm = Nm(1 + No/Nmo). The total energy per      **
c     ** cycle is therefore given by.                            **
c     **                                                         **
c     **                                                         **
      Ur = Nm*(Nmo*Ur + No*UrDec)/(Nmo+No) + Nx*Up     |[Kj]     **
c     **                                                         **
c     **                                                         **
c     **              ITERATION FOR T3 BEGINS HERE               **
```

```
c       **              ----------------------------                **
c       **                                                          **
        T3 = 1500.0             |first guess at T3
        ind = 10                |control parameter                  **
c       **
c       abundances of H, C, N and O in the chemikal equation
c       ----------
        AC = mc
        AH = mh
        AO = 2.0*Y
        AN = 2.0*(Na/2.0 + 3.76*Y)
c       **                                                          **
c       ** First step is to find the right temperature interval     **
c       **                                                          **
        do 1000 ii = 1,100  |controls the max no. of iterations
c       **
c       ** This progr. gives chose between dissoc. and no dissoc.  **
c       **                                                          **
        if(disos(:1).eq.'y'.or.disos(:1).eq.'Y') then
c       **                                                          **
c       ** call to the subpr. whitch calculates the dissociation    **
c       ** given temperature and condition at the point             **
c       **                                                          **
c       **                                                          **
c       **                  NOMENCLATURE FOR DISSOC                 **
c       **                 ------------------------                 **
c       **  V  - Constant volume combustion                         **
c       **  CR - Change in volume. Constand volume -> CR=0.0        **
c       **  P2 - Pressure at Reference state                        **
c       **  T2 - Temperature at reference state                     **
c       **  AC - Abundance of carbon in the chemical eqn            **
c       **  AH - ............Hydrogen.....................          **
c       **  AO - ............Oxigen.....................           **
c       **  AN - ............Nitrogen.....................          **
c       **  P3 - The pressure after compression. Does not play      **
c       **       role unless constant pressure condition is         **
c       **  T3 - The temperature after compression                  **
c       **  Np - The composition at P3 and T3                       **
c       **  Ntp- Total number of moles formed from combustion of    **
c       **       (Na+No) moles of fuel                              **
c       **                                                          **
        call DISSOC('v',1.0,P2,T2,AC,AH,AO,AN,0.0,T3,Np,Ntp)      |**
c       **                                                          **
c       **                                                          **
c       **                                                          **
        Cm = (nm/nmo) + (nx/ntp)        |Scale factor reducing
c                                       |mole numbers to fit the
c                                       |cylinder
c
        do 1010 i = 1,10        |This DO loop is performed
c                               |only for dissociation
        np(i) = np(i)*cm        |Fiting of mole numbers
1010        continue
        else
        Cm = (nm/nmo) + (nx/npo)
c
        do 1020 i = 1,10        |This DO loop is performed
c                               |only for no dissociation
        np(i) = 0.0             |during expansion.
1020        continue
c
```

```
      if(y.ge.Ycc) then          |Calculation of mole numbers for
      np(1) = mc*cm              |no dissociation cace
      np(3) = (Y-Ycc)*cm
      np(6) = (Na/2.0 + 3.76*Y)*cm
      np(10) = mh*cm/2.0
      else if(Y.lt.Ycc) then
      np(1) = 2.0*(Y-Ymin)*cm              |No moles formed from
      np(2) = 2.0*(Ycc-Y)*cm               |combustion of (Na + No)
      np(6) = (Y*3.76 + Na/2.0)*cm         |moles of fuel
      np(10) = mh*cm/2.0
      end if
      end if
c     **                                                          **
c     **                                                          **
c     **          Intfun calculates Internal energy at T3         **
c     **          ---------------------------------------         **
c     **                                                          **
c     write(5,*)'value of t3  ',T3                                |**
      call intfun(T3,Np,Ntp,Up3)                                  |**
c     **                                                          **
      func = (Up3 - Ur)
c     write(5,*) func,Ta,T3,Tb,Up3,Ur
      do while(ind.gt.0)
c     write(5,*)'value of T3,func,Ur,Up3',T3,func,Ur,Up3
      if(func.lt.0.0) then
      T3 = T3 + 100.0
      else
      Ta = T3 - 100.0
      Tb = T3
      ind = -10
      end if
      goto 1000
      end do
      T3 = (Ta + Tb)/2.0         |Bisection method in operation
      if(disos(:1).eq.'y'.or.disos(:1).eq.'Y') then
      call dissoc('v',1.0,P2,T2,AC,AH,AO,AN,0.0,Ta,Np,Ntp)
      cm = (nm/nmo) + (nx/ntp)
      do 1030 i = 1,10
      np(i) = np(i)*cm
1030  continue
      end if
      call intfun(Ta,Np,Ntp,Upa)
      if(disos(:1).eq.'y'.or.disos(:1).eq.'Y') then
      call dissoc('v',1.0,P2,T2,AC,AH,AO,AN,0.0,T3,Np,Ntp)
      Cm = (nm/nmo) + (nx/ntp)
      do 1040 i = 1,10
      np(i) = np(i)*cm
1040  continue
      end if
      call intfun(T3,Np,Ntp,Up3)
      if((Upa-Ur)*(Up3-Ur).lt.0.0) then
      Ta = Ta
      Tb = T3
      else
      Ta = T3
      Tb = Tb
      end if
      T3 = (Ta + Tb)/2.0
      If(abs(Ta-Tb).lt.0.05) then
      goto 10030
      end if
```

```
1000      continue
          write(5,*)'Iteration for T3 was not successfull'
          stop
c         **                                                          **
c         **                                                          **
c         **            PROPERTIES AT STATE-POINT (3)                 **
c         **            -----------------------------                 **
c         **                                                          **
10030       P3 = P2*(T3/T2)*(ntp/(nm+nx))
c         write(5,*)'I am continuing.....'
          do 1050 i = 1,10
          saveNp(K1,i) = 100.0*(Np(i)/ntp)
          saveNp(k1,11) = eq
c         **                                                          **
1050      continue                                                    |**
c         ************************************************************
c
c         ************************************************************
c         **                                                          **
c         **              BEGINING OF EXPANSION                       **
c         **              ---------------------                       **
c         **                                                          **
c         **            NOMENCLATURE FOR EXPANSION                    **
c         **            --------------------------                    **
c         **  Entropy value at points 3 and 4 clculated               **
c         **  AC3: Abundance of carbon moles at statep (3)            **
c         **  AH3: ------------ hydrogen -----------------            **
c         **  AO3: ------------ oxygen -------------------            **
c         **  AN3: ------------ nytrogen -----------------            **
c         **  Note: Values of np(i) i = 1,2,....10, have              **
c         **        units of munber of moles of specie i              **
c         **        in the cyclinder.  Therefore these                **
c         **        values have to be scaled with - cm -              **
c         **        in order to get moles per Na+No moles             **
c         **        of NH3 and C10H22                                 **
c         **  Tlook: searching value of T4, to bracet of              **
c         **         the right value                                  **
c         **  T41:  searching value for T4.                           **
c         **  T4a and T4b: T4a < T41 < t4b                            **
c         **                                                          **
c         **                                                          **
c         **   Abundances of C, H, O and N at statep 3                **
c         **   ---------------------------------------                **
          AC3 = (Np(1) + Np(2))/cm
          AH3 = (2.0*(Np(8) + Np(10)) + Np(7) + Np(9))/cm
          AO3 = (2.0*(Np(1)+Np(3))+Np(2)+Np(4)+Np(5)+Np(9)+Np(10))/cm
          AN3 = (Np(5) + 2.0*Np(6))/cm
c
          do 1060 i = 1,10
          np4(i) = np(i)/cm        |Scaling of the mole number to fit
          np(i) = np(i)/cm         |values calculated for statep (4)
1060        continue
          ntp4 = ntp/cm
          ntp = ntp/cm
c                                                                     **
c         **                                                          **
c         **          BISECTIONAL ALGORITHM TO EVALUATE T4            **
c         **          -----------------------------------             **
c         **                                                          **
          do 1070 1 = 1,1000      |max number of iterations allowed
          T4look = T3 - (1-1)*5.0
```

```
c
c       write(5,*) T4look,T3,P3,P4look,ds
        if(disaft(:1).eq.'y'.or.disaft(:1).eq.'Y') then
        if(T4look.lt.1300.0) goto 10040
        call dissoc('v',CR,P3,T3,AC3,AH3,AO3,AN3,0.0,T4look,Np4,Ntp4)
        end if
c
10040   P4look = (P3/cr)*(T4look/T3)*(Ntp4/Ntp)
        call absent(P4look,T4look,np4,S4look)
        call absent(P3,T3,np,S3)
        DS = S4look - S3        |Note that the value of S3
c       write(5,*) 'ds,s4look,s3,T4look',Ds,s4look,s3,T4look
        if (DS.le.0.0) then      |has the units of absolut entropy
        T4a = T4look              |therefore, cm is needed to make
        goto 10050               |to make the value spesific.
        end if
1070    continue
c       write(5,*)'Calculation of T4 was not successfull'
        stop
10050   T4b = T4look + 5.0
        do 1080 l = 1,100       |Max number of iterations allowed
        T41 = (T4a + T4b)/2.0
c
        if(disaft(:1).eq.'y'.or.disaft(:1).eq.'Y') then
        if(t41.lt.1300.0) goto 10060
        call dissoc('v',CR,P3,T3,AC3,AH3,AO3,AN3,0.0,T41,Np4,Ntp4)
        end if
c
10060   P41 = (P3/CR)*(T41/T3)*(Ntp4/Ntp)
        call absent(P41,T41,np4,S41)

        if(disaft(:1).eq.'y'.or.disaft(:1).eq.'Y') then
        if(t4a.lt.1300.0) goto 10070
        call dissoc('v',CR,P3,T3,AC3,AH3,AO3,AN3,0.0,T4a,Np4,Ntp4)
        end if
10070   P4a = (P3/CR)*(T4a/T3)*(Ntp4/Ntp)
        call absent(P4a,T4a,np4,S4a)
        if ((S41-S3)*(S4a-S3).gt.0.0) then
        T4a = T41
        T4b = T4b
        else
        T4a = T4a
        T4b = T41
        end if
        if(abs(T4a-T4b).lt.0.05) goto 10080
1080    continue
c       write(5,*)'Bracketing of T4 was not successful'
        stop
c       **                                                      **
c       **                                                      **
c       **              PROPERTIES AT STATE POINT (4)           **
c       **              -----------------------------           **
c       **                                                      **
c       **
10080   T4 = T41
        P4 = (P3/CR)*(T4/T3)*(Ntp4/ntp)
        do 1090 i = 1,10
        savNp4(kl,i) = 100.0*np4(i)/ntp4
1090    continue
        write(5,*)'step.......(4)....finished  ',T4,P4
        call intfun(T4,np4,Ntp4,Up4)
        call intfun(T4,np,ntp,up44)
```

```
      cm4 = (nm/nmo) + (nx/ntp4)                                        **
c     **
c     ************************************************************
c
c     ************************************************************
c     **                                                            **
c     **                      BLOWDOWN                              **
c     **                      --------                              **
c     **                                                            **
c     **                                                            **
c     **
      call gask(T4,np4,kp)          |calculates cp/cv = k at stp. (4)
c     **                                                            **
      P5 = P1 |I.e. point 5 is as if pont 4 were expanded           **
c     **        Isentropically down to manifold pressure P1         **
      T5 = T4*(P1/P4)**((kp-1.0)/kp)   |It is assumed that the      **
c     residuegases in the cyclinder expand isentropically, once     **
c     the exhaust valve opens.                                      **
      write(5,*)'step.......(5)....finished  ',T5,P1                |**
      **                                                            **
c     **
c     ************************************************************
c     **                                                            **
c     **      CALCULATION OF PERFORMANCE PARAMETERS BEGINS          **
c     **     ---------------------------------------------          **
c     **                                                            **
      cm4 = (nm/nmo) + (nx/ntp4)                                    |**
      Wexp =  Up3 - Up4*cm4          |Expansion work performed      **
      Wnet = (Wexp - Wcomp)          |Net output per cyclel         **
      Work = Wnet*Rpm/120.0          |Net output in Kw              **
      Horsp = Work/0.746             |Net output in Horspower       **
      Mep = (Wnet*4.0/(3.1415*S*Bo**2.0))/101.3     |Mean eff.     **
      **                 ressure during the expansion period.       **
c     ************************************************************
c
c     ************************************************************
c     **                                                            **
c     **    CALCULATION OF SPESIFIC FUEL CONSUMPTION [G/MJ]         **
c     **   ------------------------------------------------         **
c     **                                                            **
      spfam = 1000000.0*(Na/(Na+No+4.76*Y))*nm*17.03/Wnet           |**
      spfol = 1000000.0*(No/(Na+No+4.76*Y))*nm*142.0/wnet           |**
      **                                                            **
c     ************************************************************
c
c     ************************************************************
c     **                                                            **
c     **        CALCULATION OF THE CYCLE EFFICIENCY BEGINS          **
c     **       -------------------------------------------          **
c     **                                                            **
      eff = abs(spfam*Hrpa/17.03+spfol*Hrpf/142.0)                  |**
      eff = 100000000.0/eff                                         |**
      Voleff = 100.*(((Nmo-Na)/Nmo)*Nm)/((101.316*Vdisp)/(R*300.0))
      **                                                            **
c     ************************************************************
c
c     ************************************************************
c     **       Calculation of different ratios in the               **
c     **       fuel mixture.                                        **
c     **                                                            **
c     **        Volla: volumetric ratio NH3:C10H22                  **
c     **        Massa: Mass ratio NH3:C10H22
```

```
c       **        Enrat: Energy ratio of NH3:C10H22                    **
c       **                                                             **
c       ****************************************************************
c       **                                                             **
c       ratio = nm/(nm+nx)          |                                  **
        Volla = 100.0*(Na/(Na+No))          |                          **
        Massa = 100.0*(Na*17.03/(Na*17.03 + No*144.0))          |      **
        Enrat = 100.0*Na*17.03*Hrpa/(Na*17.03*Hrpa+No*144.0*Hrpf |**
                                                                       **
c       **                                                             **
c       ****************************************************************
c
c       ****************************************************************
c       **                                                             **
c       **          CONVERGENCE OF THE CALCULATIONS CHECKED            **
c       **         ----------------------------------------            **
c       **                                                             **
        newch(1) = voleff
        newch(2) = T3
        newch(3) = p3
        newch(4) = mep
        newch(5) = eff
        newch(6) = spfam+spfol
        ch = 0.0
        do 1100 i = 1,6
        ch = ch + abs(newch(i)-olch(i))*100.0/(6.0*newch(i))
1100        continue
        write(5,*) ch,eff,mep,voleff
        do 1110 i = 1,6                                                **
        olch(i) = newch(i)  |                                          **
1110        continue        |                                          **
c       **                                                            |**
        if(abs(ch).gt.0.007) then                                      ***
c       **                                                             **
c       **                    CALCULATION OF T1                        **
c       **                   ------------------                        **
c       **                          Specific heat,const press:         **
c       **                         ----------------------------        **
        Cpr(1) = 29.1 + 0.0248*T1          |for NH3                     **
        Cpr(2) = 27.0 + 0.0079*T1          |for O2                      **
        Cpr(3) = 27.6 + 0.0051*T1          |for N2                      **
                                                                       **
c       **                                 Mole fractions:             **
c       **                                ----------------             **
c       **                                   |of NH3                   **
        nr(1) = Na/nmo                       |of O2                    **
        nr(2) = Y/nmo                        |of N2                    **
        nr(3) = Y*3.76/nmo                                             **
        ** ---------------------------------------------------------   **
c       ** Evaluation of Specific heat values of the air and NH3       **
c       **                                                             **
c       **                                                             **
        Cprt = nr(1)*cpr(1) + nr(2)*cpr(2) + nr(3)*cpr(3)             |**
                                                                       **
c       **                                                            **
c       ***-----------------------------------------------------------**
c       ** Evaluation of Specific heat value of the product gases     **
c       ** st T1.                                                     **
c       **                                                            |**
        if(Y.ge.Ycc) then                                              **
c       **                                 Mole fractions:             **
c       **                                ----------------             **
        nr(4) = mc/Npo                       |for CO2                  **
```

```
      nr(5) = (Y-Ycc)/Npo                |for O2                          **
      nr(7) = mh/(2.0*Npo)               |for H2O                         **
      nr(8) = (Y*3.76 + Na/2.0)/Npo      |for N2                          **
c     **                                                                  **
c     **                          Specific heat,const press:              **
c     **                         ----------------------------             **
      cpr(4) = 28.8 + 0.0280*T1          |for CO2                         **
      cpr(5) = 27.0 + 0.0079*T1          |for O2                          **
      cpr(7) = 30.5 + 0.0103*T1          |for H2O                         **
      cpr(8) = 27.6 + 0.0051*T1          |for N2                          **
c     **                                                                  **
      Cppt=nr(4)*cpr(4)+nr(5)*cpr(5)+nr(7)*cpr(7)+nr(8)*cpr(8)           |**
c     **                                                                  **
      else if(Y.lt.Ycc) then                                              **
c     **                                                                  **
c     **                              Mole fractions:                     **
c     **                             ----------------                     **
      nr(4) = 2.0*(Y-Ymin)/Npo           |for CO2                         **
      nr(6) = 2.0*(Ycc-Y)/Npo            |for O2                          **
      nr(7) = mh/(2.0*Npo)               |for H2O                         **
      nr(8) = (Y*3.76 + Na/2.0)/Npo      |for N2                          **
c     **                                                                  **
c     **                          Specific heat,const press:              **
c     **                         ----------------------------             **
      cpr(4) = 28.8 + 0.0280*T1          |for CO2                         **
      cpr(6) = 27.4 + 0.0058*T1          |for CO                          **
      cpr(7) = 30.5 + 0.0103*T1          |for H2O                         **
      cpr(8) = 27.6 + 0.0051*T1          |for N2                          **
c     **                                                                  **
      Cppt=nr(4)*cpr(4)+nr(6)*cpr(6)+nr(7)*cpr(7)+nr(8)*cpr(8)           |**
c     **                                                                  **
      end if                                                              |**
c     **                                                                  **
      A = (cppt/cprt - 1.0)/(Tm*T5)
      B = -(CR + (Tm/T5) - (Cppt/Cprt))/Tm
      C = -CR
      nx = ((P1*Vtdc)/(R*T5))*101.3                                       |**
      nm = ((P1*Vbdc)/(R*T1))*101.3                                       |**
      nm = nm - nx                                                        |**
      T1 = (B + SQRT(B**2.0 - 4.0*A*C))/(2.0*A)                           **
c     **                                                                  |**
      goto 10020                                                          |**
      else
      do 1120 i = 1,6
      olch(i) = 0.0
1120  continue                                                            **
c     **
c     ********************************************************************
c
c     ********************************************************************
c     **                                                                  **
c     **          RESULTS WRITEN INTO THE FILEE = <NAME>                  **
c     **         ---------------------------------------                  **
c     **                                                                  **
      if(k1.lt.2) then
      write(21,120)
      write(21,130)
      write(21,140) CR,P1,Vdisp,Ycc,Tf,Bo,Ymin,Tm,Rpm,
     1Volla,Massa,Enrat
      write(24,*) massa,(100.0-massa)
      write(23,*)'----------(    )----dissociation---(    ) no dissoc'
```

```
      write(23,*) massa,(100.0-massa)
      write(22,*)'----------(    )----dissociation---(    ) no dissoc'
      write(22,*) massa,(100.0-massa)
      write(21,150)
      write(21,160)
      write(21,170)
      write(21,150)
4      end if
      write(21,180) Y,T1,T2,T3,T4,T5,P2,P3,P4,Kr,Kp,ratio
      1,Horsp,Eff,Mep,(Y/Ycc),Voleff,spfam,spfol
      write(22,*) (Y/Ycc),T3,P3,Eff,Mep,t4,t5,voleff,spfam,spfol
      write(23,*)      CR,T3,P3,Eff,Mep,t4,t5,voleff,spfam,spfol
      Write(24,*) Mep,(Y/Ycc),spfol,spfam,((spfol+spfam)/spfol)
      end if
c
c     ***************************************************************
c     **                                                           **
c     **       INCREMENTING OF Y/YCC IS DONE AT THIS POINT         **
C     **       ------------------------------------------          **
c     **                                                           **
c     **
      Eq = Eq + 0.2
      if(Eq.gt.Eqmax) then          |Natural stop of the program  **
      write(21,190)
      write(21,150)
      if(disos(:1).eq.'y'.or.disos(:1).eq.'Y') then
      do 193 j = 1,kl
      write(21,200) savenp(j,11),(saveNp(j,i),i=1,10)
      if(Disaft(:1).eq.'y'.or.disaft(:1).eq.'Y') then
      write(21,210) (savNp4(j,i),i=1,10)
      else
      write(21,220)
      end if
193   continue
      stop
      else
      write(21,230)
      stop
      end if
      else
      goto 10000  |Continuation if Y/Ycc is less than desired
      end if                                                      **
c     **
c     ***************************************************************
c
c     ***************************************************************
c     **                                                           **
c     **                    FORMAT STATEMENTS                      **
c     **                    -----------------                      **
c     **                                                           **
c     **
10    format('1','read in the name of
      1 the OUTPUT file',19('.'),'=',$)
20    format(A9)
30    format(' ',/,' read in memo if here -------->',$)
40    format(A70)
50    format(' ',/,' read in the mol fraction of
      1AMMONIA in the fuel..=',$)
60    format(' ',/,' read in the mol fraction of N-DECANE
      1 in the fuel..=',$)
70    format(' ',/,' dissociation after combustion.
      1.................=',$)
80    format(' ','dissociation during expansion.
```

```
     1.................=',$)
90   format(' ',/,' read in the compression ratio CR=
     1.............',$)
100  format(' ',/,' Read in the max and min equivalence ratio='
     1,f5.2,' Ymin=',f5.2,'.......',$)
110  format(' ',/,' Equivalence ratio.........=',f6.2)
120  format(' ','Table [-1-]',/,12('-'))
130  format(' ','Simulation of combustion of ammonia and n-Decane
     1 with air in a Otto cycle, for different value of
     2 equivalence ratio (Y/Ycc)',/)
140  format(' Compression ratio..=',F4.1,11x,
     1'Manifold pressure..=',f5.2,2x,'(atm)',3x,
     2'Displacement.....',f8.6,2x,'(m)',/,
     3' Stoichiom. no O2...=',f5.2,10x,
     4'Temp. of n-Decane..=',f5.1,2x,'(K)',5x,
     5'Stroke.....=',f8.6,2x,'(m)',/,
     6' Min No of O2.....=',f5.2,2x,'(mol)',3x,
     7'Manifold temp.....=',f5.1,2x,'(K)',5x,
     8'Rpm.....=',f6.1,4x,'(Rpm)',/,
     9' NH3 by volume.....=',f5.1,2x,'(%)',5x,
     1'NH3 by weight.....=',f5.1,2x,'(%)',5x,
     1'Energy from NH3....=',f5.1,5x,'(%)',/)
150  format(' ',120('-'))
```

```
160   format(' ',' Y  ',' T1 ',' T2 ',' T3  ',' T4  '
      1,' T5  ',' P2 ',' P3 ',' P4 ',' Kr ',' Kp '
      2,'  nm ',' Power',' eff ',' Imep',' Y/Ycc',' Vol'
      3,' Isfc:NH3 ','Isfc:C10H22')
170   format(' ','molO2 (k) ',' (k) ',' (k)  ','(k)  '
      1,' (K) ',' (atm)',' (atm)',' (atm)',10x,' nm+nx'
      2,'  Hp  ',4x,'(atm)',9x,'eff',5x,'g/MJ',4x,'g/MJ')
180   format(f6.2,2f6.1,3f6.0,2f6.1,f6.2,2f6.2,f6.2,f7.2,f7.2,f6.2
      1,f6.2,f6.2,f8.2,f8.2)
190   format(////,47x,'Percent dissociation',/,29x,'Y/Ycc  CO2
      1  CO   O2   O   NO   N2   H   H2   OH  H2O')
200   format(' ','Composition at state P. (3)',2x,f4.2,10f5.1)
210   format(' ','Composition at state P. (4)',6x,10f5.1)
220   format(' ',40x,'Frozen composition')
230   format(' ',40x,'No dissociation case')
      stop
      end
c      **                                                          **
c      ************************************************************
c
c     ************************************************************
c     **                                                          **
c     **                  AUXILIARY ROUTINES                      **
c     **                  ------------------                      **
c     **                                                          **
c     **  Each one of the following routines calculate thermod.   **
c     **  property for the product gases, using n(10) as the      **
c     **  weighing value.                                         **
c     **                                                          **
c     **                                                          **
c     ************************************************************
c
c     ************************************************************
c     **                                                          **
c     **                CALCULATES ENTHALPY                       **
c     **                -------------------                       **
c     **                                                          **
      subroutine entfun(T,x,xt,ht)   |calculates enthalpy
      real*4 T,x(10),xt,h(10),ht     |using x(10) as the
      call enthp('CO2',T,h(1))       |wighing values.
      call enthp('CO',T,h(2))        |NOTE: x(10) is same as
      call enthp('O2',T,h(3))        |n(10) in the mainprogram.
      call enthp('O',T,h(4))
      call enthp('NO',T,h(5))
      call enthp('N2',T,h(6))
      call enthp('H',T,h(7))
      call enthp('H2',T,h(8))
      call enthp('OH',T,h(9))
      call enthp('H2O',T,h(10))
      Ht = 0.0
      xt = 0.0
      do 400 j = 1,10
      Ht = Ht + x(j)*h(j)
      xt = xt + x(j)
400   continue
      return
      stop
      end
c      **                                                          **
c      ************************************************************
```

```
c
c      ************************************************************
c      **                                                        **
c      **              CALCULATES INTERNAL ENERGY                **
c      **              --------------------------                **
c      **                                                        **
c      ************************************************************
       subroutine intfun(T,x,xt,ut)
       real*4 T,x(10),xt,u(10),ut
       call inten('CO2',T,u(1))
       call inten('CO',T,u(2))
       call inten('O2',T,u(3))
       call inten('O',T,u(4))
       call inten('NO',T,u(5))
       call inten('N2',T,u(6))
       call inten('H',T,u(7))
       call inten('H2',T,u(8))
       call inten('OH',T,u(9))
       call inten('H2O',T,u(10))
       ut = 0.0
       xt = 0.0
       do 400 j = 1,10
       ut = ut + x(j)*u(j)
       xt = xt + x(j)
400    continue
       return
       stop
       end
c      **                                                        **
c      ************************************************************
c
c      ************************************************************
c      **                                                        **
c      **              CALCULATES THE GAS CONSTANT K             **
c      **              -----------------------------             **
c      **                                                        **
c      ************************************************************
       subroutine gasK(T,np,Kp)
       real*4 T,Kp,Ntp,np(10),Cp(10)
       call Cpres('CO2',T,cp(1))
       call Cpres('CO',T,cp(2))
       call Cpres('O2',T,cp(3))
       call Cpres('O',T,cp(4))
       call Cpres('NO',T,cp(5))
       call Cpres('N2',T,cp(6))
       call Cpres('H',T,cp(7))
       call Cpres('H2',T,cp(8))
       call Cpres('OH',T,cp(9))
       call Cpres('H2O',T,cp(10))
       Cpp = 0.0
       Ntp = 0.0
       do 100 i = 1,10
       Cpp = Cpp + np(i)*cp(i)
       Ntp = Ntp + np(i)
100    continue
       Cpp = Cpp/Ntp
       Kp = Cpp/(Cpp - 8.314)
       return
       end
c      **                                                        **
c      ************************************************************
```

```
c
c     ***************************************************************
c     **                                                           **
c     **                  CALCULATES ENTROPY                       **
c     **                  -----------------                        **
c     **                                                           **
c     **
      subroutine absent(P,T,n,S)
      real*4 P,partp,T,S,Nt,n(10),e(10)
      call entro('CO2',T,e(1))
      call entro('CO',T,e(2))
      call entro('O2',T,e(3))
      call entro('O',T,e(4))
      call entro('NO',T,e(5))
      call entro('N2',T,e(6))
      call entro('H',T,e(7))
      call entro('H2',T,e(8))
      call entro('OH',T,e(9))
      call entro('H2O',T,e(10))
      S = 0.0
      Nt = 0.0
      do 100 i = 1,10
      Nt = Nt + n(i)
100   continue
      do 200 i = 1,10
      partp = n(i)*P/Nt
      if(n(i).eq.0.0) goto 200
      S = S + n(i)*e(i) - n(i)*8.314*alog(partp)
200   continue
      return
      end                                                          **
c      **                                                           **
c      **
c      ********************************************** END ********
```

```
c     ****************************************************************
c     **              <<<<<< SUBROUTINE DISSOC >>>>>>                 **
c     ****************************************************************
c     ** PURPOSE: Calculate equilibrium composition for comb-        **
c     **          bustion of equation of of the form                  **
c     **                                                              **
c     **       C  + H  + O  + N   + Y(O + 3.76N ) ======>             **
c     **        MC   MH   MO   MN      2       2                      **
c     **                                                              **
c     **       N(1)CO + N(2)CO + N(3)O + N(4)O + N(5)NO               **
c     **            2                 2                               **
c     **                                                              **
c     **       N(6)N + N(7)H + N(8)H + N(9)OH + N(10)H O              **
c     **            2                2                    2           **
c     **                                                              **
c     **          where: MC,MH,MO,MN are the number of moles          **
c     **          of carbon, hydrogen, oxygen, and nitrogen           **
c     **          in the fuel. N(i), i=1,10 are the molenumb.          **
c     **          of the product gases. The routine is capable        **
c     **          of calculating both constant volume (dV=0)          **
c     **          and constant pressure (dP=0) combustion.            **
c     **          Control of the combustion type is done by           **
c     **          the calling parameters to the routine.              **
c     **                                                              **
c     ** INPUT:  The following is a list of input parameters          **
c     **                                                              **
c     **          INPUT                MEANING                       **
c     **          -------              ---------                     **
c     **          cond : Combustion type, i.e. dV=specified           **
c     **                 or dP=0. Correct respond is either           **
c     **                 V or P. NOTE: cond is a character            **
c     **                 variable.                                    **
c     **          cr:    Applies in the case when cond=V.             **
c     **                 The numerical value designates the           **
c     **                 compion ratio of the cycle.                  **
c     **                 NOTE: if cr>1 the condition dV=0 is          **
c     **                 not in force, but rather that the            **
c     **                 end conditions of the combustion             **
c     **                 are specified by known values of P;T         **
c     **          pr:    The reference pressure of the fuel           **
c     **                 air mixture. This parameter needs            **
c     **                 only have meaningful value for dV=           **
c     **                 specified.                                   **
c     **          tr:    The reference temp. of the fuel              **
c     **                 air mixture. This parameter needs            **
c     **                 only have meaningful value for dV=           **
c     **                 specified.                                   **
c     **          ac:    def: ac = MC in the above equation.          **
c     **          ah:    def: ah = MH in the above equation.          **
c     **          ao:    def: ao = MO in the above equation.          **
c     **          an:    def: an = MN in the above equation.          **
c     **          p:     The pressure of the fuel air mixture         **
c     **                 in the case of dP=0. NOTE: for dV=           **
c     **                 specified this variable need not have        **
c     **                 meaningful value.                            **
c     **          T:     The temperature at which calculations        **
c     **                 are to be performed. I.e. the rutine         **
c     **                 works like a vectorefuction on the           **
c     **                 scalàr temp, and returns nb(10).             **
c     **                                                              **
c     ** OUTPUT: The following is a list of output values            **
```

```
c     **                                                              **
c     **        OUTPUT              MEANING                           **
c     **        -------             ---------                         **
c     **        NB(10):The returning value of molenumbers.            **
c     **               Se above equation.                             **
c     **        NT:    The sum N(i) for i = 1,10                      **
c     **                                                              **
c     ** RESTRICTIONS: Has to have a external function which          **
c     **               controls the convergence toward corr.          **
c     **               value of the input parameter temp              **
c     **                                                              **
c     ** LANGUAGE:     FORTRAN 7.                                     **
c     **                                                              **
c     ** HISTORY:      This rutine was constructed by                 **
c     **               Gestur Valgardsson, in a partial               **
c     **               fulfillment of the requirements for            **
c     **               a MS degree at the University of               **
c     **               Tennessee, 1984.                               **
c     **                                                              **
c     ** CHANGES:      NONE                                           **
c     **                                                              **
c     ** DATE:         Completed 06:20:84                             **
c     **                                                              **
c     ****************************************************************
c     **                                                              **
      subroutine dissoc(cond,cr,pr,tr,ac,ah,ao,an,p,T,NB,NT)
c     **                                                              **
c     ****************************************************************
c     **                                                              **
c     **                DECLARATIONS OF VARIABLES                     **
c     **                -------------------------                     **
c     **                                                              **
      real*4 ac          | I
      real*4 ah          |  N
      real*4 an          |   P
      real*4 ao          |    U
      real*4 pr          |     T
      real*4 tr          |      V
      real*4 T           |       A
      real*4 p           |        R
      real*4 nb(10)      |         I
      real*4 nt          |          ABLES
      real*8 kp1,kp2,kp3,kp4,kp5,kp6 |The equilibrium constants.
      real*4 ntm
      real*4 n(10)
      real*4 c
      real*4 aom
      real*4 n7max       |Maximum value of N(7)
      real*4 Cr          |Compression ratio
      real*8 w1,w2,w3,w4,w5,w6   |Se CHAPTER VI for definitions
      integer jj
      character*20 cond
c     **                                                              **
c     ****************************************************************
c     **                                                              **
c     **         DEFINITION OF EQUILIBRIUM CONSTANTS                  **
c     **            The theory is from APENDIX D                      **
c     **            ----------------------------------                **
      kp1(t) = exp(33805.0/t+(0.7422+165.8/t)*alog(t)-16.5739) |**
      kp2(t) = exp(57126.0/t+(-0.010+599.0/t)*alog(t)-16.3201) |**
      kp3(t) = exp(-14096.0/t+(-0.6893-1375.3/t)*alog(t)+9.668)|**
```

```
      kp4(t) = exp(33587.0/t+(0.5604+3327.0/t)*alog(t)-20.8683)|**
      kp5(t) = exp(44216.0/t+(-0.1319+1298.0/t)*alog(t)-13.1303)|*
      kp6(t) = exp(42450.0/t+(-1.0740-2147.0/t)*alog(t)+3.2515)|**
      **                                                        **
c     ************************************************************
c     nt = ac + (ah+an)/2.0     |First guess at nt for dP=0 case **
      ************************************************************
c     **                                                        **
c     **                                                        **
c     **                  CONSTANT PRESSURE CASE                **
c     **                  ----------------------                **
c     **                                                        **
      if(cond(:1).eq.'P'.or.cond(:1).eq.'p') then               |**
300   w1 = kp1(T)*sqrt(p/nt)                                    |**
      w2 = kp2(T)*(p/nt)                                        |**
      w3 = kp3(T)                                               |**
      w4 = kp4(T)*(p/nt)                                        |**
      w5 = kp5(T)*(p/nt)                                        |**
      w6 = kp6(T)*sqrt(p/nt)                                    |**
      **                                                        **
c     ************************************************************
c
      ************************************************************
c     **                                                        **
c     **                  CONSTANT VOLUME COMBUSTION            **
c     **                  --------------------------            **
c     **                                                        **
      else if(cond(:1).eq.'V'.or.cond(:1).eq.'v') then          |**
      pont = (T/tr)*(pr/(ac+ah+an+ao))*(1.0/cr)                 |**
      w1 = kp1(T)*sqrt(pont)                                    |**
      w2 = kp2(T)*(pont)                                        |**
      w3 = kp3(T)                                               |**
      w4 = kp4(T)*(pont)                                        |**
      w5 = kp5(T)*pont                                          |**
      w6 = kp6(T)*sqrt(pont)                                    |**
      **                                                        **
c     ************************************************************
c     end if                                                    |**
      jj = 1                                                    |**
      ************************************************************
c     **                                                        **
c     **                  CALCUALTIONS BEGINES HERE             **
c     **                  -------------------------             **
c     **                                                        **
      n7max = AH
      n(7) = n7max/2.0
1000  n(8) = w4*n(7)**2.0
      B = (w5*n(7)/(2.0*sqrt(w2)*w6*n(8)))
      n(9) = (ah - n(7) - 2.0*n(8))*B/(1.0 + B)
      n(10) = n(9)*n(7)*w4*w6*sqrt(w2)/w5
      n(4) = (w4/w5)*(w6/w5)*(n(9)*n(9)/n(10))*sqrt(w2)
      n(3) = w2*n(4)**2.0
      n(1) = w1*sqrt(n(3))*ac/(1.0 + w1*sqrt(n(3)))
      n(2) = ac - n(1)
      c = w3*n(3)
      n(5) = 0.25*(sqrt(c**2.0 + 8.0*an*c) - c)
      n(6)= (an - n(5))/2.0                                     **
c     **                                                        **
c     ************************************************************
c
c     ************************************************************
c     **
```

```
c       **                CHECK ON THE CONVERGENCE                **
c       **                ------------------------                **
c       **                                                        **
        aom = 2.0*(n(1)+n(3)) + n(2)+n(4)+n(5)+n(9)+n(10)
        if(abs((ao-aom)/ao).lt.0.00005) then  |Convergence check
           ntm = 0.0
           do 100 i = 1,10
              ntm = ntm + n(i)
100        continue
c       **                                                        **
c       ************************************************************
c
c       ************************************************************
c       **                                                        **
c       **                CHECK FOR CONVERGENCE OF NT             **
c       **                ---------------------------             **
c       **                                                        **
          if(cond(:1).eq.'P'.or.cond(:1).eq.'p') then
            if(abs((ntm-nt)/nt).lt.0.0005) then
              nt = ntm
              goto 200
            else
              nt = ntm
              goto 300
            end if
c       **                                                        **
c       ************************************************************
c       **                                                        **
            else if(cond(:1).eq.'V'.or.cond(:1).eq.'v') then
              nt = ntm
              goto 200
            end if
          else
            jj = jj+1
            if(ao.gt.aom) then
              n(7) = n(7) - n7max/(2.0**jj)
              goto 1000
            else
              n(7) = n(7) + n7max/(2.0**jj)
              goto 1000
            end if
          end if
200       do 400 i = 1,10
            nb(i) = n(i)
400       continue
          return
          stop
          end
c       **                                                        **
c       **                                                        **
c       ************************************************ END ********
```

```
c     ************************************************************
c     **            <<<<<< SUBROUTINE PROPER >>>>>>               **
c     ************************************************************
c     ** PURPOSE:  This program is generated in order to comp.    **
c     **           thermodynamic properties for the following     **
c     **           gases:"CO","N2","CO2","H2","H2O","NO","H"      **
c     **                 "OH","O","H2O","H2"                      **
c     **                                                          **
c     **           The rutine consists of four subroutines        **
c     **                                                          **
c     **                 (1) ENTHP(subs,T,h)                      **
c     **                 (2) INTEN(subs,T,u)                      **
c     **                 (3) CPRES(subs,T,cp)                     **
c     **                 (4) CVOLU(subs,T,cv)                     **
c     **                 (5) ENTRO(subs,T,s)                      **
c     **                                                          **
c     ** INPUT:    The call to each rutine is of the form:        **
c     **                                                          **
c     **               CALL <PROPER>(subs,T,val)                  **
c     **                                                          **
c     **    Where: PROP is the property required. Allowable       **
c     **                values are:                               **
c     **                                                          **
c     **                PROP: Enthp = Enthalpy                    **
c     **                      Inten = Internal energy             **
c     **                      Cpres = Specific heat dP=0          **
c     **                      Cvolu = Specific heat dV=0          **
c     **                      Entro = Entropy                     **
c     **                                                          **
c     **             T:    Is the temperature at which            **
c     **                   properties are to be calculated.       **
c     **           val:    Is the returning thermodynamical       **
c     **                   propertie.                             **
c     **                                                          **
c     ** RESTRICTIONS: None                                       **
c     **                                                          **
c     ** LANGUAGE:     FORTRAN 7                                  **
c     **                                                          **
c     ** HISTORY:      This rutine was constructed by             **
c     **                Gestur Valgardsson, in a partial          **
c     **                fulfillment of a MS degree at the         **
c     **                Universityof   Tennessee, 1               **
c     **                                                          **
c     ** CHANGES:      None                                       **
c     **                                                          **
c     ** DATE:         Completed [06:20:84]                       **
c     **                                                          **
c     ************************************************************

c     ************************************************************
c     **                                                          **
      subroutine enthp(subst,temp,entalp)                         **
c     **                                                          **
c     ************************************************************
c     **                                                          **
c     **                DECLARATION OF VARIABLES                  **
c     **                ------------------------                  **
c     **                                                          **
      real*4 temp,entalp
      character*20 subst
      If(temp.ge.400.0.and.temp.le.1600.0) then
```

```
if(subst(:2).eq.'N2') then
entalp = 31317.0 + 37.46*temp - 4559.3*alog(temp)
return
else if(subst(:2).eq.'NO') then
entalp = 111050.0 + 37.81*temp - 2874*alog(temp)
return
else if (subst(:3).eq.'H2O') then
entalp = 88923.0 + 49.36*temp - 7940.8*alog(temp)
return
else if (subst(:2).eq.'H2') then
entalp = 326490. + 40.35*temp - 8085.2*alog(temp)
return
else if(subst(:1).eq.'H') then
entalp = 357070.0 + 20.79*temp - 7.9*alog(temp)
return
else if (subst(:3).eq.'CO2') then
entalp = 56835.0 + 66.27*temp - 11634.0*alog(temp)
return
else if (subst(:2).eq.'CO') then
entalp = 299180.0 + 37.85*temp - 4571.9*alog(temp)
return
else if (subst(:2).eq.'O2') then
entalp = 43388.0 + 42.27*temp - 6635.4*alog(temp)
return
else if (subst(:2).eq.'OH') then
entalp = 217810.0 + 37.36*temp - 5561.4*alog(temp)
return
else if(subst(:1).eq.'O') then
entalp = 265120.0 + 24.60*temp - 2729.2*alog(temp)
return
else
write(5,1000) subst(:3),temp     |end of enthalp 400-1600 K
return
end if
end if
if(temp.gt.1600.0.and.temp.le.6000.0) then
if(subst(:2).eq.'N2') then
entalp = 44639.0 + 39.32*temp - 6753.4*alog(temp)
return
else if(subst(:2).eq.'NO') then
entalp = 138670.0 + 39.92*temp - 7061.8*alog(temp)
return
else if (subst(:3).eq.'H2O') then
entalp = 154670.0 + 60.43*temp - 19212.0*alog(temp)
return
else if (subst(:2).eq.'H2') then
entalp = 461750.0 + 46.23*temp - 27649.0*alog(temp)
return
else if(subst(:1).eq.'H') then
entalp = 357010.0 + 20.79*temp - 0.0*alog(temp)
return
else if (subst(:3).eq.'CO2') then
entalp = 93048.0 + 68.58*temp - 16979.0*alog(temp)
return
else if (subst(:2).eq.'CO') then
entalp = 309070.0 + 39.29*temp - 6201.9*alog(temp)
return
else if (subst(:2).eq.'O2') then
entalp = 127010.0 + 46.25*temp - 18798.0*alog(temp)
return
else if (subst(:2).eq.'OH') then
```

```
      entalp = 298750.0 + 42.96*temp - 17695.0*alog(temp)
      return
      else if(subst(:1).eq.'O') then
      entalp = 298360.0 + 23.17*temp - 6910.3*alog(temp)
      return
      else
      write(5,1000) subst(:3),temp    |end of enthalp 1600-6000 K
      return
      end if
      end if
      write(5,2000) temp
1000  format(' ','Calculation of the property ',A4,'
     1 at the temperature ',F7.1,'was not succesfull')
2000  format(' ','calculation of properties at ',f7.1,
     1'was now succesfull')
      stop
      end
c      **                                                          **
c      ************************************************************
c      **                                                          **
      subroutine inten(subst,temp,ineg)
c      **                                                          **
c      ************************************************************
c      **                                                          **
c      **                                                          **
c      **              DECLARATION OF VARIABLES                    **
c      **              ------------------------                    **
c      **                                                          **
      real*4 temp,ineg
      character*20 subst
      If(temp.ge.400.0.and.temp.le.1600.0) then
      if(subst(:2).eq.'N2') then
      ineg = 31317.0 + 37.46*temp - 8.314*temp - 4559.3*alog(temp)
      return
      else if(subst(:2).eq.'NO') then
      ineg = 111050.0 + 37.81*temp - 8.314*temp - 2874.8*alog(temp)
      return
      else if (subst(:3).eq.'H2O') then
      ineg = 88923.0 + 49.36*temp - 8.314*temp- 7940.8*alog(temp)
      return
      else if (subst(:2).eq.'H2') then
      ineg = 326490. + 40.35*temp - 8.314*temp - 8085.2*alog(temp)
      return
      else if(subst(:1).eq.'H') then
      ineg = 357070.0 + 20.79*temp - 8.314*temp - 7.9*alog(temp)
      return
      else if (subst(:3).eq.'CO2') then
      ineg = 56835.0 + 66.27*temp - 8.314*temp - 11634.0*alog(temp)
      return
      else if (subst(:2).eq.'CO') then
      ineg = 299180.0 + 37.85*temp - 8.314*temp - 4571.9*alog(temp)
      return
      else if (subst(:2).eq.'O2') then
      ineg = 43388.0 + 42.27*temp - 8.314*temp - 6635.4*alog(temp)
      return
      else if (subst(:2).eq.'OH') then
      ineg = 217810.0 + 37.36*temp - 8.314*temp - 5561.4*alog(temp)
      return
      else if(subst(:1).eq.'O') then
      ineg = 265120.0 + 24.60*temp - 8.314*temp - 2729.2*alog(temp)
      return
      else
```

```
      write(5,1000) subst(:3),temp     |end if internal e 400-1600 K -
      return
      end if
      end if
      if(temp.gt.1600.0.and.temp.le.6000.0) then
      if(subst(:2).eq.'N2') then
      ineg = 44639.0 + 39.32*temp - 8.314*temp - 6753.4*alog(temp)
      return
      else if(subst(:2).eq.'NO') then
      ineg = 138670.0 + 39.92*temp - 8.314*temp - 7061.8*alog(temp)
      return
      else if (subst(:3).eq.'H2O') then
      ineg = 154670.0 + 60.43*temp - 8.314*temp - 19212.0*alog(temp)
      return
      else if (subst(:2).eq.'H2') then
      ineg = 461750.0 + 46.23*temp - 8.314*temp - 27649.0*alog(temp)
      return
      else if(subst(:1).eq.'H') then
      ineg = 357010.0 + 20.79*temp - 8.314*temp - 0.0*alog(temp)
      return
      else if (subst(:3).eq.'CO2') then
      ineg = 93048.0 + 68.58*temp - 8.314*temp - 16979.0*alog(temp)
      return
      else if (subst(:2).eq.'CO') then
      ineg = 309070.0 + 39.29*temp - 8.314*temp - 6201.9*alog(temp)
      return
      else if (subst(:2).eq.'O2') then
      ineg = 127010.0 + 46.25*temp - 8.314*temp - 18798.0*alog(temp)
      return
      else if (subst(:2).eq.'OH') then
      ineg = 298750.0 + 42.96*temp - 8.314*temp - 17695.0*alog(temp)
      return
      else if(subst(:1).eq.'O') then
      ineg = 298360.0 + 23.17*temp - 8.314*temp - 6910.3*alog(temp)
      return
      else
      write(5,1000) subst(:3),temp     |end of internal e 1600-6000 K
      return
      end if
      end if
      write(5,2000) temp
1000  format(' ','Calculation of the property ',A4,'
     1 at the temperature ',F7.1,'was not succesfull')
2000  format(' ','calculation of properties at ',f7.1,
     1'was now succesfull')
      stop
      end                                                          **
c      **
c      ***************************************************************
c      **                                                           **
      subroutine Cpres(subst,temp,CP)                              **
c      **
c      ***************************************************************
c      **                                                           **
c      **                                                           **
c      **                DECLARATION OF VARIABLES                   **
c      **                ------------------------                   **
c      **                                                           **
      real*4 temp,CP
      character*20 subst
      If(temp.ge.400.0.and.temp.le.1600.0) then
      if(subst(:2).eq.'N2') then
```

```
CP = 37.46 - 4559.3/temp
return
else if(subst(:2).eq.'NO') then
CP = 37.81 - 2874/temp
return
else if (subst(:3).eq.'H2O') then
CP = 49.36 - 7940.8/temp
return
else if (subst(:2).eq.'H2') then
CP = 40.35 - 8085.2/temp
return
else if(subst(:1).eq.'H') then
CP = 20.79 - 7.9/temp
return
else if (subst(:3).eq.'CO2') then
CP = 66.27 - 11634.0/temp
return
else if (subst(:2).eq.'CO') then
CP = 37.85 - 4571.9/temp
return
else if (subst(:2).eq.'O2') then
CP = 42.27 - 6635.4/temp
return
else if (subst(:2).eq.'OH') then
CP = 37.36 - 5561.4/temp
return
else if(subst(:1).eq.'O') then
CP = 24.60 - 2729.2/temp
return
else
write(5,1000) subst(:3),temp     |end of CP 400-1600 K
return
end if
end if
if(temp.gt.1600.0.and.temp.le.5000.0) then
if(subst(:2).eq.'N2') then
CP = 39.32 - 6753.4/temp
return
else if(subst(:2).eq.'NO') then
CP = 39.92 - 7061.8/temp
return
else if (subst(:3).eq.'H2O') then
CP = 60.43 - 19212.0/temp
return
else if (subst(:2).eq.'H2') then
CP = 46.23 - 27649.0/temp
return
else if(subst(:1).eq.'H') then
CP = 20.79 - 0.0/temp
return
else if (subst(:3).eq.'CO2') then
CP = 68.58 - 16979.0/temp
return
else if (subst(:2).eq.'CO') then
CP = 39.29 - 6201.9/temp
return
else if (subst(:2).eq.'O2') then
CP = 46.25 - 18798.0/temp
return
else if (subst(:2).eq.'OH') then
CP = 42.96 - 17695.0/temp
```

```
      return
      else if(subst(:1).eq.'O') then
      CP = 23.17 - 6910.3/temp
      return
      else
      write(5,1000) subst(:3),temp     |end of CP 1600-6000 K
      return
      end if
      end if
      write(5,2000) temp
1000  format(' ','Calculation of the property ',A4,'
     1 at the temperature ',F7.1,'was not succesfull')
2000  format(' ','calculation of properties at ',f7.1,
     1'was now succesfull')
      stop
      end
c      **                                                              **
c      ****************************************************************
c      **                                                              **
      subroutine Cvolu(subst,temp,CV)
c      **                                                              **
c      ****************************************************************
c      **                                                              **
c      **                                                              **
c      **                DECLARATION OF VARIABLES                      **
c      **                ------------------------                      **
c      **                                                              **
      real*4 temp,CV
      character*20 subst
      If(temp.ge.400.0.and.temp.le.1600.0) then
      if(subst(:2).eq.'N2') then
      CV = 37.46 - 8.314 - 4559.3/temp
      return
      else if(subst(:2).eq.'NO') then
      CV = 37.81 - 8.314 - 2874/temp
      return
      else if (subst(:3).eq.'H2O') then
      CV = 49.36 - 8.314 - 7940.8/temp
      return
      else if (subst(:2).eq.'H2') then
      CV = 40.35 - 8.314 - 8085.2/temp
      return
      else if(subst(:1).eq.'H') then
      CV = 20.79 - 8.314 - 7.9/temp
      return
      else if (subst(:3).eq.'CO2') then
      CV = 66.27 - 8.314 - 11634.0/temp
      return
      else if (subst(:2).eq.'CO') then
      CV = 37.85 - 8.314 - 4571.9/temp
      return
      else if (subst(:2).eq.'O2') then
      CV = 42.27 - 8.314 - 6635.4/temp
      return
      else if (subst(:2).eq.'OH') then
      CV = 37.36 - 8.314 - 5561.4/temp
      return
      else if(subst(:1).eq.'O') then
      CV = 24.60 - 8.314 - 2729.2/temp
      return
      else
      write(5,1000) subst(:3),temp     |end of CV 400-1600 K
```

```
      return
      end if
      end if
      if(temp.gt.1600.0.and.temp.le.6000.0) then
      if(subst(:2).eq.'N2') then
      CV = 39.32 - 8.314 - 6753.4/temp
      return
      else if(subst(:2).eq.'NO') then
      CV = 39.92 - 8.314 - 7061.8/temp
      return
      else if (subst(:3).eq.'H2O') then
      CV = 60.43 - 8.314 - 19212.0/temp
      return
      else if (subst(:2).eq.'H2') then
      CV = 46.23 - 8.314 - 27649.0/temp
      return
      else if(subst(:1).eq.'H') then
      CV = 20.79 - 8.314 - 0.0/temp
      return
      else if (subst(:3).eq.'CO2') then
      CV = 68.58 - 8.314 - 16979.0/temp
      return
      else if (subst(:2).eq.'CO') then
      CV = 39.29 - 8.314 - 6201.9/temp
      return
      else if (subst(:2).eq.'O2') then
      CV = 46.25 - 8.314 - 18798.0/temp
      return
      else if (subst(:2).eq.'OH') then
      CV = 42.96 - 8.314 - 17695.0/temp
      return
      else if(subst(:1).eq.'O') then
      CV = 23.17 - 8.314 - 6910.3/temp
      return
      else
      write(5,1000) subst(:3),temp     |end of CV 1600-6000 K
      return
      end if
      end if
      write(5,2000) temp
1000  format(' ','Calculation of the property ',A4,'
     1 at the temperature ',F7.1,'was not succesfull')
2000  format(' ','calculation of properties at ',f7.1,
     1'was now succesfull')
      stop
      end                                                          **
c      **
c      ************************************************************
c      **
      subroutine entro(subst,temp,entr)                            **
c      **
c      ************************************************************
c      **                                                           **
c      **                                                           **
c      **                DECLARATION OF VARIABLES                   **
c      **                ------------------------                   **
c      **                                                           **
      real*4 temp,entr
      character*20 subst
      If(temp.ge.400.0.and.temp.le.1600.0) then
      if(subst(:2).eq.'N2') then
      entr = -34.82 + 37.46*alog(temp) + 4559.3/temp
```

```
return
else if(subst(:2).eq.'NO') then
entr = -15.70 + 37.81*alog(temp) + 2874/temp
return
else if (subst(:3).eq.'H2O') then
entr = -117.0 + 49.36*alog(temp) + 7940.8/temp
return
else if (subst(:2).eq.'H2') then
entr = -121.0 + 40.35*alog(temp) + 8085.2/temp
return
else if(subst(:1).eq.'H') then
entr = -3.9 + 20.79*alog(temp) + 7.9/temp
return
else if (subst(:3).eq.'CO2') then
entr = -200.0 + 66.27*alog(temp) + 11634.0/temp
return
else if (subst(:2).eq.'CO') then
entr = -31.10 + 37.85*alog(temp) + 4571.9/temp
return
else if (subst(:2).eq.'O2') then
entr = -55.15 + 42.27*alog(temp) + 6635.4/temp
return
else if (subst(:2).eq.'OH') then
entr = -44.06 + 37.36*alog(temp) + 5561.4/temp
return
else if(subst(:1).eq.'O') then
entr = 13.86 + 24.60*alog(temp) + 2729.2/temp
return
else
write(5,1000) subst(:3),temp     |end of entr 400-1600 K
return
end if
end if
if(temp.gt.1600.0.and.temp.le.6000.0) then
if(subst(:2).eq.'N2') then
entr = -50.24 + 39.32*alog(temp) + 6753.4/temp
return
else if(subst(:2).eq.'NO') then
entr = -33.90 + 39.92*alog(temp) + 7061.8/temp
return
else if (subst(:3).eq.'H2O') then
entr = -204.6 + 60.43*alog(temp) + 19212.0/temp
return
else if (subst(:2).eq.'H2') then
entr = -176.6 + 46.23*alog(temp) + 27649.0/temp
return
else if(subst(:1).eq.'H') then
entr = -3.82 + 20.79*alog(temp) + 0.0/temp
return
else if (subst(:3).eq.'CO2') then
entr = -220.4 + 68.58*alog(temp) + 16979.0/temp
return
else if (subst(:2).eq.'CO') then
entr = -42.77 + 39.29*alog(temp) + 6201.9/temp
return
else if (subst(:2).eq.'O2') then
entr = -92.15 + 46.25*alog(temp) + 18798.0/temp
return
else if (subst(:2).eq.'OH') then
entr = -92.24 + 42.96*alog(temp) + 17695.0/temp
return
```

APPENDIX D

ALGEBRAIC EXPRESSIONS FOR THERMODYNAMIC VARIABLES

In this section algebraic expressions for the thermodynamic functions, required for the equations in Chapter II, are derived. The thermodynamic tables used for this purpose were adapted from references [19,24], and algebraic expressions from reference [18]. Expressions for the following thermodynamic variables are needed.

$h(T)$: Enthalpy at one atmospheric pressure (kJ/kmol)

$s(T,P)$: Entropy as a function of temperature and pressure (kJ/kmol K)

$c_p(T)$: Constant pressure heat capacity at one atmospheric pressure (kJ/kmol K)

$K_p(T)$: The reaction constant for all the reaction equations

The Expression for Enthalpy

Energy is associated with forces which bind atoms together into a specific compound. As a result, each reactant and product of chemical reaction has a definite bond energy at a given thermodynamic condition. When reactants form products, bonds are formed and others are broken. The total sum of the bond energies of the reactants may be quite different from that of the products, caused by the reaction. Therefore, when tables for thermodynamic properties are prepared for calculations involving chemical reactions, consideration has to be given to this difference in the bond energy of the different species.

The tables employed for this work use the heat of formation to connect tables that involve the same atoms, or groups of atoms.

Therefore, for example, if values for $h_{O_2}(T)$ are computed with an arbitrary datum, values for monatomic oxygen $h_O(t)$ can be evaluated by:

$$h_O(298.16) = \frac{1}{2}\left(\Delta h_f^o - h_{O_2}\right)_{298.16} \qquad \text{(D-1)}$$

The advantage that accompanies this choice for the monatomic values is that any difference, such as

$$2h_O(T_1) - h_{O_2}(T_2) \qquad \text{(D-2)}$$

has an unambiguous physical meaning.

In the same manner, the enthalpy of C, H_2, and N_2 can be assigned independently, since no element can be formed from any other, or combination of others.

The following algebraic relationship was employed to represent enthalpy:

$$h(T) = A + BT + C\ \ln(T) \qquad \text{(kJ/kmol)} \qquad \text{(D-3)}$$

Table D-1 lists the values of A, B, and C for two different temperature ranges, 400 K < T < 1600 K; 1600 K < T < 6000 K. In order to fix the constants the following temperatures were used. From 1600 to 6000 K: A, B, and C were evaluated at 2500, 4000, and 5500 K using values from reference [18]. For the interval 400 to 1600 K: A, B, and C were evaluated at 500, 1100, and 1600 K, using the same reference.

Table D-1. The Coefficients A, B, C and D to Be Used in Connection with Equations D-3, D-7 and D-9.

Gas	A	B	C	D
		For 400 < T < 1600 K		
CO	299180	37.85	-4571.9	-31.10
CO2	56835	66.27	-11634.0	-200.0
H	357070	20.79	-7.9	-3.900
H2	326490	40.35	-8085.2	-121.0
H2O	88923	49.36	-7940.8	-117.0
N2	31317	37.46	-4559.3	-34.82
O	265120	24.60	-2729.2	13.86
O2	43388	42.27	-6635.4	-55.15
OH	217810	37.36	-5561.4	-44.06
NO	111050	37.81	-2874.8	-15.70
N	326040	17.19	5371.4	64.67
		For 1600 < $\dot{T}$ < 6000 K		
CO	309070	39.29	-6201.9	-42.77
CO2	93048	68.58	-16979.0	-220.4
H	357010	20.79	0.0	-3.820
H2	461750	46.23	-27649.0	-176.6
H2O	154670	60.43	-19212.0	-204.6
N	44639	39.32	-6753.4	-50.24
O	298360	23.17	-6910.3	21.81
O2	127010	46.25	-18798.0	-92.15
OH	298750	42.86	-17695.0	-92.24
ON	138670	39.92	-7061.8	-33.90
N	486400	26.91	-18159.0	-20.31

Data sources:

1. A. S. Campbell, Thermodynamic Analysis of Combustion Engines, John Wiley & Sons, Inc., New York, 1979.

2. NACA TN 1037 (1951), "General Method and Thermodynamical Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions."

Enthalpy values evaluated with these functions are within 0.5% from the original source [24]. For differences between values, at two different temperatures, the accuracy proved to be even better, and in good agreement with tables based on other datum values.

The Expression for Entropy

The same problems of reference state occur also in evaluating the entropy changes of a process involving chemical reactions. Since the use of the thermodynamic property enthalpy, as used in this work, is only associated with differences between two equilibrium states, an arbitrary reference state can be chosen for each specie involved. Similar methods of assigning arbitrary reference values for the entropy of particular elements of compounds could be employed. In this case, however, a more fundamental approach is available for establishing the entropy values of substances, based on the third law of thermodynamics. Based on the third law, the entropy of a pure crystalline substance may be taken to be zero at the absolute zero thermodynamic temperature.

The entropy of an ideal gas can be found using

$$ds = c_p \, dT/T - R \, dP/P \qquad \text{(kJ/kmol K)} \qquad \text{(D-4)}$$

Based on the assumption that the specific heats of gases are not influenced by changes in pressure the expression for entropy is composed of two terms: one associated with temperature, and one with pressure. Introducing the function, defined by,

$$\phi(T) = \int_{T_o}^{T} c_p(t)/t \, dt + \phi(T_o) \qquad (D\text{-}5)$$

where $\phi(T_o)$ can be interpreted as an integration constant, the entropy difference between the two states 1 and 2 can be written as:

$$s_i(T_2,P_2) - s_i(T_1,P_1) = \phi(T_2)_i - \phi(T_1)_i - R \ln(P_2/P_1) \qquad (D\text{-}6)$$

In this work, the absolute entropy was correlated at 1 atm pressure using this algebraic expression.

$$\phi(T) = B \ln(T) - C/T + D \qquad (D\text{-}7)$$

Values for the coefficients B, C and D are listed in Table D-1.

With this result the absolute entropy of a substance can be calculated for any given temperature and pressure. For the special case, when the ratio c_p/c_v can be treated as a constant, the general expression for the reversible isentropy changes simplifies to

$$T \, p^{(k-1)/k} = \text{constant}; \quad k = c_p/c_v \qquad (D\text{-}8)$$

Use was made of this last expression during compression and "blow-down." The more accurate results of Eq. D-6 were used for calculations during the expansion stroke. In this work, it was found that the last expression gave quite accurate values, when compared with the more precise Eq. D-6.

The Specific Heat Expression

Since ideal gas behavior was assumed, the one-atmosphere values of c_p were used for all pressures. The following expression was chosen to represent the specific heat:

$$c_p(T) = B + C/T \qquad \text{(kJ/kmol K)} \qquad \text{(D-9)}$$

The coefficients B and C used for this expression can be found in Table D-1. In fact, the expression for c_p is obtained from the enthalpy function by differentiating with respect to temperature. It should be noted that this correlation is only valid for temperatures from 400 K through 6000 K. For the lower temperatures prevailing in the manifold, and at state-point (1), this linear relationship was used to evaluate $c_p(T)$.

$$c_p(T) = a + bT \qquad \text{(kJ/kmol K)} \qquad \text{(D-10)}$$

Values for the constants a and b are listed in Table D-2

Values calculated with these expressions were compared with other thermodynamic tables [18,24], and the accuracy was proven to be acceptable.

The Expression for the Reaction Coefficient

Table D-3 lists the equation and the proper constants used to calculate the reaction constant associated with each of the mass action equations.

Table D-2. The Coefficients a and b to Be Used with Equation D-10; Temperatures Lower than 500 K.

Gas	a	b	Molecular Weight
		For 298 < T < 500 K	
CO	27.4	0.0058	28.000
CO2	28.8	0.0280	44.000
H2	28.3	0.0019	2.016
H2O	30.5	0.0103	18.016
N2	27.6	0.0051	28.016
O2	27.0	0.0079	32.000
NH3	29.1	0.0248	17.040

Data sources:

1. A. S. Campbell, Thermodynamic Analysis of Combustion Engines, John Wiley & Sons, Inc., New York, 1979.
2. NACA TN 1037 (1951), "General Method and Thermodynamical Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions."

Table D-3. Coefficients for Calculation of the Reaction Constant $K_p(T)$.

Reaction	a	b	c	d
$K_p(T) = EXP(a/T + (b + c/T)\ln(T) + d)$				(D-11)
The equation is valid for 1400 < T < 6000 K				
CO + 1/2O2 -- > H2O	33805	0.7	165.8	-16.5739
2O -- > O2	57126	-0.0100	599.0	-16.3201
O2 + N2 -- > 2NO	-14096	-0.6893	-1375.3	-9.66800
2H -- > H2	33587	0.5604	3327.0	-20.8683
O + H -- > OH	44216	-0.1319	1298.0	-13.1303
H2 + 1/2O2 -- > H2O	42450	-1.0740	-2147.0	3.25150

Data sources:

1. A. S. Campbell, Thermodynamic Analysis of Combustion Engines, John Wiley & Sons, Inc., New York, 1979.
2. NACA TN 1037 (1951), "General Method and Thermodynamical Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions."

APPENDIX E

PHOTOGRAPHS OF THE EXPERIMENTAL SETUP

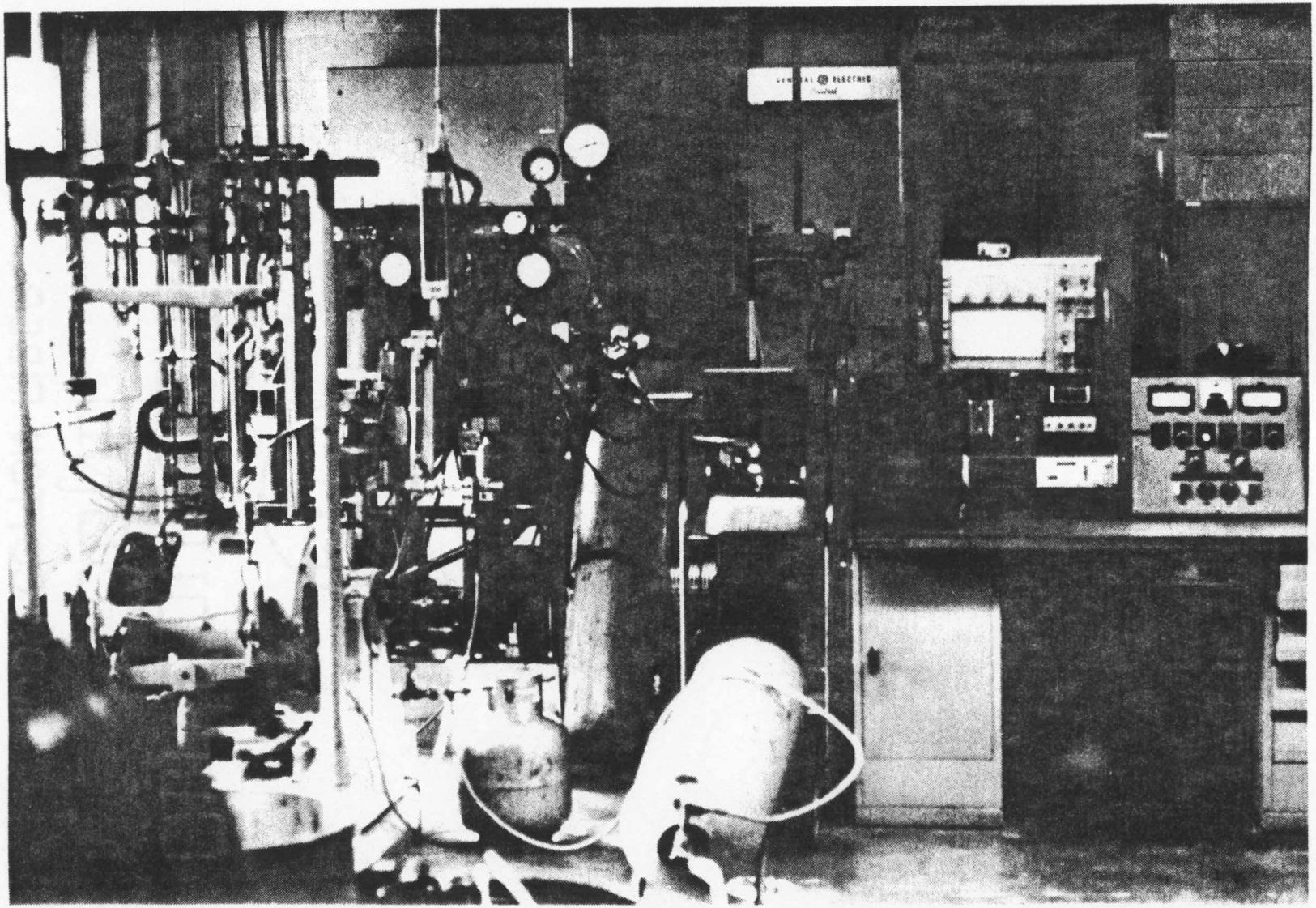


Figure E-1. Photograph of the experimental setup.

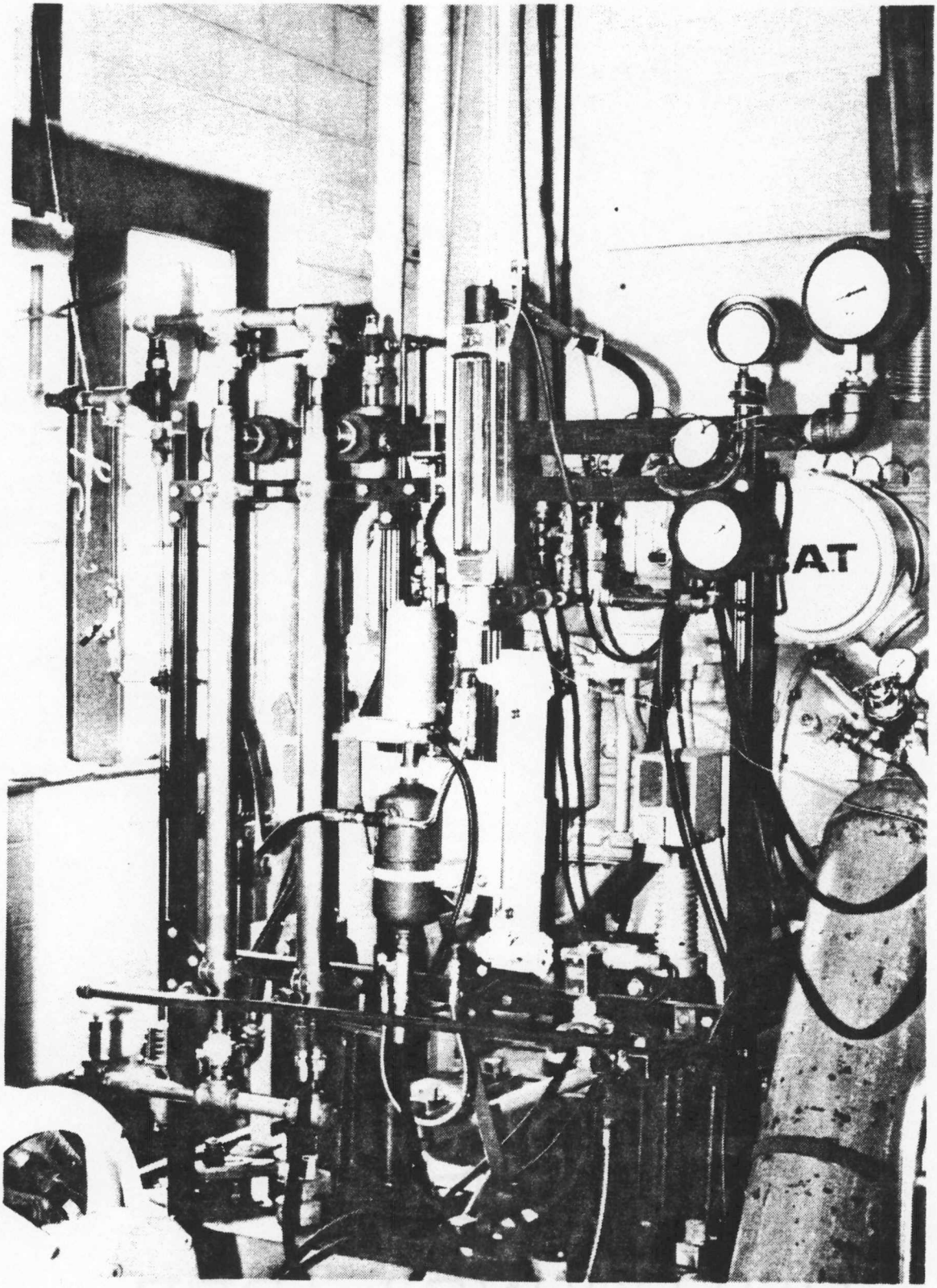


Figure E-2. Photograph of the ammonia fueling system.

APPENDIX F

ENGINE SPECIFICATIONS

The following specifications are reproduced from Caterpillar publication: CATERPILLAR D330c, DIESEL ENGINE, 021262-00 (12-67).

FOUR-CYCLE TURBOCHARGED DIESEL, Model: D330c

NUMBER OF CYLINDERS	4
BORE AND STROKE: inches	4.75x6.00
millimeters	121x152
PISTON DISPLACEMENT: cu.in	425
liters	6.9
FLYWHEEL HOUSING, Standard	SAE No. 1
ROTATION	Counterclockwise when viewed from flywheel end
NORMAL WORKING RANGE	1500-2000 RPM
LOW IDLE RPM, Standard	600
COMPRESSION RATIO	17.5:1

CAPACITIES FOR LIQUIDS:	U.S.Gal.	Imp.Gal.	Liters
Cooling System (engine only)	4.4	3.6	16.5
Cooling System (with radiator)	8.5	7.1	32.2
Lubricating Oil System (refill)	5.0	4.2	18.9

WEIGHT: Net Dry (approximate)	Lb.	Kg.
Standard Engine	1628	738

AIR CLEANERS: Dry-type with replaceable filter elements. Provide positive filtration independent of engine speed or temperature change.

BEARINGS: Corrosion-resistant, precision-type aluminum alloy. High load carrying ability and exceptional fatigue strength. Tin-plated for good "break-in."

BLOCK: High quality, close grained grey iron casting. Ribs designed for maximum strength and to assure perfect alignment for bearings.

COMBUSTION SYSTEM: Precombustion chamber system enables the engine to efficiently burn a wide variety of fuels under varied speed and load conditions. Minimizes objectionable smoke and odor characteristics of some diesel engines. Also retards combustion deposit build-up and washdown of cylinder lubricants.

COOLING: Built-in, gear driven, centrifugal pump circulates jacket water through engine at all times. Water temperature is thermostatically controlled. Heat exchanger and radiators are available.

CRANKSHAFT: Forged steel, statically and dynamically-balanced, heat-treated and shot-peened for increased toughness. Individually [with 5 to 10 millionths inch (127x10-6 mm to 254x10-6 mm) smooth main and connecting rod journals.

CYLINDER LINERS: Replaceable, full length, weth-type liners. Induction hardened, precision honed and chemically treated on inside surface.

FUEL: Burns No. 2 Fuel Oil (ASTM Specification D396), often called No. 2 furnace or burner oil, with minimum cetane rating of 35. Most of the new, lost cost economy diesel fuels are suitable. Expensive, so-called premium quality diesel fuels can be used but they are not required.

FUEL SYSTEM: Catepillar designed and manufactured fuel system features adjustment-free individual injection pumps and single orifice injection valves. Fuel is continuously filtered through replaceable cellulose filter elements.

GOVERNOR: Catepillar governor operates through entire speed range. Approximate 10% regulation is standard.

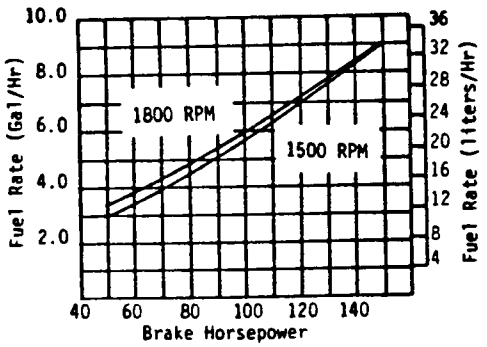
LUBRICATION: Positive displacement gear pump maintains continuous flow of lubricants under pressure to all moving parts. Full-flow filtration is provided by replaceable cellulose filter elements. Water-cooled oil cooler maintains proper oil temperature.

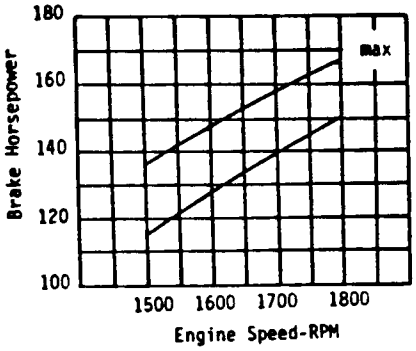
PISTONS: Elliptically-ground, contoured, aluminum alloy pistons with integrally-cast iron bands for top rings. Two chrome-faced compression rings and one chrome-faced, spring-loaded oil ring on each.

STARTING: Electric and air starting systems are offered.

VALVES: Stellite-faced valves and hard alloy steel seats. Valves rotate 3 deg each time they lift to seat in a new position each time and to allow even heat distribution.

The following power and fuel consumption ratings are a reproduction from Catepillar specifications: CATERPILLAR D330c, STANDARD ELECTRIC SET ENGINE.





VITA

Gestur Valgardsson was born in Reykjavik, Iceland, on February 2, 1955. He attended elementary school in that city and was graduated from high school in June 1972. In September 1973 he entered The Marine Engineering College of Iceland, and in June 1977 he passed the Examination for Marine Engineers First Class. In the fall of 1977 he entered The Technical College of Iceland and in June 1978, after finishing equivalent to four semesters of study he entered The University of Iceland, and in June 1982 he passed the Final Degree Examination in Mechanical Engineering. In the fall of 1982 he entered The University of Tennessee, Knoxville. He received the Master's degree, with a major in Mechanical Engineering, in March 1985.

During the years between 1973 to 1978 the author worked as an Engineering Officer on board a number of Icelandic trawlers.

The author is a member of the Marine Engineering Society of Iceland and the Icelandic Society of Engineers.

The author is married to Rannveig Maria Thorsteinsdottir, graduate student in Vocational Evaluation and Rehabilitation, at The University of Tennessee, Knoxville. They have one son, Valgardur Dadi Gestsson.