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CONTROL OF NITROGEN OXIDE EMISSIONS FROM DIESEL ENGINES: A THEORETICAL ANALYSIS

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The Project Officer for this program was Mr. Barry McNutt of the Division of Emission Control Technology, Office of Air Programs, Environmental Protection Agency.

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INTRODUCTION

Problem Description

Diesel engines are a class of reciprocating, internal-combustion engines, or "piston" engines, which are characterized by a unique ignition process. Relatively high compression ratios are used in diesel engines, and the resulting high air-charge temperatures cause ignition of fuel to occur spontaneously. Hence, the diesel is also referred to as a "compression-ignition" engine. Various references are readily available which describe the operating and design characteristics of diesel engines (e.g., Ref 1).

Exhaust emissions from diesel engines consist of the same classes of pollutants which are of concern for other combustion systems operating on petroleum-based fuels:

1. Carbon monoxide (CO).
2. Organics (hydrocarbons, aldehydes, and other organic-based materials in gaseous or liquid state).
3. Nitrogen oxides (NOx).
4. Dry particulates (DP) (materials emitted as solid particles).
5. Sulfur dioxide (SO_2).

SO_2 emissions result from the presence of sulfur-containing impurities in diesel fuels, and, hence, SO_2 emissions and their control are inevitably linked to fuel characteristics. The other emissions, however, are not inevitable, but are formed during the combustion process, and are, in a sense, results of the failure of the process to limit its products to the "ideal" constituents-- carbon dioxide and water. The nature of diesel engine emissions and their origins are discussed by Hurn in Reference 2. Hurn and others have identified the emissions of principal concern from diesel engines as nitrogen oxides and organics. Carbon monoxide emission rates are very low throughout the normal operating range of the diesel engine. Dry particulate emissions from diesel engines consist predominantly of carbon particles and their emission rates can be controlled through proper engine design, selection (or rating), and maintenance procedures, and proper fuel selection (Ref 2).

Diesel engine emissions add to the atmospheric concentrations of the pollutant classes listed above, and also result in undesirable sensory effects-- smoke and odor. Smoke is caused by excessive emissions of organics (white smoke) or particulates (black smoke), and control of smoke is achieved by control of these emission classes. The origin of diesel engine odors is unclear, though it is generally associated with emission of organics.

Program Objective

The program described in this report has been concerned with the control of NOx emissions from diesel engines. The program has been based upon an over-all approach to NOx control consisting of the following sequence of steps

1. Development of design criteria for controlling NOx emissions by theoretical analysis.
2. Verification of the theoretically-derived NOx control criteria by experimental testing.
3. Demonstration of the utility of the engine design criteria by development and operation of engines with controlled NOx emissions.

This sequence represents a logical, orderly approach to emission control which is being pursued to varying degrees for other types of sources.

The program described in this report was directed toward the first step. The objective of the program was to correlate engine design, performance, and emission characteristics by theoretical analysis, and to develop NOx-control criteria.

Program Approach

To achieve the objective defined above, the following sequence of tasks was undertaken:

1. Development of mathematical models of combustion and NO formation in diesel engines.
2. Correlation of engine design, performance, and emission characteristics.

3. Identification and evaluation of methods for controlling NO emissions.

These tasks were related through the models which were developed in the first task and subsequently employed to accomplish tasks 2 and 3. Thus, the program was oriented toward the theoretical modeling of diesel engine combustion systems.

The program was concerned primarily with diesel engines used for heavy duty vehicle propulsion. Therefore, in the modeling task, it was necessary to develop analysis techniques applicable to the types of automotive diesel engines in general use. Since the models were to represent combustion and nitrogen oxide formation processes, it was only necessary to include those features of engines and their combustion systems which directly affect these processes. For this purpose, it was necessary to distinguish between two classes of combustion chamber design. The first class consists of open-chamber or "direct-injection" engines, and the second class includes divided-chamber or "indirect-injection" engines. A separate model was developed for each engine class.

The design-performance-emission correlations, which were the objective of the second task, were produced by parametric analyses conducted with the combustion models. Engine design variables were studied to determine their effects on performance and emissions. Engine performance was monitored by calculating indicated values of power output and specific fuel consumption. The use of indicated performance parameters permitted the analyses to be limited to processes occurring within the engine combustion chamber. This limitation was justified on the grounds that indicated performance can be related to actual engine output, or "brake" performance, by means of more comprehensive engine models which have been developed earlier (e.g., Ref 3). This limitation allowed a more detailed analysis of combustion processes to be conducted which is necessary for an investigation of pollutant formation.

In the final task, the results of the previous tasks were analyzed to identify concepts for controlling NOx emissions. Two categories of control methods were defined based on these concepts-- the first category including engine design modifications, and the second category including auxiliary control devices. Design criteria were defined for

controlling NOx emissions by means of engine design modifications, and a qualitative evaluation was made of the performance of auxiliary control devices.

SUMMARY OF RESULTS

Model Development

Two mathematical models were developed-- one for direct-injection engines and the other for indirect-injection engines. To use either of these models for evaluating engine performance, a specific engine design and operating condition are represented by a set of input data. The model predicts indicated values of horsepower, specific fuel consumption, and specific NO emission rate* for the engine and its operating condition. The model also calculates the time history of combustion chamber properties, including pressure, mean temperature, and fraction of fuel burned. Thus, performance characteristics such as peak pressure and pressure rise rate can be predicted.

The models have been used to predict performance of two automotive diesel engines for which performance and emission data have been published. The performance and NO emission predictions obtained are consistent with performance generally observed for diesel engines and for these two engines in particular. No attempt was made to "calibrate" the models. That is, model parameters were not varied to attempt to obtain precise agreement between predicted and observed engine performance. The available engine performance data were not sufficiently complete to provide for calibration of the models.

Even without calibration, the models produce realistic values of engine power and fuel consumption and values of NO emission rate which agree reasonably well with measured values. Thus, the models were considered to be satisfactory for use in the remaining tasks of the program.

Design-Performance-Emission Correlations

Parametric analyses were conducted, using both engine models, to determine the sensitivity of predicted engine performance and NO emission rate to various parameters. Model sensitivity analyses were conducted to determine the relative influence of different processes occurring

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* The term "emission rate", as used in this report, indicates a normalized rate, i.e., exhaust mass fraction (ppm) or specific emission rate (gr/hp-hr).

in the combustion chamber. These analyses indicated that predicted NO emission rates are very sensitive to the values assigned to parameters which represent processes such as fuel vaporization, fuel burning, and heat transfer. This sensitivity is less pronounced in the IDI engine model than in the DI engine model.

Design sensitivity analyses were conducted to produce correlations between engine design, performance, and emission parameters. These correlations indicate the effects on performance and NO emissions of variations in design variables which are directly controlled by the engine designer. The NO emission rate from DI engines is found to be very sensitive to fuel injection variables. IDI engine emissions, however, appear to be less sensitive to fuel injection characteristics, but are very sensitive to the amount of fuel which passes unburned into the main chamber.

NOx Emission Control Methods

The design-performance-emission correlations were used in an attempt to formulate criteria for reducing NO emission rate through engine design variations. It appears from the results of this effort that NO emissions can be reduced from DI engines through variation in fuel injection characteristics. NO emissions from IDI engines might be reduced by modifying fuel spray characteristics to increase fuel residence time in the precombustion chamber. Emission rate reductions achievable by these approaches appear to be significant-- of the order of 50 per cent for DI engines-- but probably will be accompanied by reductions in engine performance.

The models also were used to investigate the effects of other engine design approaches on NO emissions. Design features examined were turbocharging, pilot injection, and fumigation. The results indicated that neither turbocharging nor pilot injection offers an effective approach to NO emission control. However, the predicted effects of fumigation included substantial reductions of NO emission rate. These effects are not considered to be conclusive since fumigation was only represented in the model in an approximate manner.

Auxiliary methods of NO emission control, such as water injection and exhaust gas recirculation, were not evaluated. However, approaches to incorporating these control methods into the engine models were indicated.

CONCLUSIONS AND RECOMMENDATIONS

The diesel engine combustion models which have been developed can be used to provide qualitative correlations between engine performance, NO emission rate, and engine design characteristics. It is anticipated that the predictive abilities of the models can be made quantitatively accurate by calibration with experimental data obtained by engine testing. These models can be used as convenient tools, either alone or in conjunction with experiments, to evaluate effects of engine design variations on indicated engine performance and NO emissions.

It has been possible to establish qualitative design criteria for reducing NO emissions from direct-injection engines. NO emission rate is found to vary monotonically with fuel injection time, injection rate, and over-all fuel-air ratio. These design variables also affect engine performance factors including specific fuel consumption, specific power, peak pressure, pressure rise rate, and smoke emission. Qualitative guidelines have been defined for reducing NO emissions by manipulation of these design variables while minimizing the associated penalties in engine performance.

The tendency for indirect-injection engines to produce lower NO emissions than direct-injection engines has been confirmed by the IDI engine model. However, this effect is strongly influenced by the fuel injection pattern of the IDI engine. If a significant fraction of the injected fuel passes directly into the main chamber, the advantage of the prechamber in reducing NO emissions is reduced.

The direct-injection engine model has been used to evaluate turbocharging, pilot injection, and fumigation as methods for reducing NO emissions. Of the approaches considered, only fumigation was found to decrease NO emissions. Further evaluation of this control method will be required to determine the extent of NO emission control actually attainable. With minor modifications, the models also can be used to evaluate water injection and exhaust gas recirculation, and combinations of these and other emission control methods.

It is recommended that the development of predictive techniques for diesel engine performance and emissions be continued. These predictive techniques are likely to be useful to engine manufacturers in their efforts to

comply with future emission standards. Therefore, it is important that the tehcniques be as accurate as possible and have broad applicability.

Two specific recommendations for additional effort are as follows:

1. The engine models developed in this program should be modified and extended to increase their general utility in research on emission control. Modifications recommended involve the introduction of more general, or flexible, sub-models of combustion processes which have been found to affect NO emissions strongly, including ignition delay, fuel burning, and heat transfer. Extensions recommended include the incorporation of water injection and exhaust gas recirculation into the models.
2. A carefully-controlled experimental program should be undertaken to calibrate the engine models developed in this program, and to verify the predicted correlations between engine design, performance, and emission parameters. The experimental program should include measurements of engine performance and emissions with variations in design characteristics which appear to affect NO emissions most strongly. Primary emphasis should be directed toward the effects of fuel injection characteristics.

This recommended additional effort constitutes a logical continuation of the work that has been accomplished and should lead to the development of effective emission control methods for diesel engines.

GENERAL DESCRIPTION OF ENGINE MODELS

Nature of the Models

The engine models are sets of mathematical relationships which relate the performance and emission characterictics of diesel engines to their design characteristics and operating conditions. The models include those factors and processes normally considered in calculating engine performance. These processes are:

Heat release rate

Heat losses

Internal losses

The models also include additional factors which are believed to affect the rate of NO emission most strongly:

Nonuniform gas composition

Nonuniform gas temperature

Real gas composition and thermal properties

Finite-rate kinetics of NO formation

The models represent explicitly the processes of fuel injection, vaporization, ignition, and combustion so that heat release rate is calculated instead of being prescribed as input data. Thus, the models provide a utilitarian procedure for relating engine performance and emission rate to design variables and operating conditions.

Modeling Concept

Mathematical models of combustion chambers can be developed with varying degrees of complexity. The complexity of a model is dependent upon the degree to which fluid properties within the combustion chamber are represented as functions of time and spatial dimensions. For discussion purposes, such models can be classifed as follows:

1. Homogeneous.
2. Heterogeneous, nondimensional.
3. Heterogeneous, dimensional.

Within each class, a model can be either steady or unsteady (i.e., time-dependent).

In a homogeneous model of a combustion chamber, fluid properties within the chamber are uniform and particles of fluid do not retain their identity as they pass through the chamber. A common example of this type of model is the "perfectly-stirred reactor" concept which has been used to model many combustion systems.* Unsteady homogeneous models can be used to represent systems where the over-all system properties, such as volume, mass, or composition vary with time.

In a heterogeneous, nondimensional model, certain nonuniform fluid properties can be represented. Distributions of properties such as composition and temperature can be assigned to the fluid within the chamber. However, the spatial distribution of these properties is not represented. An example of this type of model is the "well-stirred" or "partially-stirred reactor" concept which has been utilized as an extension of the perfectly-stirred reactor. Heterogeneous, nondimensional models may be unsteady in their over-all properties or in the distribution of fluid properties within the chamber.

In a heterogeneous, dimensional model, the distribution of all fluid properties can be represented and their spatial distributions are indicated. Such models can be of one, two, or three dimensions and may be either steady or unsteady.

Of the model types discussed above, the steady, homogeneous model is the simplest, and the unsteady, heterogeneous, three-dimensional model is the most complex. As model complexity increases, the number of features of the combustion system represented by the model also increases. However, the effort required to develop and use a model increases very rapidly with model complexity. Therefore, when selecting a model for a particular application, it is good practice to choose the least complex model which will meet the requirements of the specific application. The use of an unnecessarily complex model always results in a waste of resources.

In the case of diesel engine combustion chambers, most models used in the past (e.g., Ref 3) have been of the unsteady, homogeneous type. This simple model form has been found to be entirely adequate for predicting cylinder pressure and heat transfer rates from which over-all engine performance can be derived. It has not been found necessary to

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* For example, see Reference 18.

model the heterogeneous fluid properties in the cylinder to predict engine performance.

In this program, the requirements of the models include the prediction of exhaust gas NOx concentration as well as engine performance. For this purpose it is necessary to calculate the rate at which NO is formed and to integrate this rate over the duration of the engine cycle. The formation rate of NO is dependent upon gas composition and temperature, and the temperature dependence is highly nonlinear. Thus, average properties of the cylinder gases cannot be used. The heterogeneous character of the gases must be modeled, and NO formation rates must be calculated individually for each portion of the gas mixture. Thus, it is necessary to model the distribution of fluid properties in the cylinder gases as a function of time during the cycle. It is not necessary, however, to model the spatial distribution of gas properties. The formation of NO in an element of the gas mixture, is not dependent on the location of the element in the cylinder. The properties of the element may be dependent upon its location, but in the case of the diesel combustion chamber this spatial dependence is only of secondary importance. Therefore, it is not necessary to model the spatial distribution of elements of gas mixture to determine their properties.

On the basis of these considerations, the class of models selected for this program is the unsteady, heterogeneous, nondimensional type. In this model type, the gas mixture is represented as a finite number of elements or "systems". The properties of each system are uniform at any time, but vary with time during the cycle. It is not assumed that a system exists as one continuous volume of fluid in the cylinder. It may take any shape and may consist of many individual fluid elements, all with the same properties. This type of model is well suited to the diesel combustion chamber since the fluid systems present in the early stages of the cycle, i.e., air and liquid fuel, are well defined. The properties of these systems and other systems which are formed can be determined during the remainder of the cycle by appropriate modeling of transport processes.

A critical aspect of the combustion chamber models is the representation of chemical rate processes occurring within fluid systems

and mass and energy transport processes occurring among systems and between systems and the chamber walls. These processes, which are referred to in this report as "rate processes", result in changes in properties of fluid systems and the formation of new systems. Models of rate processes can become very complex and can incorporate dimensional features of the combustion chamber and its contents. In modeling diesel engine combustion, several rate processes must be modeled which are not well understood. In these instances, the approach used here is the formulation of heuristic models which embody the correct functional dependencies among the variables involved, and the incorporation in these models of accessible empirical constants which can be used to obtain quantitative agreement between theoretical predictions and experimental observations. Generally, the over-all combustion model is constructed in a way which will allow these empirical rate process models to be replaced by theoretically-based models as they become available.

The intent of this discussion has been to present the rationale for the selection of the model concept used in this program. The detailed nature of each model is presented in subsequent sections of this report.

Model Assumptions

A number of significant assumptions are involved in the engine models. Certain of these assumptions result directly from the selection of the model concept, and others result from the formulation of the model and its analysis procedure. These assumptions are identified and discussed here so that the reader may have a clearer understanding of the capabilities and limitations of the models.

Two separate models have been developed, one for direct-injection (DI) engines and the other for indirect-injection (IDI) engines. These assumptions, in general, pertain separately to the two chambers of the IDI engine combustion chamber. That is, the two chambers are treated independently in the specification of fluid systems and rate processes.

Fluid Systems

It is assumed in each model that the contents of the engine combustion chamber consist of a finite number of fluid systems, each of which

has uniform properties. These systems and the mass transport processes occurring among them are indicated in Figures 1 and 2 for the DI and IDI models, and are discussed below.

1. Air - One system which may contain an initial NOx concentration. Mass is lost from this system through fuel burning and dilution of burned mixture systems.
2. Liquid fuel - One system which gains mass through fuel injection and loses mass through fuel vaporization.
3. Gaseous fuel - One system which gains mass through vaporization of liquid fuel and loses mass through fuel burning.
4. Burned mixture - The burned mixture consists of the products of combustion which exist in the combustion chamber at any given time, and is highly nonuniform in composition. This mixture is represented in the model by a large number of uniform systems with individual properties which are determined by the time at which the combustion of each system occurred and its subsequent air dilution history. Once formed, there is no loss of mass from a burned mixture system. However, the system gains mass by dilution with air.

In this formulation of fluid systems, fuel and air mixing and burning are assumed to occur simultaneously. The presence of a fuel vapor-air mixture is not represented, even though such mixtures exist during early stages of combustion. The omission of a fuel vapor-air mixture as a system was justified on the basis that the additional complexity would not improve the ability of the model to predict engine performance or NO emission rate. The effects of fuel and air mixing processes on fuel burning rate must be incorporated in the fuel burning rate model.

Mass Transport Processes

Fuel Vaporization

Fuel vaporization is represented by an empirical model based upon the description of the "preparation-to-burn" process by Lyn (Ref 4). The

model includes one variable parameter which controls the vaporization schedule of each increment of fuel injected into the combustion chamber. This modeling method was selected because it combines all of the processes affecting fuel vaporization into one simple model which has been shown to be a realistic representation of vaporization rate. The model is limiting in that it does not explicitly represent fuel injector design variables which may affect vaporization.

Fuel Burning

Fuel burning is considered to occur in two distinct phases. In the first, fuel vapor and air are assumed to be premixed and to burn over a range of fuel-air ratios. Ignition is assumed to occur in a near-stoichiometric fuel-air mixture, and combustion proceeds by flame spreading through rich and lean fuel-air mixtures. The burning rate in the initial burning phase exceeds the vaporization rate so that eventually all gaseous fuel is consumed. The final burning phase commences when all gaseous fuel has been burned. Burning in the final phase proceeds at the same rate as fuel vaporization and occurs at a fixed fuel-air ratio, usually stoichiometric. This burning rate model also is patterned after Lyn's description of diesel combustion processes (Ref 4). The assumption that ignition and final stages of burning occur at stoichiometric mixture ratios is based upon laboratory observations of thermal ignition and diffusion flame combustion. This modeling concept was selected because it is considered to represent the processes which determine the time and mixture ratio at which each increment of fuel burns-- factors which strongly influence the formation of NO.

Ignition Delay

The interval between the start of fuel injection and fuel burning (ignition) is determined by an empirical ignition delay correlation, or alternatively, it may be specified as an input data item. The empirical correlation included in the model was developed by Tsao (Ref 5). This correlation did not provide realistic ignition delay times at all operating conditions, and thus was not used in the analyses conducted in this program.

Burned Mixture Dilution

The dilution of the burned mixture with additional air is included in the model because the dilution process significantly affects combustion efficiency and NO formation. Burned mixture systems with rich fuel-air ratios require additional air for completion of fuel burning. Once burned, the NO concentration in each system would be predicted to reach unrealistically high levels if dilution were ignored. The rate of dilution of each burned mixture system is assumed to be proportional to both the amount of excess air present and the mass of the burned mixture system. This modeling concept is based upon the assumption that mixing occurs at a uniform rate throughout the combustion chamber and across the boundaries between systems.

Inter-Chamber Mass Flow (IDI Engine)

In the IDI model, ignition is assumed to occur first in the precombustion chamber. Prior to ignition, fluid flows from the chamber with the higher pressure to the other. The composition of the flow is the same as the over-all composition of the fluid in the chamber of origin. After ignition in the precombustion chamber, flow occurs only from this chamber to the main chamber, and the composition of this flow is equal to the mass average composition of burned mixture systems in the precombustion chamber. This assumption-- that after ignition, only burned mixture flows from the prechamber-- is based on the concept that the fluid issuing from the prechamber is well-mixed and can be represented effectively as a burned mixture system. The burned mixture entering the main chamber is not combined with existing burned mixture systems, but is retained in separate systems. This assumption is made to avoid the analysis procedures which would be required to model mixing of burned mixture systems. The effect of this assumption on predicted performance probably is negligible.

Other Mass Transport Processes

It is assumed that no other mass transfer between fluid systems occurs other than that represented by the processes listed above. Specifically neglected are mixing of different burned mixture systems and mixing of fuel vapor with burned mixture systems. Omission of these

processes simplifies the model analysis procedures without detracting significantly from the ability of the model to predict engine performance and NO emission rate.

Other Rate Processes

Heat Transfer

Heat transfer is assumed to occur between all gaseous fluid systems and the chamber wall in accordance with a Newtonian rate expression. The heat transfer rate is a fixed parameter and the driving temperature difference is that between the wall temperature and a mean fluid temperature. The wall temperature is assumed to be uniform and constant. The mean fluid temperature is derived from an empirical temperature-energy correlation using a fuel-air ratio based on total fuel burned and total air present. The energy transferred is distributed among all gaseous systems in proportion to their masses. It is assumed that no heat transfer occurs between fluid systems except for the convective transfer associated with the mass transport processes described above. This heat transfer model represents effectively that portion of the cycle prior to ignition where heating of the air system occurs over a relatively long time period. A uniform distribution of heat transfer is a reasonable assumption because of the high turbulence level in the chamber during this period.

The model is less effective after ignition where the heat loss from burned mixture systems is more dependent upon the individual system temperature than on the mean fluid temperature. Also, heat loss from burned mixture systems is dependent upon location within the chamber-- systems near the wall losing energy at the highest rate. These effects could be represented by using a model with heat transfer rate based upon individual system temperature and introducing a distribution of heat transfer coefficients to account for spatial effects. This additional complexity was not considered to be justified in this initial program. However, in view of the apparent influence of heat transfer on NO formation (discussed in later sections of the report), modification of the heat transfer model should be considered in a future program.

Compression and Expansion Work

The transfer of energy due to compression and expansion work is distributed among all gaseous systems present in the chamber. All systems are assumed to expand or contract polytropically with the same polytropic index.

Nitrogen Oxide Formation

The formation of nitric oxide (NO) is modeled and the concentration of all nitrogen oxides (NOx) in the exhaust gas is assumed to be equal to the NO concentration predicted by the model. This assumption implies that conversion of NO to other oxides (predominantly NO_2) does not affect the NO formation rate. NO formation is assumed to proceed in each burned mixture system in accordance with a model developed by Fletcher and Heywood (Ref 6). This model is based upon a six reaction NO formation scheme, and the formation rate increases with the departure of the NO concentration from its equilibrium value.

The NO formation rate in the air system is assumed to be zero. This assumption has been substantiated by observing the temperature history of the air system as calculated by each model. The air system temperature remains well below the temperature regime wherein NO formation occurs at a significant rate.

Chamber Pressure

Combustion chamber pressure is calculated by means of a homogeneous fluid model integrated within the over-all model. The homogeneous system is assumed to consist of combustion products from all fuel burned and the total air charge. The gaseous and liquid fuel systems are neglected. Chamber pressure is calculated by an energy conservation equation and an equation of state using real gas property correlations by Borman (Ref 3). Calculation of chamber pressure by means of a homogeneous fluid model is a key assumption in that the resulting analysis procedures are greatly simplified. The assumption that pressure can be predicted effectively by this approach is justified by past experience in the successful prediction of chamber pressure and engine performance by means of homogeneous fluid models (Refs 3 and 4).

Model Descriptions

The direct-injection (DI) and the indirect-injection (IDI) engine models are described in the following sections of this report. The discussion of each model is divided into four topics:

1. Physical description.
2. Governing relationships.
3. Rate processes.
4. Analysis procedure.

The physical description indicates the concept of the diesel combustion process which forms the basis for the model, and the governing relationships are the conservation and state equations which are relevant to the combustion concept. The discussion of rate processes indicates the approaches used to prescribe transport and chemical processes occurring during the combustion cycle. The discussion of analysis procedures outlines the technique used to solve the mathematical relationships to obtain the predicted engine performance and NO emission rate.

DESCRIPTION OF THE DIRECT-INJECTION ENGINE MODEL

Physical Description

The model is concerned with the properties of the fluid system contained in a direct-injection engine cylinder, as represented in Figure 3. The variables which define the cylinder design for modeling purposes are:

B = cylinder bore

V_c = clearance volume

L = connecting rod length

R = crank length

θ = crank position (θ = 0 at TDC)

N = engine speed = $d\theta/dt$.

The model includes only those processes occurring during the portions of the compression and expansion strokes when all valves are closed. Thus, the model treats a fixed mass of air and residual gas trapped in the cylinder when the intake valves close. The model, therefore, is applicable to either two-stroke or four-stroke cycle engines, and valve design characteristics need not be considered in formulating the model. However, inlet valve design features may be included in prescribing certain transport processes as discussed in the next section.

The fluid within the cylinder is considered to be uniform in pressure and to consist of a set of open or variable mass systems as follows:

1. Air-residual-gas mixture (referred to as "air" in this discussion) - one system designated by subscript a.
2. Liquid fuel - one system designated by subscript $f\ell$.
3. Vaporized fuel - one system designated by subscript fg.
4. Burned mixture (combustion products and excess air) - i systems designated by subscript bm,i.

These systems are assumed to exist within the cylinder, but their locations or distributions are not prescribed by the model.

The conditions within each of the systems are controlled by the following rate processes:

1. Liquid fuel injection, $\dot{m}_{f\ell}$.
2. Fuel vaporization, $\dot{m}_{fg}$.

3. Ignition delay, τ_{ig}.
4. Fuel burning, $\dot{m}_{fb}$.
5. Burned mixture dilution, $(dm/d\theta)_a$.
6. Heat transfer, $\dot{Q}$.
7. Nitrogen oxide formation, $\dot{r}_{bm,i}$.

The interaction of these rate processes in determining system properties is described in terms of a five-phase cycle in which the phases are defined by certain crank positions, as indicated in Figure 4:

1. Valve closure, θ_{vc}.
2. Start of fuel injection, θ_{in}.
3. Ignition, θ_{ig}.
4. Start of final burning, θ_{fb}.
5. End of combustion, θ_{eb}.
6. Valve opening, θ_{vo}.

The phases in the cycle are described as follows.

1. Initial Compression ($\theta_{vc} \leq \theta \leq \theta_{in}$). Only the air system is present in the chamber.
2. Ignition Delay ($\theta_{in} \leq \theta \leq \theta_{ig}$). Physically, liquid fuel is injected into the chamber and begins to vaporize and mix with the air to form a mixture of varying fuel-air ratio in both chambers. In the model, consideration of this mixing process is deferred until the next phase, so that in general three systems (m_a, m_{fl}, m_{fg}) are present in the chamber.
3. Initial Burning ($\theta_{ig} \leq \theta \leq \theta_{fb}$). Physically, ignition occurs during this phase and burning occurs via flame propagation through all elements of combustible mixture, resulting in combustion over a wide range of fuel-air ratios, until all of the vaporized fuel accumulated during the ignition delay phase has been burned. In the model, an elemental quantity of fuel vapor is assumed to mix with an appropriate amount of air to burn instantaneously at a specified fuel-air ratio during each crank-angle increment. The specification of the fuel-air ratio at which burning occurs, as a function of crank angle, simulates the quality of fuel-air mixing achieved during the ignition delay phase.

Subsequent to the formation of each element of burned mixture, it is diluted by mixing with part of the excess air. In general, then, there are three $+i$ systems ($m_a, m_{fl}, m_{fg}, m_{bm,i}$) present in the chamber during this phase, where i is the number of crank-angle increments taken.

4. Final Burning ($\theta_{fb} \leq \theta \leq \theta_{eb}$). During this phase, it is assumed that burning is diffusion controlled, and hence, that combustion occurs at a constant fuel-air ratio near stoichiometric. Thus, in the model, there are two $+i$ systems ($m_a, m_{fl}, m_{bm,i}$) present in the chamber.
5. Final Expansion ($\theta_{eb} \leq \theta \leq \theta_{no}$). All fuel burning is complete in this phase, and the only significant process occurring is the further dilution of the burned mixture systems with excess air. One $+i$ systems ($m_a, m_{bm,i}$) are present in the chamber.

The above cycle is based upon phenomenological descriptions of diesel combustion by various workers, such as Obert (Ref 1) and Lyn (Ref 4).

The temperature and composition of each burned mass system are assumed to be equal to thermodynamic equilibrium values, except for concentrations of N, N_2O, and NO. Formation reactions for N and N_2O are assumed to be in steady state. These assumptions lead to a single reaction rate equation governing the increase in NO concentration from its initial value. This "pseudo-equilibrium" assumption is reasonable in modeling NO formation, since these reactions are not energetically significant to the over-all hydrocarbon combustion process. Thus, in general, the properties of any system are completely determined from the pressure (p), the fuel mass fraction (F), the NO mass fraction ($[NO]$), and the temperature (T) or the internal energy (ε) or the enthalpy(h).

Governing Relationships

The governing equations for the properties of the fluid systems are the conservation of mass (air and fuel), conservation of species (NO), conservation of energy, and thermal and caloric equations of state. Appropriate forms of the conservation relations for the over-all mixture are

used to determine the chamber pressure, while the conservation relations for each system are used to determine the system properties in terms of the mass of the air system, the mass of fuel in the other systems, the fuel mass fraction in the burned mixture systems ($F_{bm,i}$), the internal energy of all systems, and the NO mass fraction of all systems. Mathematical relationships describing the various rate processes complete the model formulation.

Over-All Relationships

To determine chamber pressure and mean temperature, it is assumed that the mixture within the chamber is homogeneous and in thermodynamic equilibrium. These assumptions exclude the presence of unburned fuel, and the relevant relationships are as follows:

Conservation of mass:

$$m_h = m_a + \sum_i \frac{m_{fbm,i}}{F_{bm,i}} \tag{1}$$

Conservation of energy:

$$\frac{d}{d\theta}(m_h \varepsilon_h) = -KP\dot{V} - \dot{Q} \tag{2}$$

Equation of state:

$$PV = m_h R_h T_h \tag{3a}$$

$$R_h = R_h (T_h, F_h) \tag{3b}$$

Caloric equations of state.

$$\varepsilon_h = \varepsilon_h (T_h, F_h, P) \tag{4a}$$

$$h_h = h_h (T_h, F_h, P) \tag{4b}$$

where h = subscript referring to properties of homogeneous mixture

F_h = mass fraction of burned fuel = $\left(\sum_i m_{fbm,i}\right) / m_h$

m = mass

K = polytropic index

$\dot{V}$ = rate of change of chamber volume per unit crank angle

$\dot{Q}$ = rate of energy transfer to chamber walls per unit crank angle

R = gas constant.

System Equations of State

Each system is assumed to behave as a semiperfect gas, and hence, the caloric equations of state are of the following form:

$$\varepsilon_a, h_a = f(P, T_a) \tag{5a,b}$$

$$\varepsilon_{f\ell}, h_{f\ell} = f(P, T_{f\ell}) \tag{6a,b}$$

$$\varepsilon_{fg}, h_{fg} = f(P, T_{fg}) \tag{7a,b}$$

$$\varepsilon_{bm,i}, h_{bm,i} = f(P, T_{bm,i}, F_{bm,i}) \tag{8a,b}$$

The exact relationships used are described at the end of this section of the report.

Conservation of System Energy

The energy conservation relations for the air system can be written as:

$$\frac{d}{d\theta}(m_a \varepsilon_a) = -\varepsilon_a \left(\frac{Dm}{D\theta}\right)_a + v_a \left(\frac{V_{up}\dot{P}}{n P} - \dot{Q}\right) \tag{9}$$

where $$\left(\frac{Dm}{D\theta}\right)_a = -\int_{\theta_{vc}}^{\theta} \left(\frac{dm}{d\theta}\right)_a d\theta - \int_{\theta_{ig}}^{\theta} \frac{1 - F^o_{bm}}{F^o_{bm}} \dot{m}_{fb}\, d\theta$$

For the liquid fuel system:

$$\frac{d}{d\theta}\left(m_{f\ell}\, \varepsilon_{f\ell}\right) = h_{f\ell}\left(\dot{m}_{fc} - \dot{m}_{fg}\right) \tag{10}$$

For the vapor fuel system:

$$\frac{d}{d\theta}\left(m_{fg}\varepsilon_{fg}\right) = h_{f\ell}\dot{m}_{fg} - \varepsilon_{fg}\dot{m}_{fb} + \nu_{fg}\left(\frac{V_{ap}\dot{P}}{n P} - \dot{Q}\right) \tag{11}$$

For already formed burned mixture systems:

$$\frac{d}{d\theta}\left(\frac{m_{fbm,i}\varepsilon_{bm,i}}{F_{bm,i}}\right) = \varepsilon_a\left(\frac{dm}{d\theta}\right)_{abm,i} + \nu_{bm,i}\left(\frac{V_{ap}\dot{P}}{n P} - \dot{Q}\right) \tag{12a}$$

For burned mixtures forming as a result of combustion:

$$\frac{d}{d\theta}\left(\frac{m_{fbm,i}\varepsilon_{bm,i}}{F_{bm,i}}\right) = \varepsilon_{fg}\dot{m}_{fb} + \varepsilon_a\frac{1 - F^{\circ}_{bm}}{F_{bm}}\dot{m}_{fb} - \left(KP\dot{V} + \frac{V_{ap}\dot{P}}{n P}\right) \tag{12b}$$

where the "ν's" determine the distribution of energy transfer to each system by compression or expansion work and heat transfer:

$$\nu_a = m_a R_a T_a / V_{ap} \tag{13}$$

$$\nu_{fg} = m_{fg} R_{fg} T_{fg} / V_{ap} \tag{14}$$

$$\nu_{bm,i} = m_{fbm,i} R_{bin,i} T_{bm,i} / F_{bm,i} V_{ap} \tag{15}$$

where

$$V_{ap} = m_a R_a T_a + m_{fg} R_{fg} T_{fg} + \sum_i\left(\frac{m_{fbm,i} R_{bm,i} T_{bm,i}}{F_{bm,i}}\right) \tag{16}$$

$$n = 1 + K(\gamma - 1) \quad = \text{polytropic exponent} \tag{17}$$

The energy transfer distribution assumed here is, in physical terms, equivalent to assuming that all nonreacting systems expand or contract polytropically, with the volume available for the reacting system being

equal to the remaining chamber volume plus the initial volume of the reactants. While this is not a completely accurate distribution of energy transfer, it incorporates the essential processes.

Conservation of System Mass

The conservation of air in the air system can be written as:

$$m_a = m_a^\circ + \int_{\theta_{vc}}^{\theta} \left(\frac{\partial M}{\partial \theta}\right)_a d\theta \tag{18}$$

The fuel contents of the various systems are determined by the following equations:

$$m_{f\ell} = \int_{\theta_{vc}}^{\theta} (\dot{m}_{f\ell} - \dot{m}_{fg})\, d\theta \tag{19}$$

$$m_{fg} = \int_{\theta_{vc}}^{\theta} (\dot{m}_{fg} - \dot{m}_{fb})\, d\theta \tag{20}$$

$$m_{fbm,i} = \int^{\Delta\theta_i} \dot{m}_{fb}\, d\theta \tag{21}$$

where $\Delta\theta_i$ is the crank-angle interval during which the i^{th} system is formed.

Finally, it is necessary to specify the initial fuel mass fraction (F_{bm}°) in each burned mass system. During the initial burning period, $\theta_{ig} \leq \theta \leq \theta_{fb}$, this specification is:

$$F_{bm}^\circ = F_m - \frac{i-1}{2}\Delta F \quad , \; i \text{ odd} \tag{22a}$$

$$F_{bm}^\circ = F_m + \frac{i}{2}\Delta F \quad , \; i \text{ even} \tag{22b}$$

where F_m = specified mean mixture ratio at which burning occurs

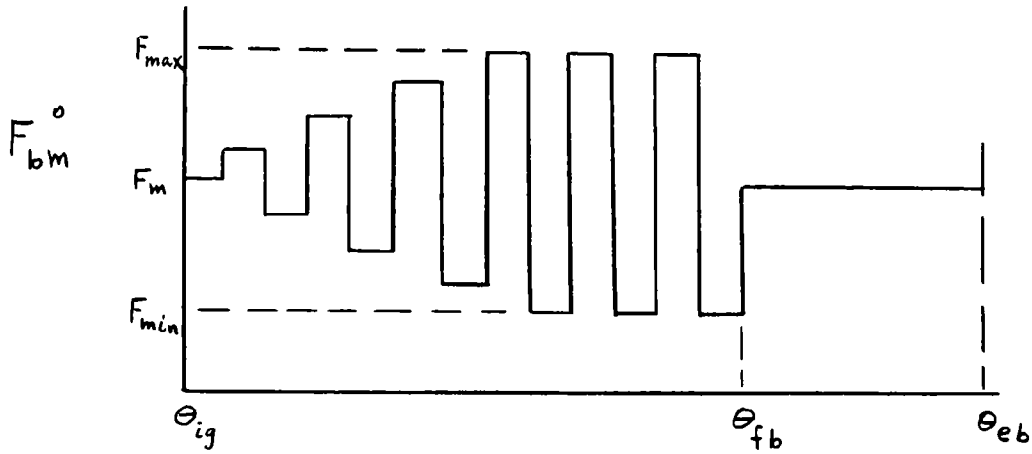
ΔF = specified increment in mixture ratio for each crank-angle interval

i = number of crank-angle increments after ignition (which is also equal to the number of burned mixture systems present).

As i increases, the values of F^{o}_{bm} diverge from F_m in accordance with Equations 22a and 22b. However, divergence limits, F_{min} and F_{max}, are imposed so that the fuel fraction at burning is constrained within realistic limits (e.g., flammability limits). After the initial burning period, it is assumed that burning occurs at a constant mixture ratio*:

$$F^{o}_{bm} = F_m \tag{22c}$$

Thus, the initial fuel fractions of the burned mixture systems varies as shown below:



Conservation of air in the burned mixture systems is represented by the instantaneous values of the fuel mass fractions:

$$\frac{dF_{bm,i}}{d\theta} = \frac{F^{2}_{bm,i}}{m_{fbm,i}} \frac{dm_{abm,i}}{d\theta} \tag{23}$$

where $dm_{abm,i}/d\theta$ is the rate of dilution of system i.

Conservation of Nitric Oxide

It is assumed that the NO reactions do not proceed in the air system, so that $[NO]_a$ is constant, and hence, the only relevant NO conservation relations are those for the burned mixture systems.

$$\frac{d[NO]_{bm,i}}{d\theta} = \frac{1}{6N}\left[\dot{r}_{bm,i} + \frac{[NO]_a}{F_{bm,i}}\left(\frac{dF_{bm,i}}{d\theta}\right)\right] \tag{24}$$

where N is the engine speed in rpm.

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* The fuel fraction at burning is automatically increased if for any reason there is insufficient air to burn all fuel present at $F^{o}_{bm} = F_m$.

Rate Processes

Fuel Injection Rate

Fuel injection rate is assumed to be a function of crank angle only and is prescribed arbitrarily as input data.

Fuel Vaporization Rate

To represent the rate of fuel vaporization, a rate equation was adopted which is patterned after Lyn's description of the "preparation to burn" process (Ref 4). Each increment of liquid fuel, injected during a crank-angle interval j is assumed to vaporize at a rate described as follows:

$$\frac{dm_{fl,j}}{d\theta} = -C\,\frac{\theta-\theta_{in,j}}{C_1^2}\,\exp\left[-\frac{\theta-\theta_{in,j}}{C_1}\right] \tag{25}$$

where $m_{fl,j}$ = mass of liquid fuel injected during j^{th} fuel injection interval $\Delta\theta_j$

C and C_1 are vaporization rate factors, C_1 being considered independent, and C determined by the requirement:

$$\int_{\theta_{in,j}}^{+180} -\frac{dm_{fl,j}}{d\theta}\,d\theta = m^{\circ}_{fl,j} \tag{26}$$

where $m^{\circ}_{fl,j}$ = initial value of $m_{fl,j}$

The total fuel vaporization rate in the cylinder at any crank position θ is the sum of the rates for all fuel elements:

$$\dot{m}_{fg} = -\sum_j \frac{dm_{fl,j}}{d\theta} \tag{27}$$

There remains, then, one rate factor to be specified (C_1) which has units of crank angle and determines the rate or "schedule" of fuel vaporization.

Ignition Delay

To specify the ignition delay, an empirical correlation developed by Tsao (Ref 5) can be used as shown below, or the ignition delay can be specified arbitrarily as an item of input data.

$$\tau_{ig} = \frac{\theta_{ig} - \theta_{in}}{N} = \left(\frac{123}{P_{in}} + 0.415\right)\left\{\left(-\frac{36.3}{T_{a,in}} + 0.022\right) N + \left(\frac{47.45 \times 10^3}{T_{a,in}} - 26.66\right) + \left(\frac{T_{a,in}}{10^3} - 1.45\right)\left(\frac{10^3 - N}{60}\right)\right\} \quad (28)$$

where P_{in} = cylinder pressure at $\theta = \theta_{in}$ (psia)
$T_{a,in}$ = air temperature at $\theta = \theta_{in}$ (deg R)
N = engine speed (rpm)
τ_{ig} = ignition delay (msec).

Fuel Burning Rate

After ignition, fuel burning is assumed to occur at a rate exceeding the fuel vaporization rate until the fuel vaporized during the ignition delay has been consumed, as described by Lyn (Ref 4). During this initial burning period, the fuel burning rate is specified as follows:

$$\dot{m}_{fb} = \dot{m}_{fg} + \frac{dm_{fg}}{d\theta} \quad (29)$$

where

$$\frac{dm_{fg}}{d\theta} = \frac{4 m^{o}_{fg}}{C_2^2}(\theta - \theta_{ig}) \qquad \text{for } (\theta - \theta_{ig}) < \frac{C_2}{2}$$

$$\frac{dm_{fg}}{d\theta} = \frac{4 m^{o}_{fg}}{C_2^2}(C_2 + \theta_{ig} - \theta) \qquad \text{for } (\theta - \theta_{ig}) > \frac{C_2}{2}$$

and m^{o}_{fg} = mass of fuel vapor present at $\theta = \theta_{ig}$

The parameter C_2 is the crank-angle interval $\theta_{fb} - \theta_{ig}$ corresponding to the initial burning period. This formulation of the initial burning rate provides a "spike" burning rate profile of the form obtained from cylinder pressure analyses (Ref 4). The parameter C_2 must be specified as input data. During the final burning period where $\theta > \theta_{fb}$, the fuel burning and vaporization rates are equal.

Burned Mixture Dilution Rate

Mixing of air with each burned mixture system is assumed to proceed at a rate proportional to the mass of the system as follows:

$$\left(\frac{dm}{d\theta}\right)_a = C_3 \left[\frac{1}{m_a} + \frac{1}{\sum_i \left(m_{fbm,i} / F_{bm,i}\right)}\right]^{-1} \tag{30}$$

where C_3 is a mixing-rate parameter which should be specified as a function of engine design variables and operating conditions. It is assumed that this dilution is proportioned according to the mass of individual burned mixture systems.

$$\left(\frac{dm}{d\theta}\right)_{abm,i} = \frac{m_{fbm,i} / F_{bm,i}}{\sum_i \left(m_{fbm,i} / F_{bm,i}\right)} \left(\frac{dm}{d\theta}\right)_a \tag{31}$$

Specification of the dilution rate parameter, C_3, therefore, determines the distribution of air in burned mixture systems throughout the cycle.

Heat Transfer Rate

The energy transfer to the walls is expressed as:

$$\dot{Q} = C_4 A \left(T_h - T_w\right) \tag{32}$$

where A is the surface area of the chamber

and T_h = mean temperature of the fluid in chamber (spatial mean)

T_w = mean wall temperature of chamber (constant)

C_4 = average heat transfer coefficient in chamber (constant).

Nitric Oxide Reaction Rate

The NO reaction rate is expressed in the form developed by Fletcher and Heywood (Ref 6):

$$\dot{r}_{bm,i} = \frac{2 M_{NO}}{6 N \rho_{bm,i}} \left(1 - \alpha_{bm,i}^2\right)\left(\frac{R_{1,bm,i}}{1 - \alpha K_{1,bm,i}} + \frac{R_{6,bm,i}}{1 + \alpha K_{2,bm,i}}\right) \tag{33}$$

where $\dot{r}_{bm,i}$ = NO formation rate (per unit crank angle) in burned mixture system i

$\rho_{bm,i}$ = fluid density

$\alpha_{bm,i}$ = ratio of NO mass fraction to equilibrium NO mass fraction

K_1, K_2, K_6 = reaction rate parameters

$R_1 = K_1 [N]_e [NO]_e$

$R_6 = K_6 [O]_e [N_2O]_e$

$[\ ]_e$ = equilibrium mole fraction.

Equilibrium concentrations of the various species are determined by means of a program developed by the NASA Lewis Research Laboratory (Ref 7).

Engine Performance Parameters

The following relationships are used to calculate indicated performance parameters for the engine (Ref 1):

$$IMEP = P_i = \frac{2}{\pi B^2 R}\left[\int_0^{\theta_{nro}} P\frac{dV}{d\theta}\,d\theta - \int_{\theta_{nrc}}^{0} P\frac{dV}{d\theta}\,d\theta\right] + P_{i,nro} \qquad (34)$$

$$ISFC = \frac{2cx}{\pi B^2 RN}\frac{\dot{\bar{m}}_{fl}}{P_i} \qquad (35)$$

where c = appropriate conversion constant for horsepower units

x = number of revolutions per power stroke

$\dot{\bar{m}}_{fl}$ = mean fuel consumption rate per cylinder.

The fraction of IMEP generated during the portions of the cycle when inlet or outlet valves are open is indicated by $P_{i,nro}$ and, in principle, is calculated as follows:

$$P_{i,nro} = \frac{2}{\pi B^2 R}\left[\int_{\theta_{nro}}^{+180} P\frac{dV}{d\theta}\,d\theta - \int_{-180}^{\theta_{nrc}} P\frac{dV}{d\theta}\,d\theta\right]$$

This quantity generally is positive, but is a small fraction of the total IMEP. It may be neglected in comparing performance of engines of the same type, but must be included when comparing engines with widely differing valve timing or manifold pressures.

Model Summary

The model described here treats the fluid within cylinder as composed of distinct systems, and results, in general, in the determination of the pressure, the thermodynamic variables ε, T, h, and m for each system present, and the mixture ratio F and NO concentration for each burned mixture system present. In addition, the total fluid within the cylinder is described in terms of average quantities (ε_h, h_h, T_h, m_h). Thus, in general, the system of equations described above results in $6_i + 13$ unknowns, where i is the number of burned mixture systems. Specification of appropriate initial conditions and the use of the previously defined rate processes complete the model formulation.

Analysis Procedure

The technique for solving the model equations to predict engine performance consists of the following sequence of steps:

1. Pressure Calculation - Cylinder pressures at all values of θ are calculated using Equations 1 through 4 assuming that the contents of the cylinder are homogeneous. IMEP and ISFC also are calculated during this step using Equations 34 and 35.
2. Fuel Distribution Calculation - The mass of fuel in each system is calculated at the end of each crank angle interval $\Delta\theta_i$ using Equations 19, 20, and 21.
3. Fuel Mass Fraction Calculation - The fuel mass fraction of each burned mass system is calculated using Equation 22 for the system formed during the interval $\Delta\theta$ and Equation 23 for systems formed in previous intervals.
4. Air System Mass Calculation - Mass of the air system remaining at the end of each θ interval is calculated using Equation 18.
5. Thermodynamic Property Calculations - The temperature and enthalpy of each system at the end of each θ interval are calculated using Equations 5 through 17. Equations for the internal energy and enthalpy of the various systems (Equations 5 through 8) are described below.
6. NO Concentration Calculation - The NO concentration in each

burned mass system is calculated for the end of each interval using Equation 26.

7. NO Emission Rate Calculation - Engine NO emission rate is calculated at the end of the cycle by summing the masses of NO in all burned mass systems and in the air system.

Thermodynamic Properties

The thermodynamic properties of the various systems are as follows:

Air Properties

These properties are obtained from Borman (Ref 3):

$$R_a = 0.06855 \times 778 \times 32.2 \quad (ft\text{-}lbf/slug\text{-}^\circ R)$$

$$\varepsilon_a = 778 \times 32.2 \times [0.16528\, T_a + 5.1979 \times 10^{-6} T_a^2 + 3.9016 \times 10^{-9} T_a^3 - 9.3632 \times 10^{-13} T_a^4 + 6.3156 \times 10^{-17} T_a^5] \quad (ft\text{-}lbf/slug)$$

$$h_a = \varepsilon_a + R_a T_a$$

Liquid Fuel Properties

These properties are:

$$\varepsilon_{f\ell} = c_{p,f\ell}\, T_{f\ell}$$

$$h_{f\ell} = c_{p,f\ell} \cdot T_{f\ell}$$

where $c_{p,f\ell}$ is the specific heat of the liquid fuel.

Vapor Fuel Properties

Vapor fuel is assumed to behave as a perfect gas with:

$$R_{fg} = 1.9857 \times 778 \times 32.2 / M_{fg}$$

$$\mathcal{E}_{fg} = h_{fg} - R_{fg} T_{fg}$$

$$h_{fg} = c_{p,fg} T_{fg} - \Delta h_{fg}$$

where M_f is the molecular weight of the fuel vapor, $C_{p,fg}$ is the specific heat of the vapor (assumed constant), and Δh_{fg} is the heat of vaporization of the fuel.

Burned Mixture Properties

For lean mixtures, $F \leq F_s$ where F_s is the stoichiometric mixture ratio, the curve-fits of Borman (Ref 3) are used.

$$R_{bm} = 778 \times 32.2 \times (1-F) \times (0.06855 + 0.004788\ \phi)$$

$$\mathcal{E}_{bm} = 778 \times 32.2 \times (1-F) \times (A - B\phi + C)$$

$$h_{bm} = \mathcal{E}_{bm} + R_{bm} T_{bm}$$

where

ϕ = equivalence ratio = $F(1-F_s)/F_s(1-F)$

$$A = 0.16528\, T_{bm} + 5.1979 \times 10^{-6} T_{bm}^2 + 3.9016 \times 10^{-9} T_{bm}^3 - 9.3632 \times 10^{-13} T_{bm}^4 + 6.3156 \times 10^{-17} T_{bm}^5$$

$$B = \Delta h_c - 1.3623 \times 10^{-2} T_{bm} - 1.2605 \times 10^{-5} T_{bm}^2 + 1.587 \times 10^{-9} T_{bm}^3 - 8.2022 \times 10^{-14} T_{bm}^4$$

$$C = \exp(D_1 + D_2 + D_3)$$

$$D_1 = 10.41066 + 7.85125\ \phi - 3.71257\ \phi^3$$

$$D_2 = (-27.00107 - 28.5087\ \phi + 17.30375\ \phi^3)(1000/T_{bm})$$

$$D_3 = [0.154226\ \phi^3 - 0.38656\ \phi - 0.10329 + (0.21289\ \phi - 0.026574)(1000/T_{bm})] \ln(P/14.4)$$

$\left(\frac{1-F_s}{F_s}\right)\Delta h_c$ = lower heating value of fuel in Btu/lbm

P = pressure in lbf/ft^2.

For rich mixtures, the properties are obtained by the crude approximation that the mixture can be represented by a mixture of stoichiometric combustion products and excess fuel vapor provided that a suitable value for the vapor specific heat is selected. Thus, for $F > F_s$:

$$R_{bm} = \frac{1}{1+f}\left[(1+f_s)R_s + (f-f_s)R_{fg}\right]$$

$$\varepsilon_{bm} = \frac{1}{1+f}\left[(1+f_s)\varepsilon_s + (f-f_s)(h_{fg} - R_{fg}T_{bm})\right]$$

$$h_{bm} = \varepsilon_{bm} + R_{bm}T_{bm}$$

where

$$f = F/(1-F)$$

$$R_s = R_{bm} \text{ and } \varepsilon_s = \varepsilon_{bm} \text{ for } F = F_s$$

$$h_{fg} = c_{p,fgd}T_{bm} - \Delta h_{fg}$$

$c_{p,fgd}$ = fictitious value of vapor specific heat.

It is anticipated that this approximation will be adequate since only the peak temperature range is of interest in determining NO formation rates.

Homogeneous Mixture Properties

For those calculations where the mixture in the chamber is assumed to be homogeneous, the above equations for burned mixtures are used. The fuel fraction F is based on the total amount of fuel which has been burned and the initial air mass.

DESCRIPTION OF THE INDIRECT-INJECTION ENGINE MODEL

Physical Description of the Model

The model is concerned with the properties of the fluid system contained in an indirect-injection engine cylinder, as represented in Figure 5. The variables which define the cylinder for modeling purposes are:

B = cylinder bore
V_1 = volume of precombustion chamber
A = interchamber port area
A_1 = surface area of precombustion chamber
V_c = clearance volume
L = connecting rod length
R = crank length
Θ = crank position
N = engine speed.

The model includes only those processes occurring during the portions of the compression and expansion strokes when all valves are closed. Thus, the model treats a fixed mass of air and residual gas trapped in the cylinder when the intake valves close.

The pressure in each chamber is assumed to be uniform with values P_1 and P_2, where the subscripts 1 and 2 refer to quantities in the precombustion chamber and the main chamber, respectively. Within each chamber, the fluid is considered to consist of a set of open or variable mass systems as follow.

1. Air-residual-gas mixture (referred to as "air" in this discussion) - one system in each chamber designated by the subscripts $a,1$ and $a,2$.
2. Liquid Fuel - one system in each chamber designated by the subscripts $f\ell,1$ and $f\ell,2$.
3. Vaporized fuel - one system in each chamber designated by the subscripts $fg,1$ and $fg,2$.
4. Burned mixture - i systems in each chamber designated by the subscripts $bm,i,1$ and $bm,i,2$.

These systems are assumed to exist within each chamber, but their locations or distributions are not prescribed by the model.

The conditions within each of the systems are controlled by the following rate processes:

1. Liquid fuel injection, $\dot{m}_{f\ell}$.
2. Fuel vaporization, $\dot{m}_{fg,1}$ and $\dot{m}_{fg,2}$.
3. Fuel burning, $\dot{m}_{fb,1}$ and $\dot{m}_{fb,2}$.
4. Burned mixture dilution, $\dot{m}_{abm,i,1}$ and $\dot{m}_{abm,i,2}$.
5. Heat transfer, $\dot{Q}_1$ and $\dot{Q}_2$.
6. Nitrogen oxide formation, $\dot{r}_{bm,i,1}$ and $\dot{r}_{bm,i,2}$.
7. Interchamber mass flow, $\dot{m}_{12}$ and $\dot{m}_{21}$.

As in the case of the direct-injection engine, the interaction of these rate processes in determining system properties is described in terms of a five-phase cycle which is similar in each chamber, and in which the phases are defined by certain crank positions, as indicated in Figure 4:

1. Valve closure, θ_{vc} .
2. Start of fuel injection, θ_{in}.
3. Ignition, θ_{ig} .
4. Start of final burning, θ_{fb}.
5. End of combustion, θ_{eb} .
6. Valve opening, θ_{vo}.

The phases in the cycle are described as follows.

1. Initial Compression ($\theta_{vc} \leq \theta \leq \theta_{in}$). Only air is present in each chamber, and in general mass flows from the main chamber to the precombustion chamber.
2. Ignition Delay ($\theta_{in} \leq \theta \leq \theta_{ig}$). Physically, liquid fuel is injected into the precombustion chamber or, in some cases, into both chambers, and begins to vaporize and mix with the air to form a mixture of varying fuel-air ratio in both chambers. In the model, consideration of this mixing process is deferred until the next phase, so that in general three systems (m_a, $m_{f\ell}$, m_{fg}) are present in each chamber, and mass flows from the main chamber to the precombustion chamber.
3. Initial Burning ($\theta_{ig} \leq \theta \leq \theta_{fb}$). Physically, ignition occurs during this phase and burning occurs via flame

propagation through all elements of combustible mixture, resulting in combustion over a wide range of fuel-air ratios, until all of the vaporized fuel accumulated during the ignition delay phase has been burned. In the model, an elemental quantity of fuel vapor is assumed to mix with an appropriate amount of air to burn instantaneously at a specified fuel-air ratio during each crank angle increment. The specification of the fuel-air ratio at which burning occurs, as a function of crank angle, simulates the quality of fuel-air mixing achieved during the ignition delay phase. Subsequent to the formation of each element of burned mixture, it is diluted by mixing with remaining excess air. In general, then, there are three $+i$ systems (m_a, m_{fl}, m_{fg}, $m_{bm,i}$) present in each chamber during this phase, where i is the number of crank-angle increments taken. It is assumed that ignition in the main chamber occurs later than in the precombustion chamber, and hence, in general, some mass of the burned mixture in the precombustion chamber flows into the main chamber.

4. Final Burning ($\theta_{fb} \leq \theta \leq \theta_{eb}$). During this phase, it is assumed that burning is diffusion controlled, and hence, that combustion occurs at a constant fuel-air ratio near stoichiometric. Thus, in the model, there are two $+i$ systems (m_a, m_{fl}, $m_{bm,i}$) present in each chamber, and mass flows from the precombustion chamber to the main chamber.
5. Final Expansion ($\theta_{eb} \leq \theta \leq \theta_{no}$). Burning of fuel is complete in this phase, and the only significant process occurring is the further dilution of the burned mixture systems with excess air. One $+i$ systems (m_a, $m_{bm,i}$) are present in each chamber, and flow continues from the precombustion chamber to the main chamber.

As in the case of the direct-injection engine, the temperature and composition of each burned-mixture system are assumed to be the thermodynamic equilibrium values corresponding to the known pressure and elemental composition, except for concentrations of NO-related species. Thus, in general, the properties of any system are completely determined from the

pressure (P), the fuel mass fraction (F), the NO mass fraction ($[NO]$), and the temperature (T) or the internal energy (ε) or the enthalpy (h).

Rate Processes

Various rate processes, involving transport and convective phenomena identified previously, must be formulated in terms of the model variables.

Fuel Injection Rate

It is assumed that the total fuel injection rate into the cylinder, $\dot{m}_{f\ell}$, is prescribed as a function or crank angle, in units of mass per unit crank angle. It is further assumed that a specified fraction of this fuel, $K_{f\ell}(\theta)$, is injected into the main chamber while the remainder is injected into the precombustion chamber. Hence,

$$\dot{m}_{f\ell,1} = (1 - K_{f\ell})\,\dot{m}_{f\ell} \tag{1}$$

$$\dot{m}_{f\ell,2} = K_{f\ell}\,\dot{m}_{f\ell} \tag{2}$$

where the subscripts 1 and 2 refer to the precombustion chamber and main chamber, respectively.

Fuel Vaporization Rate

The fuel vaporization rate in each chamber, which physically includes all processes necessary to form the combustible mixture elements, is assumed to be analogous to that in the direct-injection engine. Hence, the vaporization rate is given by

$$\dot{m}_{fg,k}(\theta) = \int_{\theta_{in}}^{\theta} \left[\dot{m}_{f\ell,k}(\theta') - \dot{m}_{f\ell,k\ell}(\theta') + \dot{m}_{f\ell,\ell k}(\theta')\right] f_k(\theta',\theta)\,d\theta' \tag{3}$$

where

$$f_k(\theta',\theta) = \frac{\theta'-\theta}{C_{1,K}^2} \; \frac{\exp\left[-(\theta'-\theta)/C_{1,K}\right]}{1-\left[1+(\theta_{vo}-\theta')/C_{1,K}\right]\exp\left[-(\theta_{vo}-\theta')/C_{1,K}\right]} \tag{4}$$

$\dot{m}_{f\ell,k\ell}$ = liquid fuel flow from chamber k to chamber ℓ due to droplet entrainment (always non-negative)

$C_{1,K}$ = rate parameter specified as input

and the latter subscripts K and ℓ refer to either chamber with the understanding that $K \neq \ell$.

Ignition Delay

In the precombustion chamber, the same empirical correlation for ignition delay used with the DI engine model can be used, or the ignition delay can be specified as input data. It is assumed that ignition in the main chamber is further delayed by a specified time

$$\tau_{ig,2} = \tau_{ig,1} + \tau_{d,2}$$

Fuel Burning Rate

As in the direct-injection engine, fuel burning after ignition is assumed to occur at a rate exceeding the fuel vaporization rate until the fuel vaporized during the ignition delay period has been consumed. Hence, for chamber K.

$$\dot{m}_{fb,K} = \dot{m}_{fg,K} - \dot{m}_{fg,K\ell} + \dot{m}_{fg,\ell K} + \frac{4\, m^{o}_{fg,K}}{C^{2}_{2,K}} (\theta - \theta_{ig,K}) \qquad (5)$$

for $\theta < (\theta - \theta_{ig,K}) < \frac{C_{2,K}}{2}$, and

$$\dot{m}_{fb,K} = \dot{m}_{fg,K} - \dot{m}_{fg,K\ell} + \dot{m}_{fg,\ell K} + \frac{4\, m^{o}_{fg,K}}{C^{2}_{2,K}} (C_{2,K} + \theta_{ig,K} - \theta) \qquad (6)$$

for $\frac{C_{2,K}}{2} < (\theta - \theta_{ig,K}) < C_{2,K}$, and

$$\dot{m}_{fb,K} = \dot{m}_{fg,K} - \dot{m}_{fg,K\ell} + \dot{m}_{fg,\ell K} \qquad (7)$$

for $(\theta - \theta_{ig,K}) > C_{2,K}$, where

$C_{2,K}$ = crank-angle interval $\theta_{fb,K} - \theta_{ig,K}$ defining the initial burning period

$m^{o}_{fg,K}$ = mass of fuel vapor present in chamber K at $\theta = \theta_{ig,K}$

$\dot{m}_{fg,K\ell}$ = rate of fuel vapor flow from chamber K to chamber ℓ.

The mixing process of the air with the fuel vapor necessary to sustain these burning rates is described by means of a specification of the fuel mass fraction (F^{o}_{bm}) at which burning occurs. During the initial

burning period, $\theta_{ig,K} < \theta < (\theta_{ig,K} + C_{2,K})$, this specification is:

$$F^{\circ}_{bm,i,K} = F_{m,K} - \frac{i-1}{2}\Delta F_K \quad , \; i \text{ odd} \tag{8a}$$

$$F^{\circ}_{bm,i,K} = F_{m,K} + \frac{i}{2}\Delta F_K \quad , \; i \text{ even} \tag{8b}$$

where $F_{m,K}$ = specified mean mixture ratio at which burning occurs in chamber K

ΔF_K = specified increment in mixture ratio for each crank-angle interval

i = number of crank-angle increments after ignition (which is also equal to the number of burned mixture systems present) in chamber K.

As in the DI model, divergence limits, F_{mLn} and F_{max}, are imposed on the range of values which can be assigned to $F^{\circ}_{bm,i,K}$. After the initial burning period, it is assumed that burning occurs at constant mixture ratio:

$$F^{\circ}_{bm,i,K} = F_{m,K} \tag{8c}$$

The mixture ratio at burning ($F^{\circ}_{bm,i,K}$) is automatically increased by the model if, in either chamber, there is insufficient air to burn all fuel present at $F^{\circ}_{bm,i,K} = F_{m,K}$.

Burned Mixture Dilution Rate

In a manner which is again completely analogous to the treatment of the direct-injection engine, it is assumed that mixing of air with the burned mixture systems is proportional to the amount of air present:

$$\left(\frac{dm}{d\theta}\right)_{a,K} = C_{3,K}\left[\frac{1}{m_{a,K}} + \frac{1}{\sum_i \left(m_{fbm,i,K}/F_{bm,i,K}\right)}\right]^{-1} \tag{9}$$

where $C_{3,K}$ is a mixing-rate parameter which should be specified as a function of engine design variables and operating conditions. It is assumed that this dilution is proportioned according to the mass of individual burned mixture systems:

$$\left(\frac{dm}{d\theta}\right)_{abm,i,K} = \frac{m_{fbm,i,K}/F_{bm,i,K}}{\sum_i \left(m_{fbm,i,K}/F_{bm,i,K}\right)}\left(\frac{dm}{d\theta}\right)_{a,K} \tag{10}$$

Heat Transfer Rate

The energy transfer to the walls is expressed as.

$$\dot{Q}_K = C_{4,K} A_K (T_{h,K} - T_{w,K}) \tag{11}$$

Where A_K is the surface area of the chamber:

$A_1 = A_1$ (specified)

$A_2 = \frac{\pi B^2}{2} + \frac{4V_2}{B}$

and

$T_{h,K}$ = mean temperature of the fluid in chamber K (spatial mean)

$T_{w,K}$ = mean wall temperature of chamber K (constant)

$C_{4,K}$ = average heat transfer coefficient in chamber K (constant).

Nitrogen Oxide Reaction Rate

The NO reaction rate in either chamber is expressed in a manner identical to that for the direct-injection engine:

$$\dot{r}_{bm,i,K} = \frac{2M_{NO}}{6N\rho_{bm,i,K}} (1-\alpha^2_{bm,i,K}) \left(\frac{R_{1,bm,i,K}}{1+\alpha K_{1,bm,i,K}} + \frac{R_{6,bm,i,K}}{1+\alpha K_{2,bm,i,K}} \right) \tag{12}$$

where $\dot{r}_{bm,i,K}$ = NO formation rate (per unit crank angle) in burned mixture system i, chamber K

$\rho_{bm,i,K}$ = fluid density

$\alpha_{bm,i,K}$ = ratio of NO mass fraction to equilibrium NO mass fraction

K_1, K_2, K_6 = reaction rate parameters

$R_1 = K_1 [N]_e [NO]_e$

$R_6 = K_6 [O]_e [N_2O]_e$

$[\ ]_e$ = equilibrium mole fraction.

Interchamber Mass Flow

The total interchamber flow is assumed to obey the usual orifice-type relationship, before ignition.

$$\dot{m}_{Kl} = \frac{P_K}{\sqrt{T_{h,K}}} A f(P_K/P_l), \quad P_K > P_l \tag{13a}$$

$$\dot{m}_{Kl} = 0, \quad P_K < P_l \tag{13b}$$

where $\dot{m}_{K\ell}$ = total mass flow from chamber K to chamber ℓ (always non-negative)

and

$$f\left(P_K/P_\ell\right) = 2.2\left(1-\exp\left[-\tfrac{1}{2}\sqrt{\tfrac{P_K-P_\ell}{P_\ell}}\right]\right), \quad \frac{P_K}{P_\ell} < 1.3 \qquad (14a)$$

$$f\left(P_K/P_\ell\right) = 0.53, \quad \frac{P_K}{P_\ell} \geq 1.3 \qquad (14b)$$

Equation 14 is an approximate relationship which gives accurate results up to pressure ratios of approximately 1.2, but less accurate results for pressure ratios between 1.2 and 1.3. It is also assumed that after ignition in the precombustion chamber, the flow is always from this chamber to the main chamber ($\dot{m}_{21} = 0$).

The composition of the interchamber flow is in general, assumed to be identical to that in the chamber of origin, with the exception that after ignition in the precombustion chamber, it is assumed that only burned mixture flows from this chamber to the main chamber.* Thus, the constituent flows are given by:

$$\dot{m}_{a,K\ell} = \left(m_{a,K}/m_K\right)\dot{m}_{K\ell} \qquad (15)$$

$$\dot{m}_{f\ell,K\ell} = \left(m_{f\ell,K}/m_K\right)\dot{m}_{K\ell} \qquad (16)$$

$$\dot{m}_{fg,K\ell} = \left(m_{fg,K}/m_K\right)\dot{m}_{K\ell} \qquad (17)$$

$$\dot{m}_{bm,i,K\ell} = \left(m_{fbm,i,K}/m_K F_{bm,i,K}\right)\dot{m}_{K\ell} \qquad (18)$$

$$\dot{m}_{fbm,i,K\ell} = F_{bm,i,K}\,\dot{m}_{bm,i,K\ell} \qquad (19)$$

for $K=1$, $\theta_{VC} \leq \theta \leq \theta_{ig,1}$ and for $K=2$, $\theta_{VC} \leq \theta \leq \theta_{VO}$, where

$$m_K = m_{a,K} + m_{f\ell,K} + m_{fg,K} + \sum_i \left(m_{fbm,i,K}/F_{bm,i,K}\right)$$

After ignition in the precombustion chamber, constituent flows from this chamber are:

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* Interchamber port is considered to act as an ignition source, or "flame-holder" so that any fuel in the flow burns during passage.

$$\dot{m}_{a,12} = \dot{m}_{fl,12} = \dot{m}_{fg,12} = 0 \tag{20}$$

$$\dot{m}_{bm,i,12} = \left[\left(m_{fbm,i}\right) / F_{bm,i,1}\right) \Big/ \sum_{i} \left(m_{fbm,i,1} / F_{bm,i,1}\right)\right] \dot{m}_{kl} \tag{21}$$

$$\dot{m}_{fbm,i,12} = F_{bm,i,1}\, \dot{m}_{bm,i,12} \tag{22}$$

Governing Equations

The governing equations for the properties of the fluid systems are the conservation of mass (air and fuel), conservation of species (NO), conservation of energy, and thermal and caloric equations of state. Consistent with the approach employed for the direct-injection engine, appropriate forms of the conservation relations for the over-all mixture in each chamber will be used to determine the pressures, while the conservation relations for each system will be used to determine the system properties in terms of the mass of the air systems, the mass of fuel in the other systems, the fuel mass fraction in the burned mixture systems ($F_{bm,i}$), the internal energy of all systems, and the NO mass fraction of all systems. Mathematical relationships describing the various rate processes complete the model formulation.

Over-All Relationships

For the purposes of determining chamber pressures, it is assumed that the mixture within each chamber is homogeneous and in thermodynamic equilibrium. These assumptions exclude the presence of unburned fuel, and the relevant relationships are as follows (in all of the following, as before, the subscripts 1 and 2 refer to the precombustion chamber and the main chamber, respectively, for convenience, the subscripts k and l are often used to represent these numerical subscripts with the understanding that k and l may both take the value of either 1 or 2 , except that when they appear in the same equation, $k \neq l$):

Conservation of mass.

$$m_{h,K} = m_{a,K} + \sum_i \frac{m_{fbm,i,K}}{F_{bm,i,K}} \tag{23}$$

Conservation of energy (before ignition):

$$\frac{d}{d\theta}(m_{h,K}\,\varepsilon_{h,K}) = \dot{m}_{a,\ell K}\,h_{a,\ell} - \dot{m}_{a,K\ell}\,h_{a,K} - \kappa_K P_K \dot{V}_K - \dot{Q}_K \tag{24}$$

Conservation of energy (after ignition).

$$\frac{d}{d\theta}(m_{h,K}\,\varepsilon_{h,K}) = \dot{m}_{\ell K}\,h_{h,\ell} - \dot{m}_{K\ell}\,h_{h,K} - \kappa_K P_K \dot{V}_K - \dot{Q}_K \tag{25}$$

Equation of state:

$$P_K V_K = m_{h,K}\, R_{h,K}\, T_{h,K} \tag{26}$$

$$R_{h,K} = R_{h,K}(T_{h,K}, F_{h,K}) \tag{27}$$

Caloric equations of state:

$$\varepsilon_{h,K} = \varepsilon_{h,K}(T_{h,K}, F_{h,K}, P_K) \tag{28}$$

$$h_{h,K} = h_{h,K}(T_{h,K}, F_{h,K}, P_K) \tag{29}$$

where h = subscript referring to properties of homogeneous mixture

$F_{h,K}$ = mass fraction of burned fuel = $\left(\sum_i m_{fbm,i,K}\right) / m_{h,K}$

m = mass

$\dot{m}_{K\ell}$ = rate of mass transfer from chamber K to chamber ℓ per unit crank angle (always non-negative)

κ = polytropic index

$\dot{V}$ = rate of change of chamber volume per unit crank angle ($\dot{V} = 0$ for precombustion chamber)

$\dot{Q}$ = rate of energy transfer to chamber walls per unit crank angle

R = gas constant.

Conservation of System Mass

Conservation of liquid fuel can be written:

$$m_{fl,K}(\theta) = \int_{\theta_{vc}}^{\theta} (\dot{m}_{fl,K} - \dot{m}_{fg,K} - \dot{m}_{fl,Kl} + \dot{m}_{fl,lK})\, d\theta \tag{30}$$

The conservation of vapor fuel is:

$$m_{fg,K}(\theta) = \int_{\theta_{vc}}^{\theta} (\dot{m}_{fg,K} - \dot{m}_{fb,K} - \dot{m}_{fg,Kl} + \dot{m}_{fg,lK}).d\theta \tag{31}$$

where $\dot{m}_{fb,K}$ = rate of fuel burning in chamber K

$\dot{m}_{fg,Kl}$ = rate of vapor fuel transfer from chamber K to chamber l .

The conservation of fuel in the burned mixture systems is, for all systems except those which form in the main chamber as a result of flow of burned mixture from the precombustion chamber.

$$m_{fbm,i,K}(\theta) = \int^{\Delta\theta_i} \dot{m}_{fb,K}\, d\theta - \int_{\theta_i+\Delta\theta_i}^{\theta} \dot{m}_{fbm,i,Kl}\, d\theta \tag{32a}$$

where $\Delta\theta_i$ is the crank-angle interval during which the ith system is formed and θ_i is the crank angle at the beginning of this interval. It should be noted that $\dot{m}_{fbm,i,21} = 0$. For the burned mixture systems formed in the main chamber as a result of flow of burned mixture from the precombustion chamber, the conservation of fuel can be written as.

$$\tilde{m}_{fbm,i,2}(\theta) = \sum_i \int^{\Delta\theta_i} \dot{m}_{fbm,i,12}\, d\theta \tag{32b}$$

The conservation of air in the air system can be written as:

$$m_{a,K}(\theta) = m^{\circ}_{a,K} + \int_{\theta_{vc}}^{\theta} \left(\frac{Dm}{D\theta}\right)_{a,K} d\theta - \int_{\theta_{vc}}^{\theta} \dot{m}_{a,Kl}\, d\theta + \int_{\theta_{vc}}^{\theta} \dot{m}_{a,lK}\, d\theta \tag{33}$$

where

$$\left(\frac{Dm}{D\theta}\right)_{a,K} = -\int_{\theta_{vc}}^{\theta} \left(\frac{dm}{d\theta}\right)_{a,K} d\theta - \int_{\theta_{ig,K}}^{\theta} \frac{1 - F^{\circ}_{bm,K}}{F^{\circ}_{bm,K}}\, \dot{m}_{fb,K}\, d\theta$$

where $F^{\circ}_{bm,K}$ is the mixture ratio at which burning occurs in chamber K .

The conservation of air in the burned mixture systems can be expressed in terms of fuel mass fraction as:

$$F_{bm,i,K}(\theta) = F^{o}_{bm,i,K}(\theta_i) + \int_{\theta_i}^{\theta} \frac{F^{2}_{bm,i,K}}{m_{fbm,i,K}} \left(\frac{dm}{d\theta}\right)_{abm,i,K} d\theta \qquad (34)$$

where θ_i is the crank-angle position defining the formation of the ith burned system. $F^{o}_{bm,i,K}$ is given by Equations 8a through 8c for all burned systems except those which form in the main chamber due to flow of burned mixture from the prechamber. For these systems the composition of the burned mixture is assumed to be a mass-weighted average of the burned mixture systems existing in the prechamber.

$$\tilde{F}^{o}_{bm,i,2}(\theta) = \frac{\sum_i \int^{\Delta\theta_i} \dot{m}_{fbm,i,12}\, d\theta}{\sum_i \int^{\Delta\theta_i} (\dot{m}_{fbm,i,12}/F_{bm,i,1})\, d\theta} \qquad (35)$$

Conservation of System Energy

The energy conservation relations for the air system can be written as.

$$\frac{d}{d\theta}(m_{a,K}\,\varepsilon_{a,K}) = -\varepsilon_{a,K}\left(\frac{Dm}{D\theta}\right)_{a,K} - \dot{m}_{a,K\ell}\,\varepsilon_{a,K} + \dot{m}_{a,\ell K}\,\varepsilon_{a,\ell} + \nu_{a,K}\left(\frac{V_{ap,K}\,\dot{P}_K}{n_K\,P_K} - \dot{Q}_K\right) \qquad (36)$$

For the liquid fuel system.

$$\frac{d}{d\theta}(m_{f\ell,K}\,\varepsilon_{f\ell,K}) = h_{f\ell}\,(\dot{m}_{f\ell,K} - \dot{m}_{fg,K} - \dot{m}_{f\ell,K\ell} + \dot{m}_{f\ell,\ell K}) \qquad (37)$$

For the vapor fuel system.

$$\frac{d}{d\theta}(m_{fg,K}\,\varepsilon_{fg,K}) = h_{f\ell}\,\dot{m}_{fg,K} - \varepsilon_{fg,K}\,\dot{m}_{fb,K} - \dot{m}_{fg,K\ell}\,\varepsilon_{fg,K} + \dot{m}_{fg,\ell K}\,\varepsilon_{fg,\ell} + \nu_{fg,K}\left(\frac{V_{ap,K}\,\dot{P}_K}{n_K\,P_K} - \dot{Q}_K\right) \qquad (38)$$

For already formed burned mixture systems

$$\frac{d}{d\theta}\left(\frac{m_{fbm,i,K}\,\varepsilon_{bm,i,K}}{F_{bm,i,K}}\right) = \varepsilon_{a,K}\left(\frac{dm}{d\theta}\right)_{abm,i,K} - \varepsilon_{bm,i,K}\,\frac{\dot{m}_{fbm,K}\,\ell}{F_{bm,i,K}} + \nu_{bm,i,K}\left(\frac{V_{ap,K}\,\dot{P}_K}{n_K\,P_K} - \dot{Q}_K\right) \tag{39a}$$

For burned mixtures forming as a result of combustion.

$$\frac{d}{d\theta}\left(\frac{m_{fbm,i,K}\,\varepsilon_{bm,i,K}}{F_{bm,i,K}}\right) = \varepsilon_{fg,K}\,\dot{m}_{fb,K} + \varepsilon_{a,K}\,\frac{1-F^{o}_{bm,K}}{F^{o}_{bm,K}}\,\dot{m}_{fb,K} - \left(\kappa_K P_K \dot{V}_K + \frac{V_{ap,K}\,\dot{P}_K}{n_K P_K}\right) \tag{39b}$$

For burned mixtures forming in the main chamber as a result of flow from the precombustion chamber.

$$\frac{d}{d\theta}\left(\frac{m_{fbm,i,2}\,\varepsilon_{bm,i,2}}{F_{bm,i,2}}\right) = \sum_i \frac{\dot{m}_{fbm,i,12}}{F_{bm,i,1}}\,\varepsilon_{bm,i,1} \tag{39c}$$

where the "ν's" determine the distribution of energy transfer to each system by compression or expansion work and heat transfer:

$$\nu_{a,K} = m_{a,K}\,R_{a,K}\,T_{a,K} \,/\, V_{ap,K} \tag{40}$$

$$\nu_{fg,K} = m_{fg,K}\,R_{fg,K}\,T_{fg,K} \,/\, V_{ap,K} \tag{41}$$

$$\nu_{bm,i,K} = m_{fbm,i,K}\,R_{bm,i,K}\,T_{bm,i,K} \,/\, F_{bm,i,K}\,V_{ap,K} \tag{42}$$

where

$$V_{ap,K} = m_{a,K}R_{a,K}T_{a,K} + m_{fg,K}R_{fg,K}T_{fg,K} + \sum_i\left(m_{fbm,i,K}R_{bm,i,K}T_{bm,i,K}/F_{bm,i,K}\right)$$

$$n_K = 1 + \kappa_K\,(\gamma-1) \qquad = \text{polytropic exponent} \tag{43}$$

The energy transfer distribution assumed here is, in physical terms, equivalent to assuming that all nonreacting systems expand or contract polytropically, with the volume available for the reacting system being equal to the remaining chamber volume plus the initial volume of the reactants. While this is not a completely accurate distribution of energy transfer, it incorporates the essential processes.

Equations of State

Each system is assumed to behave as a semiperfect gas, and hence, the caloric equations of state are:

$$\varepsilon_{a,K},\ h_{a,K} = f(P_K, T_{a,K}) \tag{44a,b}$$

$$\varepsilon_{fl,K},\ h_{fl,K} = f(P_K, T_{fl,K}) \tag{45a,b}$$

$$\varepsilon_{fg,K},\ h_{fg,K} = f(P_K, T_{fg,K}) \tag{46a,b}$$

$$\varepsilon_{bm,i,K},\ h_{bm,i,K} = f(P_K, T_{bm,i,K}, F_{bm,i,K}) \tag{47a,b}$$

The form of these equations is given at the end of the description of the DI engine model.

NO Conservation

It is assumed that the NO reactions do not proceed in the air system, so that $[NO]_{a,K}$ is constant, and hence, the only relevant NO-conservation relations are those for the burned mixture systems.

$$\frac{d[NO]_{bm,i,K}}{d\theta} = \frac{1}{6N}\left[\dot{r}_{bm,i,K} + \frac{[NO]_{a,K}}{F_{bm,i,K}}\left(\frac{d F_{bm,i,K}}{d\theta}\right)\right] \tag{48}$$

where N is the engine speed in rpm. For the burned mixture systems which are formed in the main chamber as a result of flow from the precombustion chamber, the initial NO mass fraction is given by:

$$[\tilde{NO}]_{bm,i,2} = \frac{\tilde{F}^{\,o}_{bm,i,2}}{m_{fbm,i,2}} \sum_i \int^{\Delta\theta_i} \frac{\dot{m}_{fbm,i,12}}{F_{bm,i,1}} [NO]_{bm,i,1} \tag{49}$$

Model Summary

In its most general form, the model proposed here treats the fluid within cylinder as composed of distinct systems within each chamber, and results in general in the determination of the pressure, the thermodynamic variables ε, T, h, and m for each system present, and the mixture ratio F and NO concentration for each burned mixture system present. In addition,

the total fluid within each chamber is described in terms of average quantities (ε_h, h_h, T_h, m_h). Thus, in general, the system of equations described above results in $5 + 4i + 2i_{bm}$ unknowns for each chamber, where i is the total number of systems present and i_{bm} is the total number of burned mixture systems present. The basic system of equations containing these unknown quantities are, for each chamber.

1. The five over-all relations (Equations 23, 24 or 25, 26, 28, 29).
2. The four conservation and state relations for the air system (Equations 33, 36, 46a, 46b).
3. The four conservation and state relations for the liquid fuel (Equations 30, 37, 45a, 45b).
4. The four conservation and state relations for the vapor fuel (Equations 31, 38, 46a, 46b).
5. The six conservation and state relations for each burned mixture system (Equations 32a or 32b, 34 or 35, 39a or 39b or 39c, 47a, 47b, 48).

Specification of appropriate initial conditions and the use of the previously defined rate processes complete the model formulation. Of the rate processes, those governing the interchamber mass flow (Equations 13 through 22) deserve special mention, since they represent the only coupling between the two chambers.

Analysis Procedure

The technique for solving the model equations is essentially a stepwise procedure for successive increments $\Delta\theta$ in crank-angle position from θ_{vc} to θ_{vo}. For any interval, in which the initial conditions are always known, the procedure is as follows.

1. Interchamber Mass Flow Calculation. The interchamber mass flows are calculated for the interval from Equations 13 through 22.
2. Pressure Calculation. Chamber pressures are determined from Equations 23 through 29.
3. Fuel Distribution Calculation. The mass of fuel in each system is determined from Equations 30 through 32.

4. Fuel Mass Fraction Calculation. The fuel mass fraction in each burned mixture system is determined from Equation 34.
5. Air System Mass Calculation. The mass of the air system is determined from Equation 33.
6. Internal Energy Calculation. The internal energy of each system is determined from Equations 36 through 39.
7. Thermodynamic Property Calculation. The thermodynamic properties T and h for each system are determined from Equations 44 through 47.
8. NO Concentration Calculation. The NO concentration in each burned mixture system is determined from Equation 48.
9. NO Emission Rate Calculation. The total NO emission rate is determined by summing the masses of NO in all of the burned mixture systems and the air system.

ENGINE DESIGN-PERFORMANCE-EMISSION CORRELATIONS

Methodology

Parametric analyses of NO emissions rates from diesel engines were conducted using the direct-injection (DI) and indirect-injection (IDI) engine models. The objectives of the parametric analyses were twofold:

1. The relative importance of different combustion processes in the production of NO were evaluated. This evaluation was accomplished by "model sensitivity" analyses wherein model parameters, representing processes such as fuel vaporization and mixing, were varied parametrically. Correlations between these model parameters and NO emission rate developed in this manner indicate the combustion processes which must be modeled most accurately.
2. Relationships between engine design variables and NO emission rate also were evaluated. This evaluation was accomplished by "design sensitivity" analyses wherein engine design parameters were varied parametrically. Design-emission correlations resulting from these analyses will be used in the formulation of design criteria for minimizing NO emissions. These analyses were conducted by using sets of input data describing "reference engines". Individual parameters were varied to determine the sensitivity of the predicted engine performance and NO concentration to each input variable.

Direct-Injection Engine

Reference Engine Description

Two reference engines were used with the DI engine model. The reference engines are identical except for their chamber wall heat transfer characteristics. The reference engine data sets are listed in Table 1. The values of the model parameters used are, as far as possible,

based upon experimental evidence relevant to the combustion processes occurring in the cylinder. The heat transfer coefficient (C_4) is based on engine heat transfer data (Ref 8), and the mean fuel fraction (F_m) is assigned a stoichiometric value in accordance with observations that combustion rates in diffusion flames are greatest in regions where stoichiometric mixtures exist. The minimum and maximum fuel fractions (F_{min} and F_{max}) correspond approximately to flammability limits for diesel engine fuels. The values of other model parameters, however, are estimates based upon phenomenological descriptions of diesel combustion (Refs 1 and 4).

The values of the design parameters used correspond to an engine for which emission data are available (Engine E, Ref 9). This engine is an eight-cylinder automotive direct-injection engine with a design power output of 200 bhp and 3200 rpm. An inlet manifold pressure of 0.9 atm was selected to represent a volumetric efficiency of 90 per cent. Valve timing and inlet manifold flow losses were represented in this manner since their principal effects are to reduce the mass of the air charge.

Reference Engine Performance

The predicted performance parameters for the reference direct-injection engines operating at their design point (3200 rpm) are as follows:

Performance Parameter	Predicted Value	
	Engine A	Engine B
IMEP (psi)	139	107
IHP	323	247
ISFC	0.249	0.325
Exhaust NO Concentration (ppm)	1750	2210
Specific NO Emission Rate (gr/IHP-hr)	5.89	9.73

The predicted exhaust NO concentrations of 1750 and 2210 ppm are reasonably consistent with reported values of 1300 ppm and 5.20 gr/BHP-hr for approximately the same operating condition (186 bhp at 3000 rpm, Ref 9).

The mean chamber pressure, temperature, and NO concentration, as predicted by the model, are shown in Figure 6 for the two engines.

In the analysis leading to these performance predictions, 51 burned mixture systems were formed during the combustion cycle. The properties of the over-all air charge and five of the burned mixture systems for Engine A are shown in Figure 7. The initial characteristics of the five burned mixture systems described in the figure are as follows:

Burned Mixture System Number	θ at Formation (DCA)	Initial Fuel Fraction (F/F_S)
1	2.05	1.0
3	3.32	0.843
4	3.87	1.31
18	11.14	1.0
40	30.4	1.0

The first three systems were formed during the initial burning period. The first was formed with a stoichiometric fuel fraction, and the second and third were lean and rich, respectively. The last two systems were formed during the final burning period when combustion is assumed to occur in diffusion flames at stoichiometric fuel concentrations.

These results for the DI reference engines reveal a number of significant features of the DI engine model and the NO formation process. It appears that the model predicts engine performance parameters and NO emission rates quite well. The pressure-time curves shown in Figure 6 match closely the characteristics which are observed in actual engines. The power, fuel consumption, and emission parameters listed above are consistent with the values of these quantities reported for the engine. No attempt has been made to adjust the model to achieve better agreement between measured and predicted values of performance parameters. Better agreement could be obtained by varying several different parameters, and there is no basis at this time for choosing one over another. The agreement achieved by the model in its "uncalibrated" form was considered sufficient for the purposes of this program.

With regard to NO formation, the most striking observation from the results with the DI reference engines is that nearly all NO is formed during a small fraction of the total combustion cycle. NO formation occurs primarily during the early stages of the final burning phase. Very little NO is formed during its initial burning period. The NO concentrations

in a few burned mixture systems do reach high levels as seen in system 4 in Figure 7. However, this behavior is limited to those systems which burn at fuel fractions slightly richer than stoichiometric. The over-all NO formation rate increases abruptly when fuel begins to burn in diffusion flames at stoichiometric mixture ratios during the final burning phase. The high NO formation rate continues for about 30 degrees of crank angle after which the rate slows due to reduced chamber temperatures.

The concentrations of NO formed in the burned mixture systems vary widely. NO is formed rapidly in each system while its temperature is high. As observed in Figure 7, when the temperature of a system falls below about 4500 deg R, the NO formation rate effectively becomes zero. The factors which appear to affect the final NO concentration in each system most strongly are:

1. Initial fuel fraction at burning.
2. Time (crank angle) at burning.
3. Heat transfer rate.
4. Rate of dilution with excess air.

These factors determine the temperature history of the system and, in particular, the length of time the system temperature is in the regime where NO formation proceeds at significant rates.

Model Parameter Sensitivity

To determine the sensitivity of predicted engine performance to the evaluation of model parameters; a series of analyses were conducted using the data for reference DI Engine A in Table I. Each of the first six model parameters was varied individually about its reference value, and the performance predictions obtained are shown in Figure 8. The power output (IHP) and efficiency (ISFC) of the engine are found to be insensitive to these parameters except for weak effects of the fuel vaporization rate parameter (C_1) and the heat transfer coefficient (C_4). Reducing the fuel vaporization rate (increasing C_1) reduces power and efficiency by delaying heat release, and increasing the heat transfer rate increases the energy lost to the cooling system.

The exhaust NO concentration, on the other hand, is observed to be very sensitive to all model parameters except the dilution rate

parameter (C_3). All of these sensitivities can be explained in terms of the characteristics of the model.

Increasing the fuel vaporization rate parameter (C_1), the fuel burning rate parameter (C_2), or the fuel fraction increment (ΔF) causes the NO concentration to decrease. The effect of C_1 is to prolong burning into later portions of the expansion stroke so that flame temperatures are lower. The effects of C_2 and ΔF are similar in that they both increase the portion of fuel burned late in the premixed burning period in lean or rich systems.

Increasing the heat transfer rate is seen to increase the NO concentration. This effect results from heating of the air charge during the compression stroke which increases the initial temperatures of the burned mixture systems. The magnitude of this effect also is dependent upon the assumed cylinder wall temperature. A more detailed analysis of the effects of heat transfer parameters was conducted and the results are shown in Figure 9. Changes in heat transfer rate and wall temperature produce large changes in NO concentration, even though the corresponding changes in peak temperature are small.

Finally, it is observed that varying the mean fuel fraction (F_m) in either direction from stoichiometric reduces the NO concentration strongly. This effect is due primarily to reduced flame temperatures.

Design Parameter Sensitivity

Sensitivities of engine performance to design parameters were determined in a manner similar to the model parameter sensitivity analysis. Six design parameters were varied independently about their reference values and the resulting variations in engine performance are shown in Figure 10. In this figure, NO emissions are indicated both as exhaust concentration and specific emission rate expressed in gr/IHP-hr.

An increase in clearance volume reduces power, efficiency, and NO concentration. The reduced NO is a result of lower flame temperatures, due to lower compression ratios and peak temperatures. The rate of NO emission increases, but the effect is small.

An increase in engine speed increases power output because of the increased frequency of power strokes, and reduces NO concentration because of reduced time available for NO formation. The rate of NO emission also decreases when expressed in gr/IHP-hr as in Figure 10.

Increasing inlet pressure increases power output and efficiency, and strongly reduces NO concentration. The decrease in NO concentration results from more rapid dilution and cooling of burned mixture systems. The rate of NO emission also is reduced as the inlet pressure is increased to 2 atm, but is increased with further increases in pressure. The increase in emission rate at higher inlet pressures results from higher peak temperatures due to the suppression of dissociation. This effect appears to outweigh the dilution rate effect at inlet pressures above 2 atm. It should be noted here that in this analysis inlet pressure alone was varied so that the effect is not fully representative of turbocharging where inlet temperature and heat transfer rate would vary also.

Changing the fuel injection time has the effect of changing the time of heat release in the cycle. When injection and heat release are delayed, the power output and efficiency are reduced, and the NO concentration and emission rate are reduced because of lower flame temperatures.

Changing the injection rate changes the time period over which fuel is injected. A low injection rate prolongs the heat release period leading to reduced power, efficiency, NO concentration, and emission rate. A high injection rate increases power and efficiency but reduces NO concentration and emission rate. The latter effect is a result of burning all or most of the fuel during the premixed burning period wherein many systems are burned at lean or rich fuel fractions and, hence, low flame temperatures. Increasing fuel injection rate increases pressure rise rate and peak pressure which also are important engine performance parameters. High pressure rise rates lead to engine "knock" and high peak pressures increase mechanical stresses. These performance characteristics are predicted by the engine model as shown in Figure 6.

The effect of reduced fuel rate (over-all fuel-air ratio) was analyzed by keeping the injection time and rate constant, but reducing the injection period (constant beginning-variable ending injection). Reducing the fuel rate in this manner has the effect of reducing power output, improving efficiency because of earlier burning, and reducing NO concentration and emission rate. The NO reduction results from elimination of the final burning portion of the combustion cycle wherein the highest NO concentrations are formed.

Some of these design parameter effects can be compared with experimental data, and the comparisons indicate generally that the effects predicted by the model are qualitatively realistic. The effect of clearance volume has been shown to have a mild effect on NO exhaust concentration (Ref 10) as predicted here. The predicted effects of injection time and over-all fuel-air ratio also are consistent with observed performance of similar engines (Ref 11).

Indirect-Injection Engine

Reference Engine Description

The reference engine data set used with the IDI model is listed in Table II. The values of the model parameters are, in most cases, the same as those used with the DI model reference engines. The values of the design parameters used correspond to an engine for which performance and emission data are available (Engine I, Ref 9). This engine is a six-cylinder automotive indirect-injection engine with a design power output of 270 bhp at 2200 rpm. Intake air is turbocharged to approximately 2 atms and aftercooled.

Reference Engine Performance

The predicted performance parameters for the reference indirect-injection engine, operating at its design point, are as follows:

Indicated Mean Effective Pressure (IMEP)	214 psi
Indicated Specific Fuel Consumption (ISFC)	0.295 lbm/IHP-hr
Indicated Horsepower (IHP)	378 hp
Exhaust NO Concentration	1275 ppm
Specific NO Emission Rate	5.46 gr/IHP-hr

The predicted exhaust NO concentration is higher than the reported value of 700 ppm and 3.48 gr/BHP-hr for this engine operating at its design point (279 ghp at 2200 rpm, Ref 9).

The properties of the air charge in the engine cylinder, as predicted by the model, are shown in Figure 11 for the compression and expansion strokes. Peak pressure, temperature, and NO concentration are

predicted to be higher in the prechamber than in the main chamber. The reversal in the prechamber NO concentration is due partly to dissociation of NO with decreasing temperature and partly to the efflux of burned mixture from the prechamber.

Model Parameter Sensitivity

The model parameter sensitivity analysis was conducted in the same manner as with the direct-injection engine model. Each model parameter for each chamber was varied about its reference value with all other parameters held constant, and the variations in predicted engine performance are shown in Figure 12. The engine performance parameters, ISFC and IHP, were found to be insensitive to all model parameters. This lack of sensitivity is more pronounced than with the direct-injection engine. Slight effects on performance are observed with variations in the fuel vaporization rate parameter and the heat transfer coefficient. The trends are similar to those with the DI engine.

The predicted exhaust NO concentration was found to be more sensitive to model variables than engine performance, but again less than with the DI engine. The NO concentration is seen to be rather insensitive to fuel vaporization rate parameter, the burning rate parameter, the heat transfer coefficient, and the fuel fraction increment. Increases in the dilution rate parameter in the main chamber, however, cause pronounced increases in the NO concentration. This effect is the result of incomplete fuel burning in the prechamber due to rich fuel mass fractions. When the burned mixture systems pass into the main chamber, they are diluted with air and their temperatures rise as the burning process is completed. With increased dilution rates, burning is completed earlier in the cycle leading to increased NO concentrations.

The dependence of engine performance and NO concentration on the mean fuel fraction at burning is shown in Figure 12 in tabular form. The mean fuel fraction is expressed as a fraction of the stoichiometric fuel fraction. The maximum NO concentration is predicted for the condition where combustion occurs initially at stoichiometric conditions ($F_m/F_{st} = 1.0$). Changes in the initial fuel fraction in either chamber cause a reduction in

NO concentration. This result is consistent with the results for the DI engine. In the IDI engine analysis, changes in F_m were evaluated in the rich direction in the prechamber and in the lean direction in the main chamber since these are the directions in which variations are most likely to occur.

Design Parameter Sensitivity

Sensitivities of engine performance, exhaust NO concentration, and specific NO emission rate were determined for eight engine design and operating parameters, and the results are shown in Figure 13. The first six parameters are the same ones which were investigated with the DI engine. The last two parameters-- prechamber volume and the fraction of fuel injected into the main chamber-- are specific to the indirect-injection engine.

The clearance volume was varied with the fraction occupied by the prechamber held constant at 30 per cent. As with the DI engine, an increase in clearance volume is accompanied by a degradation of engine performance and a slight reduction in NO concentration. As with the DI engine, the specific NO emission rate increases slightly with clearance volume.

Changes in engine speed are accompanied by changes in power output, as with the DI engine, but also by changes in ISFC. The exhaust NO concentration and the specific emission rate vary inversely with engine speed. All of these effects are observed to be mild.

Increases in inlet pressure are seen to improve performance, but the exhaust NO concentration passes through a minimum at about 2 atms pressure. The specific NO emission rate, which is dependent upon both pressure and exhaust concentration, is a minimum at a somewhat lower inlet pressure. The existence of a minimum emission rate is observed with both the DI and IDI engines, and occurs at inlet pressures above ambient.

The effects of fuel injection time and injection rate on engine performance and NO concentration appear to be small. This lack of sensitivity can be attributed to the influence of the divided chamber. The heat release rate is controlled partly by the flow of fuel from the prechamber so that the dependence upon injection parameters is reduced.

Somewhat greater sensitivity of NO emissions to fuel injection parameters has been observed in experimental tests (Ref 12).

The over-all fuel-air ratio was investigated by keeping the injection time and rate constant and reducing the injection duration (constant beginning-variable ending injection). The same procedure was used with the DI engine. As the fuel rate is reduced from the design point, the power output and ISFC decrease. The exhaust NO concentration increases to a maximum and then decreases. A maximum NO concentration such as that predicted here is actually observed with some indirect-injection engines (Ref 13). However, a maximum was not reported for the reference engine (Ref 9). Such a maximum can be attributed to near-stoichiometric fuel-air mixtures and high flame temperatures in the prechamber which will occur at intermediate engine power levels.

Variations in prechamber volume were investigated by keeping the total clearance volume constant and varying the fraction occupied by the prechamber. This variation is observed to have only mild effects on engine performance and NO concentration. Increasing the prechamber volume reduces performance and increases NO emission rate.

The fraction of fuel injected directly into the main chamber is defined to represent that portion of the fuel which passes directly through the interchamber port upon injection. This parameter was found to have a strong effect on NO concentration and lesser effects upon engine performance. Reducing this fraction appears to result in strong reductions in NO concentration, but at the expense of milder reductions in engine performance.

Summary of Results

The results of the parametric analyses which have been conducted indicate that exhaust NO concentrations and specific NO emissions rates in both direct- and indirect-injection engines are influenced by a number of combustion processes (represented in these models by model parameters) and a number of engine design parameters. Because of this interdependence of parameters, it has not been possible to calibrate either of the prediction techniques by means of existing performance and

emission data. To calibrate the models it will be necessary to conduct carefully controlled experiments wherein the engine design parameters are known and can be controlled. Further evaluation of certain combustion processes also will be necessary to evaluate those model parameters which influence NO emissions.

The performance and emission predictions appear to be in qualitative agreement with results reported for actual engines. Direct-injection engine NOx emissions are sensitive to fuel injection parameters-- injection time, injection rate, and over-all fuel-air ratio. Indirect-injection engines are less sensitive to fuel injection parameters. A general tendency of indirect-injection engines to produce lower NO emissions than direct-injection engines has been observed. However, the distribution of fuel between the chambers appears to be an important factor in this effect.

ENGINE DESIGN CRITERIA FOR NOx EMISSION CONTROL

Direct-Injection Engines

In the previous section, it was observed that NOx emissions from the DI engine are affected by various engine design parameters, particularly those related to fuel injection characteristics. Specifically, NOx exhaust concentrations and specific emission rates (gr/IHP-hr) can be reduced by the following variations in design parameters:

1. Delay injection time.
2. Increase injection rate.
3. Reduce engine power level (over-all fuel-air ratio).

These variations are, of course, accompanied by changes in engine performance parameters which include:

1. Specific fuel consumption (lb-fuel/HP-hr).
2. Specific power (HP/lb-engine).
3. Peak chamber pressure.
4. Pressure rise rate.

Design parameter variations may also affect the emission of pollutants other than nitrogen oxides.

Different combinations of design parameter variations will have different effects on engine performance. However, it is reasonable to assume that engines currently are designed to attain a near optimum combination of the performance parameters listed above. Any modification of design parameters is likely to move engine performance away from this optimum condition. Thus, NOx emission control attained through engine design modifications will result in a performance penalty.

The degree of NOx emission control attainable with DI engines appears to be dependent upon the amount of performance loss the engine designer can tolerate. However, by carefully combining different emission control approaches, it appears that significant reductions in specific NOx emission rate-- of the order of 50 per cent-- should be attainable with small losses in engine performance.

Of the three design parameter variations listed above, the most attractive is the increased injection rate since this variation also

improves specific fuel consumption. Delaying injection time increases specific fuel consumption and smoke emission (Ref 11). Reducing fuel-air ratio reduces specific engine power, but also reduces smoke and CO emissions. Thus, a logical approach to NOx emission control with DI engines might involve the following sequence of steps:

1. Increase injection rate to maximum degree possible within limits imposed by a peak pressure or pressure rise rate criterion.
2. Simultaneously retard injection timing and reduce over-all fuel-air ratio (or engine power rating). Combined variations of these two quantities should allow control of smoke emission to be maintained while NOx emission rate is reduced.

Indirect-Injection Engines

The use of indirect injection has been observed to reduce NOx emissions from the levels characteristic of DI engines. The results of this study indicate that this natural advantage of IDI engines can be accentuated by restricting the injection of fuel to the precombustion chamber. Changes in fuel injection rate and timing appear to have little effect on NOx emissions in contrast to the DI engine where these factors have the greatest influence. As mentioned earlier, the precombustion chamber appears to act as a fuel injection device. NOx emissions can be minimized by retaining the fuel in the prechamber until burning occurs, and then allowing the rich burned mixture to pass into the main chamber where further burning and dilution occur quickly. It seems likely that this approach could be exploited by modifications of fuel spray characteristics which reduce the quantity of fuel injected directly through the interchamber port and increase the fuel residence time in the precombustion chamber. This approach appears from Figure 13 to involve an increase in specific fuel consumption, and it is possible that other performance penalties would be incurred which are not evident from the theoretical results. However, the NOx emission reduction effectiveness of this approach appears to be high.

AUXILIARY METHODS OF NOx EMISSION CONTROL

Control Methods Considered

Auxiliary methods of reducing the rate of NO emission from diesel engines have been identified during this study and in investigations by other workers. One of the objectives of this study was to evaluate these approaches, as far as possible, using the emission prediction techniques which have been developed for direct and indirect-injection engines. The control approaches which have been identified are the following:

1. Turbocharging.
2. Staged fuel injection.
3. Water injection.
4. Exhaust gas recirculation.

Analyses of turbocharging and staged injection have been conducted. Water injection and exhaust gas recirculation have not been evaluated since they would require modifications to the models to account for the changes in properties of the initial air charge. With these modifications, it will be possible to investigate these control methods for both types of engines.

Evaluation Results

Turbocharging

The effect of turbocharging was investigated using the direct-injection engine model and a series of data sets representing different engines. These engines were as follows:

Engine B - Nonturbocharged reference engine. (Engine B in Table I).

Engine C - Same as Engine B with turbocharging to double the inlet pressure. Compressor efficiency assumed to be 82 per cent, and no aftercooling.

Engine D - Same as Engine C with aftercooling.

Engine E - A high MEP, low compression ratio engine. Displacement equal to Engine B. Turbocharged to approximately

6 atms with aftercooling, and compression ratio reduced to 10:1.

This series of engines represents the introduction of turbocharging without and with aftercooling, and the extension of the turbocharging concept to very high operating pressure engines. The engine parameters which were varied and the predicted performance for the engines are listed in Table III.

The predicted results indicate that a reduction in NO emission will not result directly from the use of conventional turbocharging. The exhaust NO concentration is reduced only slightly because the increase in inlet temperature offsets the effect of the reduction in fuel-air ratio. The rate of NO emission from the engine is predicted to increase substantially either with or without aftercooling. It is possible, however, that changes in fuel injection timing and ignition delay, associated with the use of turbocharging, could result in reduced NO emission rates. Fuel injection and ignition delay effects were not included in this analysis, but investigation of these effects would appear to be warranted.

The results for Engine E indicate that the use of high MEP engines with reduced compression ratios may lead to reduced NO emissions. However, the reduction does not appear to be large, and it is obtained at the expense of a severe increase in peak cylinder pressure. The favorable power and specific fuel consumption predicted by the model are not realistic because the pumping losses are not included.

Staged Fuel Injection

Modeling Techniques

The term "staged injection" is used to describe diesel engine fuel injection systems wherein fuel is introduced into the combustion chamber in two steps. Typically, a portion of the fuel is injected as in conventional engines, while another portion is introduced earlier in the combustion cycle. Three methods of early introduction of fuel have been developed (Ref 1):

1. Pilot injection - injection early in the compression stroke.
2. Vigom injection - injection into the residual gas at the end of the exhaust stroke.
3. Fumigation - injection or carburetion into the inlet air.

These methods of early fuel introduction were developed as methods for improving combustion performance or to allow operation with alternate fuels. Descriptions of engine performance resulting from these fuel introduction techniques are contained in References 14 through 17.

In this program, separate models were not required to represent combustion in diesel engines with staged fuel injection. The pilot injection approach was investigated with the existing direct-injection model by appropriate variation of the fuel injection schedule. The Vigom and fumigation approaches were represented by introducing minor changes in the existing DI model.

In both Vigom injection and fumigation, the fuel introduced early can be assumed to be completely vaporized and uniformly mixed with the air charge by the time the main fuel injection process begins. The fuel premixed in the air charge was represented in the DI model by introducing two new variables:

$F_{i,t}$ - The <u>true</u> fuel fraction of system i.

F_a - The fuel fraction of the air charge due to early introduction of fuel.

These variables are related to the fuel fraction F_i in the model as follows:

$$F_{i,t} = F_i (1 - F_a) + F_a$$

With no early introduction of fuel ($F_a = 0$), the fuel fraction F_i and the true fuel fraction $F_{i,t}$ are equal. If fuel is introduced early ($F_a > 0$), the fuel fraction F_i must be interpreted as the mass fraction of <u>injected</u> fuel.

The true fuel fraction $F_{i,t}$ must be utilized in determining the internal energy or enthalpy of a burned mass system, and in calculating the NO formation rate in a burned mass system. The injected fuel fraction F_i continues to serve in the conservation of injected fuel.

This approach to modeling staged injection is adequate as long as the fraction of fuel introduced early is small. The physical properties

of the air charge need not be modified to account for the effect of the premixed fuel.

Pilot Injection Results

Pilot injection was investigated in a series of direct-injection engines with variations in the quantity and timing of the early injected fuel. The engine parameters varied and the predicted performance are listed in Table IV. The reference engine is similar to the reference DI Engine B described in Table I, but with one model parameter changed as follows:

Fuel fraction increment = 0.005.

The other engines listed in Table IV are similar to the reference engine, but with pilot injection of a part of the fuel. Variations in pilot injection time, pilot injection fraction, and main fuel injection time were investigated. No significant changes in engine performance were predicted, and in all cases exhaust NO concentration was predicted to increase or remain unchanged.

In modeling pilot injection with the direct-injection engine model, it is being assumed implicitly that no fundamental differences in combustion processes result from pilot injection. Early injection of fuel results in an increase in the quantity of fuel vapor present at ignition, and a larger fraction of the fuel burned during the initial burning period. This fuel burns at rich and lean fuel fractions (in the model) because of the fuel burning model employed. The effect of pilot injection on ignition delay is not known precisely, but a reduced delay time would be expected. Therefore, a shorter ignition delay was assumed with all engines with pilot injection, and one variation in delay time (engine F) was examined to determine its effect. The net result of this investigation of pilot injection is that, within the constraints imposed by the use of the DI model, there is no indication of a reduction in NO emissions from the use of pilot injection.

Fumigation Results

The effects of fumigation (or Vigom injection) on performance and NO concentration were investigated in a series of engines with variations in the quantity of early-injected fuel and the injection time of the main charge. The results of this investigation are listed in Table V. The ignition time was varied since the effect of fumigation on ignition time was not incorporated in the model.

The reference engine is a direct-injection engine similar to that described in Table I and the same reference engine used to study pilot injection. With fumigation, the mean fuel fraction at burning (F_m), which now only represents injected fuel, was adjusted so that the total fuel fraction at burning was stoichiometric. Also, the total amount of fuel burned per cycle, including injected and fumigated fuel, was held constant.

With 20 per cent of the fuel introduced by fumigation, a large reduction in NO concentration is predicted with a modest penalty in engine performance. At higher fumigation rates, NO concentration is further reduced, but the predicted engine performance reductions are more severe. These results appear to represent an attractive approach to NO emission control. However, limited data available on the effects of fumigation (Ref 11) do not confirm the degree of NO emission reduction which is predicted. It appears that there is a strong possibility that the model does not represent the effects of fumigation accurately and that the effects on NO emission are exaggerated. Nevertheless, because of the predicted trend, which is qualitatively consistent with experimental results, it seems that fumigation deserves further investigation as a means for NO emission control.

Water Injection

The addition of water to the inlet air of diesel engines has been found to reduce NOx emissions (Ref 11), and similar results are observed with other combustion systems. With certain modifications, the engine models developed in this program can be used to evaluate the effectiveness of water injection as an emission control method. The

modifications of the models required to conduct this evaluation are as follows:

1. The thermodynamic properties of the air charge must be modified to represent a mixture of air and water vapor.
2. Equilibrium composition of burned mixtures must be calculated for combustion of fuel-air-water mixtures.
3. Caloric equations of state must be introduced for burned mixtures resulting from fuel-air-water combustion.

Other changes due to water injection, such as variations of inlet air conditions, can be represented by variations of model input data.

Exhaust Gas Recirculation

Exhaust gas recirculation also has been found to be effective in reducing NOx emissions from diesel engines (Ref 11). This effectiveness can be evaluated with the engine models developed in this program with modifications. The modifications required are as follows:

1. The thermodynamic properties of the air charge must be modified to represent a mixture of air and exhaust gas.
2. The exhaust gas concentration must be incorporated in the burned mixture composition calculation procedure.

Other modifications, such as changes in stoichiometric air-fuel ratios, can be made by varying model input data.

Effects of Control Methods on Other Emissions

Exhaust concentrations or emission rates of other pollutants of concern-- CO, hydrocarbons, and particulates-- are not predicted by the engine models. However, sufficient experimental data on these emissions exist to allow qualitative predictions to be made of the effects of the various control methods examined in this study. A comprehensive review of published data on diesel engine design-emission correlations has been prepared recently by Bascom, Broering, and Wulfhorst (Ref 11).

Observations of the effects of control methods on other emissions are as follows:

1. Turbocharging reduces exhaust particulates (smoke) and has no appreciable effect on CO or hydrocarbons.
2. Fumigation is found to increase CO and hydrocarbon emissions, particularly at intermediate power levels. Effects on particulate emissions depend upon the nature of the fuel, but fumigation with kerosene appears to increase smoke. Effects of pilot injection on emissions have not been reported.
3. Water injection does not appear to have significant effects on other emissions. However, the relevant data are limited.
4. Exhaust gas recirculation tends to increase CO and particulate emission because of the reduced availability of oxygen.

Summary of Effects

The effects of the various control methods on emissions are summarized qualitatively in Table VI. Certain of these methods can be combined to produce more effective emission control. A very attractive combination which is included in the table is exhaust gas recirculation with turbocharging and aftercooling (Ref 11).

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TABLES

TABLE I

REFERENCE ENGINE INPUT DATA USED WITH DIRECT-INJECTION ENGINE MODELS*

Model Parameters

Fuel Vaporization Rate Parameter (C_1)	10 DCA**
Fuel Burning Rate Parameter (C_2)	10 DCA
Dilution Rate Parameter (C_3)	0.05 DCA^{-1}
Heat Transfer Coefficient (C_4)	0.001 $\frac{lbf - ft}{ft^2 - deg\ R - DCA}$ (Engine A)
	0.010 $\frac{lbf - ft}{ft^2 - deg\ R - DCA}$ (Engine B)
Mean Fuel Fraction at Burning (F_m)	0.0636 (stoichiometric)
Fuel Fraction Increment (ΔF)	0.01
Minimum Fuel Fraction at Burning (F_{min})	0.0318
Maximum Fuel Fraction at Burning (F_{max})	0.0955
Ignition Delay (DCA)	15

Design Parameters

Cylinder Bore (B)	0.375 ft
Crank Length (R)	0.1875 ft
Compression Ratio	17:1
Clearance Volume (V_c)	0.00259 ft^3/cylinder
Inlet Manifold Pressure	1900 psfa
Inlet Air and Fuel Temperature	520 deg R
Average Wall Temperature	1200 deg R (Engine A)
	1000 deg R (Engine B)
Engine Speed	3200 rpm
Injection Time	15 DCA-BTC**
Fuel Injection Rate	5.23×10^{-6} $\frac{lbm}{DCA - cylinder}$
Mean Injection Rate	10.46×10^{-5} $\frac{lbm}{cycle - cylinder}$

* The same input data were used for both reference Engines A and B except where indicated.

** DCA = degrees crank angle; BTC = before top center.

TABLE II

REFERENCE ENGINE INPUT DATA USED WITH INDIRECT-INJECTION ENGINE MODEL

Model Parameters

	Prechamber	Main Chamber
Fuel Vaporization Rate Parameter (C_1)	10 DCA	5 DCA*
Fuel Burning Rate Parameter (C_2)	10 DCA	10 DCA
Dilution Rate Parameter (C_3)	0.05 DCA^{-1}	0.05 DCA^{-1}
Heat Transfer Coefficient (C_4)	0.01 $\frac{lbf - ft}{ft^2 - deg\ R - DCA}$	0.01 $\frac{lbf - ft}{ft^2 - deg\ R - DCA}$
Mean Fuel Fraction at Burning (F_m)	0.0636	0.0636
Fuel Fraction Increment (ΔF)	0.005	0.005
Minimum Fuel Fraction at Burning (F_{min})	0.0318	0.0318
Maximum Fuel Fraction at Burning (F_{max})	0.0955	0.0955
Ignition Delay (DCA)	11.5	14.0

Design Parameters

Cylinder Bore (B)	0.396 ft
Crank Length (R)	0.250 ft
Compression Ratio	12:1
Clearance Volume (V_C)	0.0056 ft^3/cylinder
Prechamber Volume (V_{PC})	0.00168 ft^3/cylinder
Inlet Manifold Pressure	4000 psfa
Inlet Air Temperature	580 deg R
Inlet Fuel Temperature	520 deg R
Average Wall Temperature (both chambers)	1000 deg R
Engine Speed	2200 rpm
Fraction of Fuel Injected to Main Chamber	0.25
Injection Time	14 DCA-BTC*
Fuel Injection Rate	1.4×10^{-5} $\frac{lbm}{DCA - cylinder}$
Mean Injection Rate	2.8×10^{-4} $\frac{lbm}{cycle - cylinder}$

* DCA = degrees crank angle; BTC = before top center.

TABLE III

PREDICTED EFFECTS OF TURBOCHARGING ON DIRECT-INJECTION ENGINE PERFORMANCE AND NO EMISSION

Parameter	Engine			
	B	C	D	E
Inlet Pressure (psia)	13.2	26.5	26.5	80.0
Inlet Temperature (deg R)	520	655	590	590
Compression Ratio	17	17	17	10
Peak Pressure (psia)	945	1360	1440	1930
ISFC (lbm/IHP-hr)	0.325	0.262	0.253	0.166
IMEP (psi)	107	132	138	210
IHP	247	306	317	486
Over-All f/a	0.0375	0.0218	0.0197	0.0062
Exhaust NO (ppm)	2213	2058	1803	619
NO Emission Rate (gr/IHP-hr)	9.73	11.47	10.52	7.49
Ignition Delay (DCA)	15.0	15.0	15.0	15.0

Note: Engine configuration same as DI reference Engine B (Table I).

TABLE IV

PREDICTED EFFECTS OF PILOT INJECTION ON DIRECT-INJECTION ENGINE PERFORMANCE AND NO EMISSION

Parameter	Engine					
	Ref*	F	G	H	I	J
Pilot Fuel Quantity (fraction of total)	0	0.3	0.3	0.3	0.4	0.3
Pilot Injection Time (DCA)	-	-35	-35	-55	-35	-35
Main Fuel Injection Time (DCA)	-15	-15	-15	-15	-15	-7
Ignition Time (DCA)	0	-5	-8	-8	-8	0
IHP	247	256	256	256	257	245
ISFC (lbm/IHP-hr)	0.325	0.315	0.314	0.315	0.312	0.325
Exhaust NO (ppm)	3227	3656	4507	4031	4000	3182
NO Emission Rate (gr/IHP-hr)	14.2	15.6	19.2	17.2	16.95	14.0

* Reference Engine B (Table I) with $\Delta F = 0.005$.

TABLE V

PREDICTED EFFECTS OF FUMIGATION ON DIRECT-INJECTION ENGINE PERFORMANCE AND NO EMISSION

Parameter	Engine				
	Ref*	K	L	M	N
Quantity of Fumigated Fuel (fraction of total)	0	0.2	0.2	0.4	0.4
Main Fuel Injection Time (DCA)	-15	-15	-15	-15	-7
Ignition Time (DCA)	0	-8	0	-8	0
IHP	247	206	206	163	154
ISFC (lbm/IHP-hr)	0.325	0.389	0.391	0.492	0.520
Exhaust NO (ppm)	3227	1003	603	214	105
NO Emission Rate (gr/IHP-hr)	14.2	5.29	3.19	1.43	0.74

* Reference Engine B (Table I) with $\Delta F = 0.005$.

TABLE VI

SUMMARY OF CONTROL METHOD EFFECTIVENESS

Control Method	Effect on Emission Rates (gr/bhp-hr)			
	NOx	CO	HC	Particulates
Turbocharging	Increase	Decrease	Decrease	Decrease
Pilot Injection	Increase	U	U	U
Fumigation	Decrease	Increase	Increase	Increase
Water Injection	Decrease	N	N	N
Exhaust Gas Recirculation	Decrease	Increase	U	Increase
Exhaust Gas Recirculation with Turbocharging and Aftercooling*	Decrease	N	N	N

* Results actually dependent on extent of EGR and TC.
Code: N = little or no effect.
U = effect unknown.

FIGURES

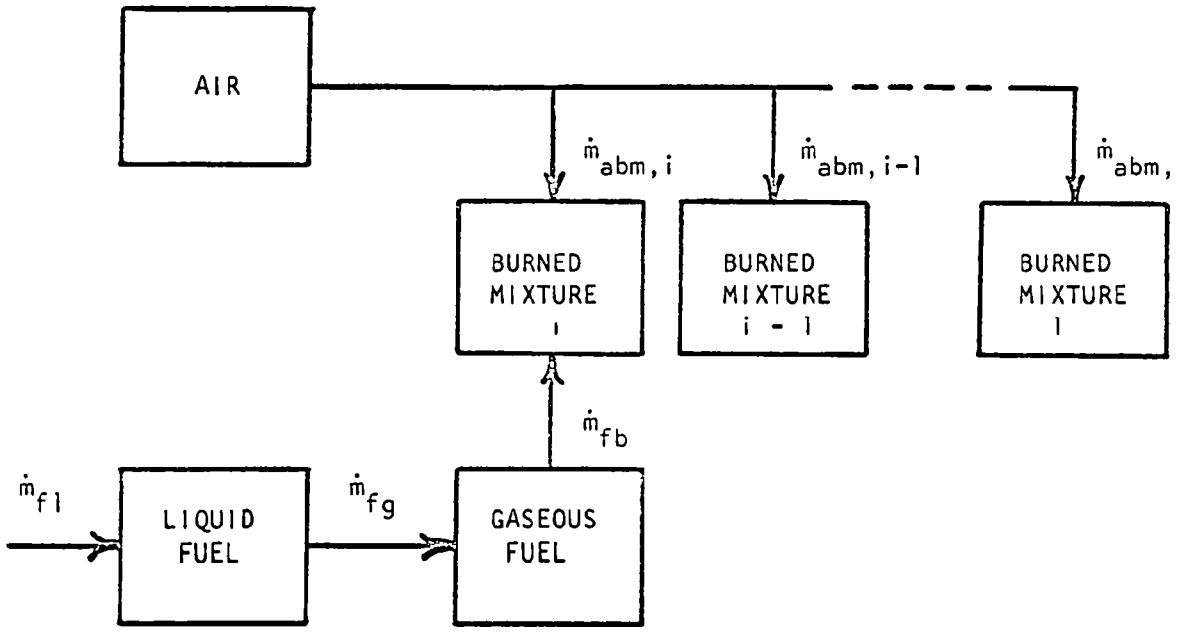


FIGURE 1 - FLUID SYSTEMS AND MASS TRANSPORT PROCESSES: DIRECT-INJECTION ENGINE MODEL

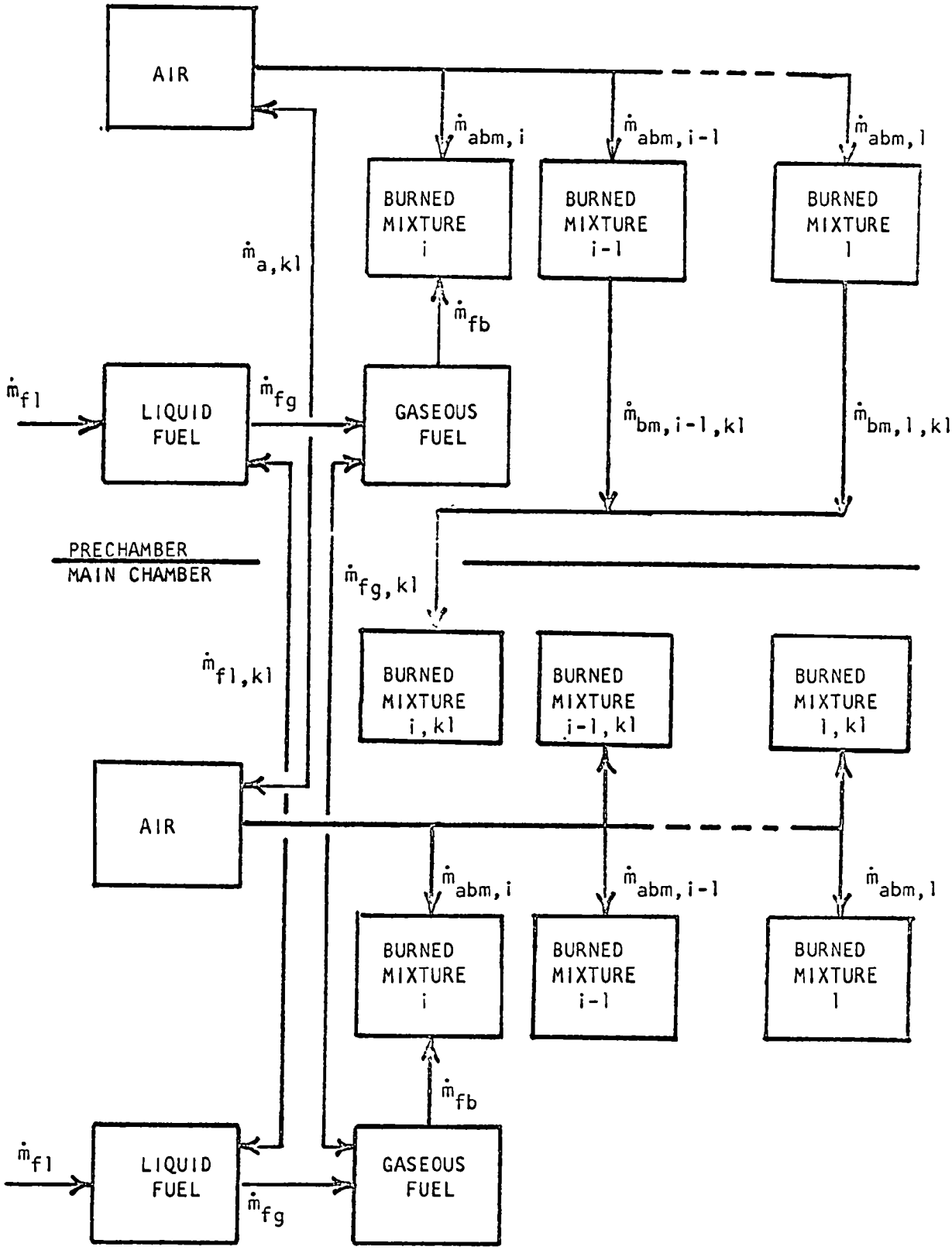


FIGURE 2 - FLUID SYSTEMS AND MASS TRANSPORT PROCESSES: INDIRECT-INJECTION ENGINE MODEL

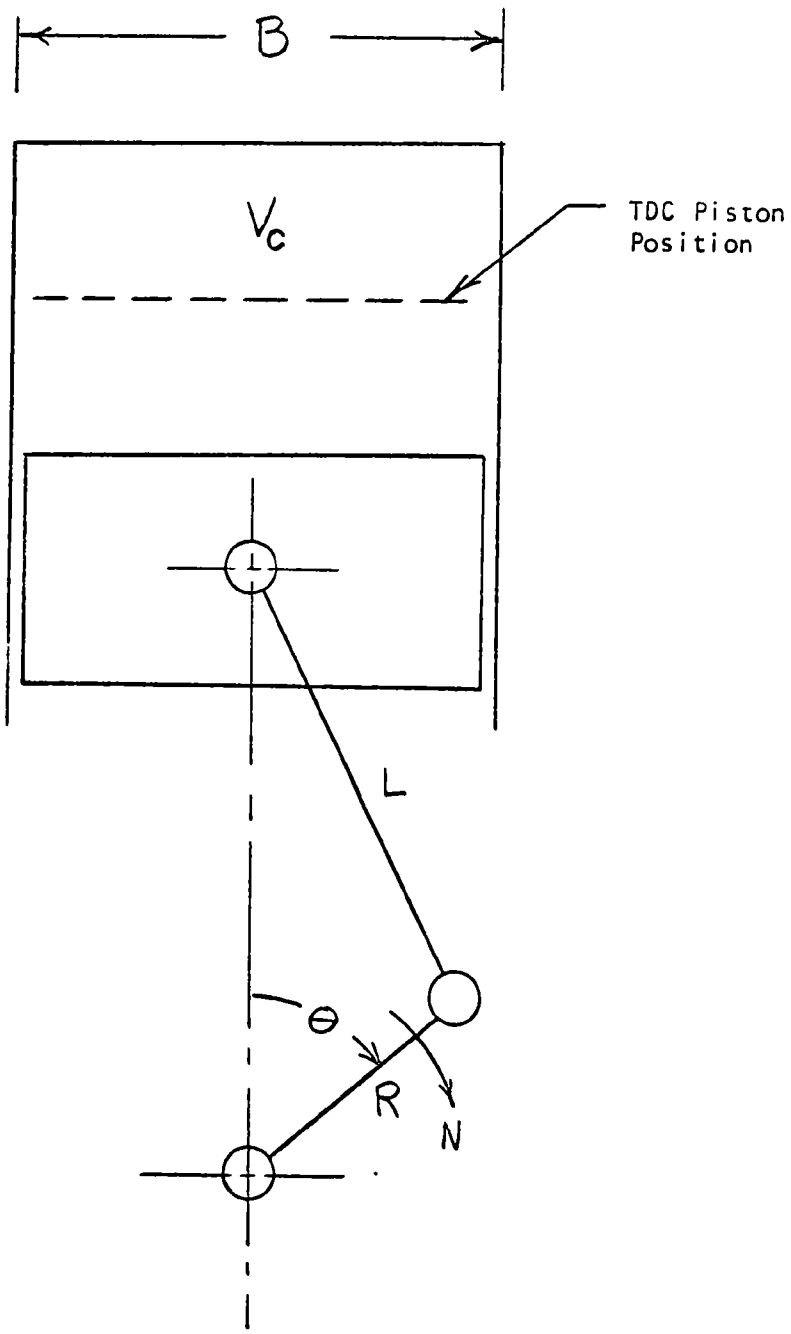


FIGURE 3 - DIRECT-INJECTION ENGINE CYLINDER DESIGN VARIABLES

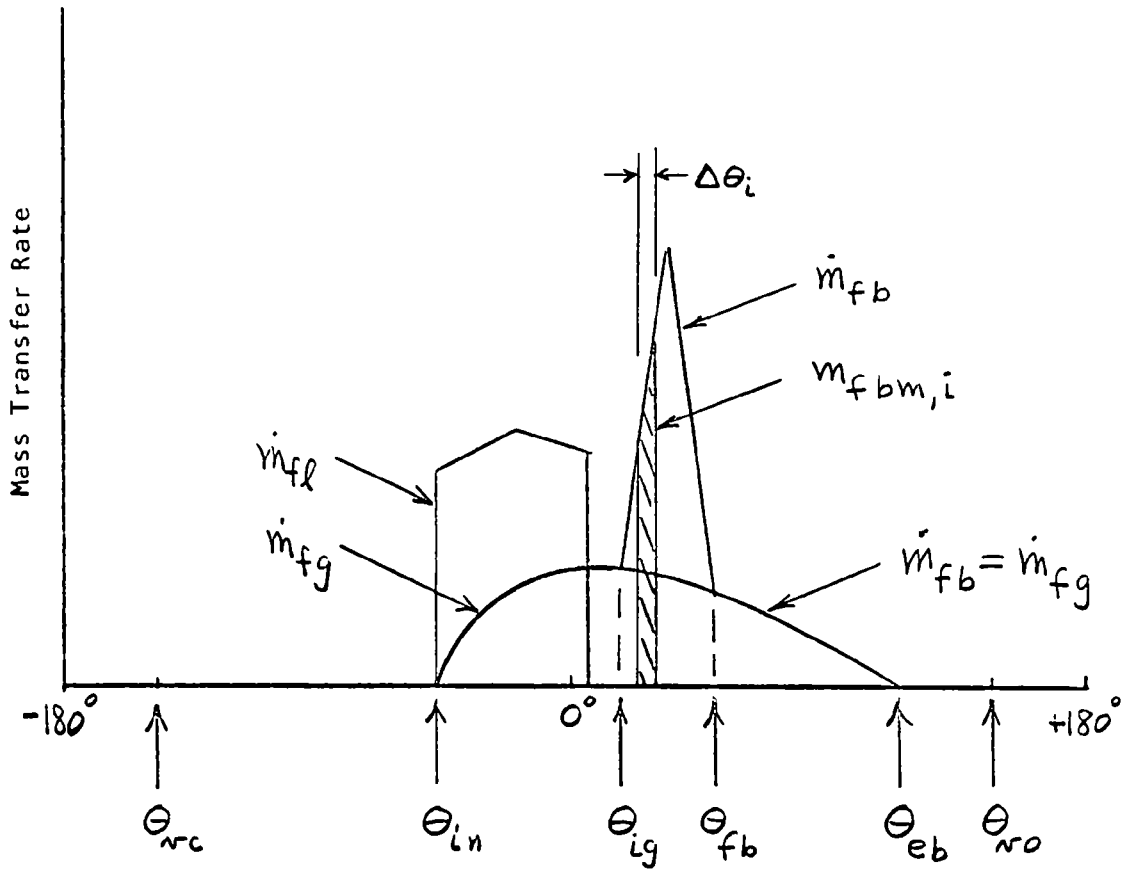


FIGURE 4 - DIRECT-INJECTION ENGINE COMBUSTION CYCLE AND MASS TRANSPORT PROCESSES

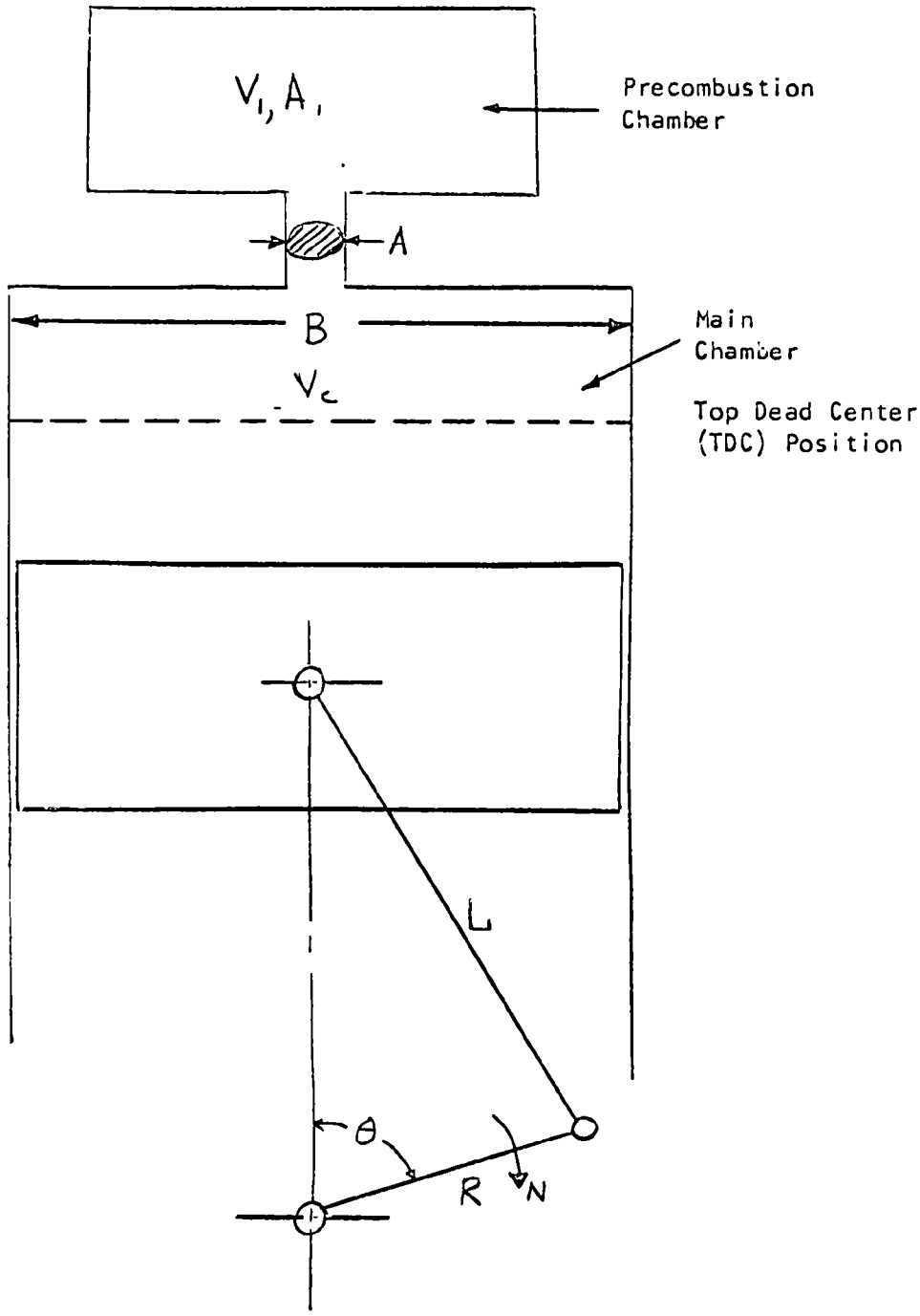


FIGURE 5 - INDIRECT-INJECTION ENGINE CYLINDER DESIGN VARIABLES

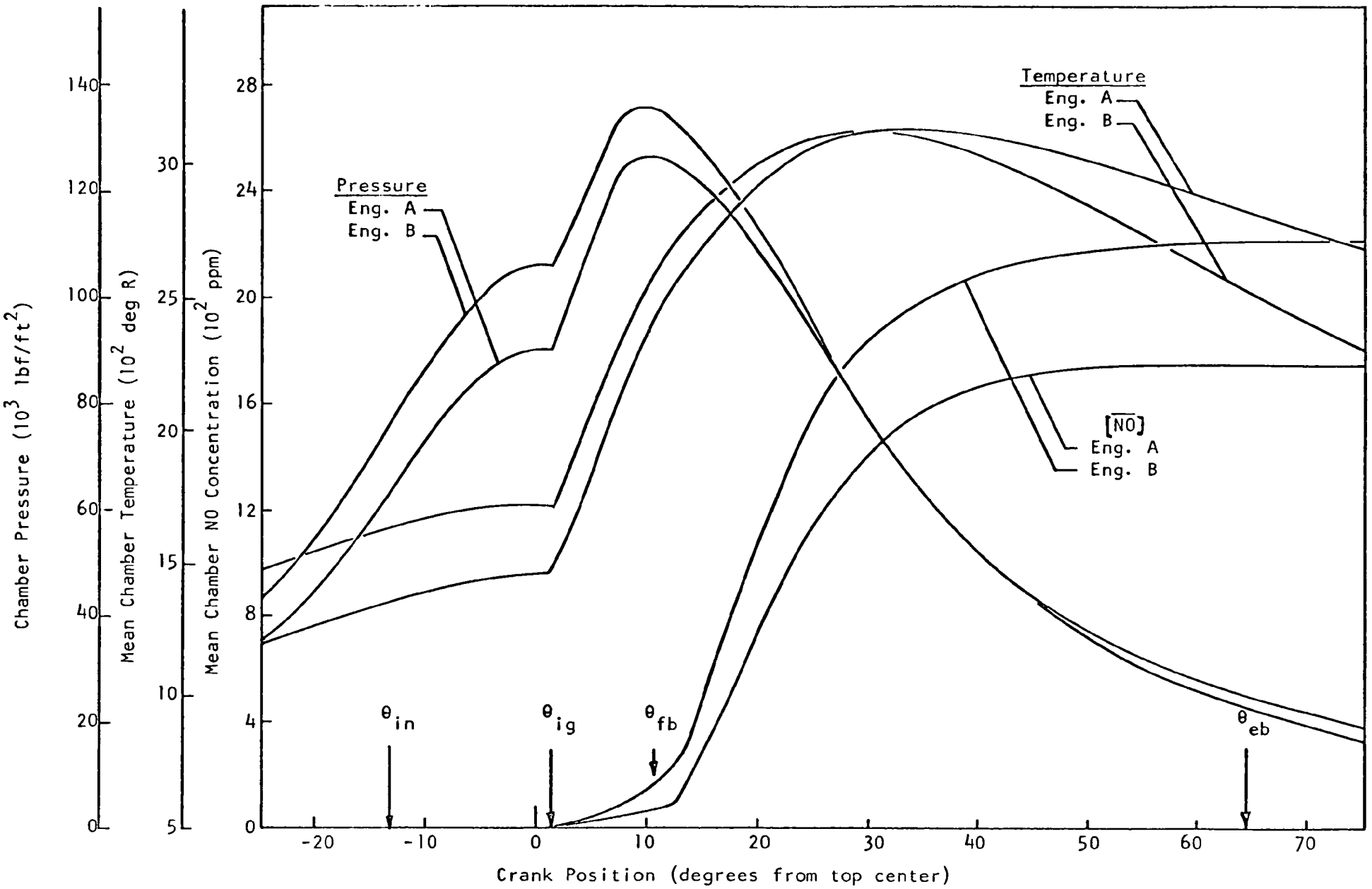


FIGURE 6 - MEAN CHAMBER GAS PROPERTIES, DIRECT-INJECTION REFERENCE ENGINES

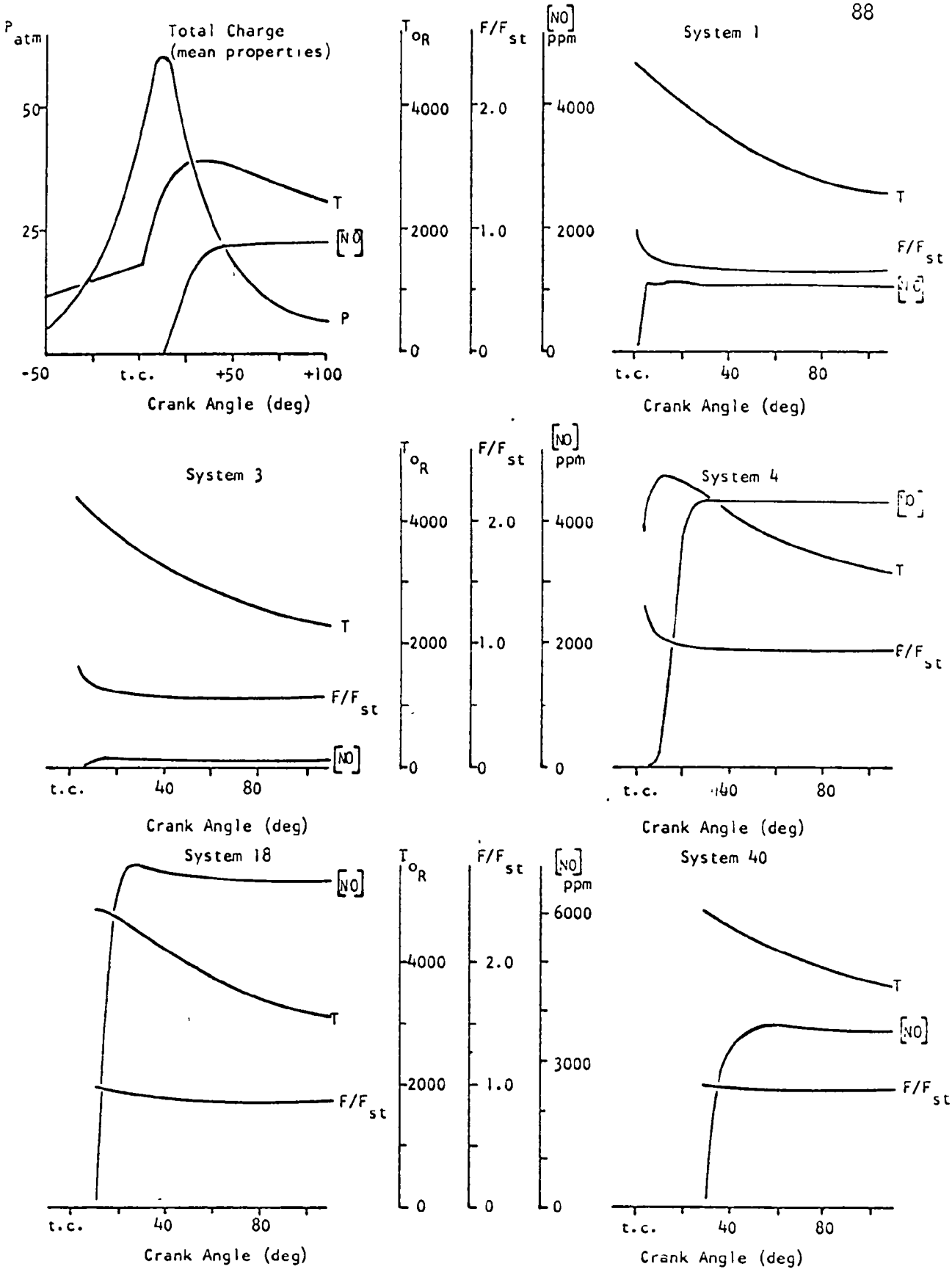


FIGURE 7 - PREDICTED PERFORMANCE OF THE REFERENCE DIRECT-INJECTION ENGINE

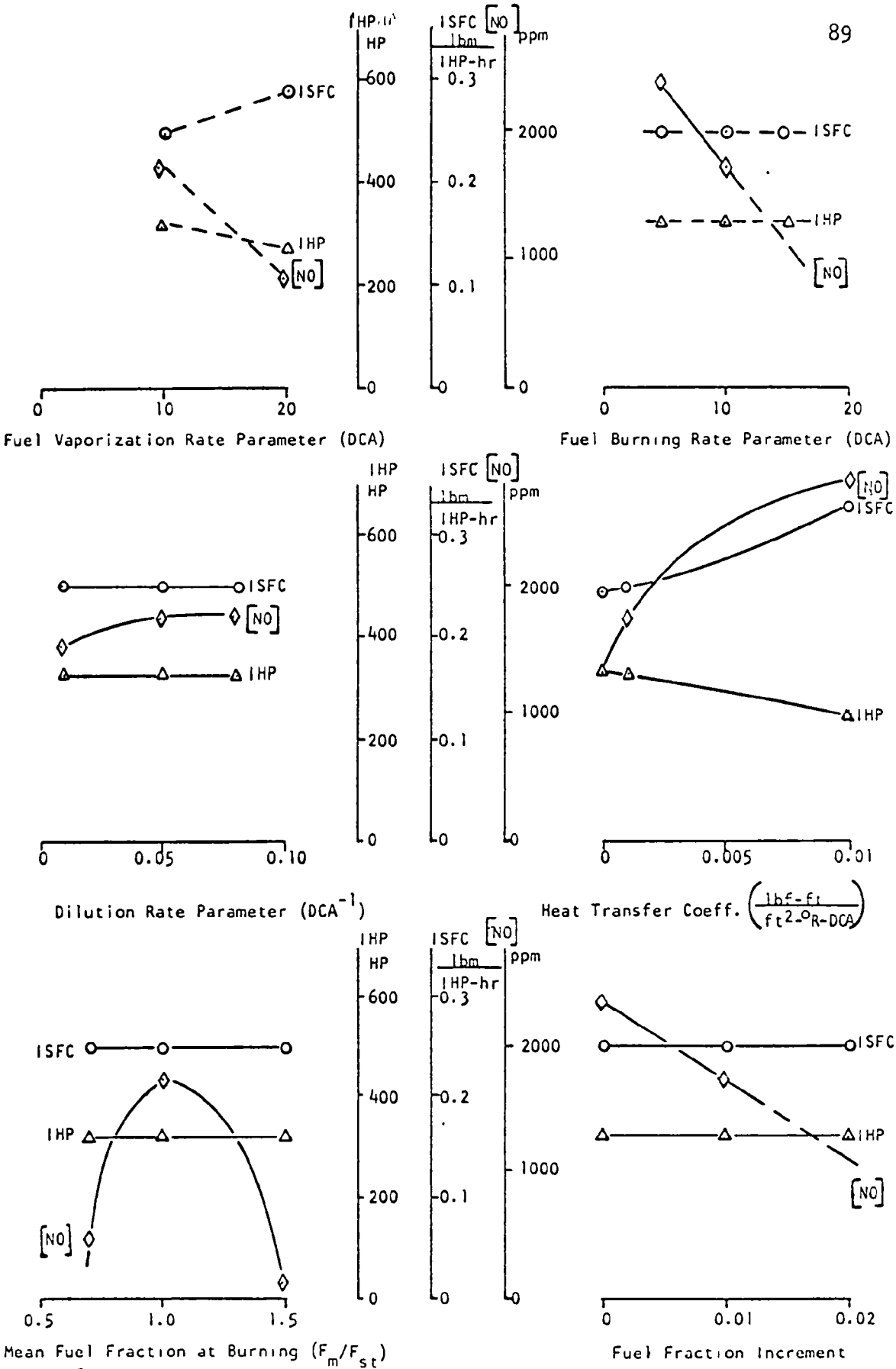


FIGURE 8 - SENSITIVITY OF PREDICTED DIRECT-INJECTION ENGINE PERFORMANCE TO MODEL PARAMETERS

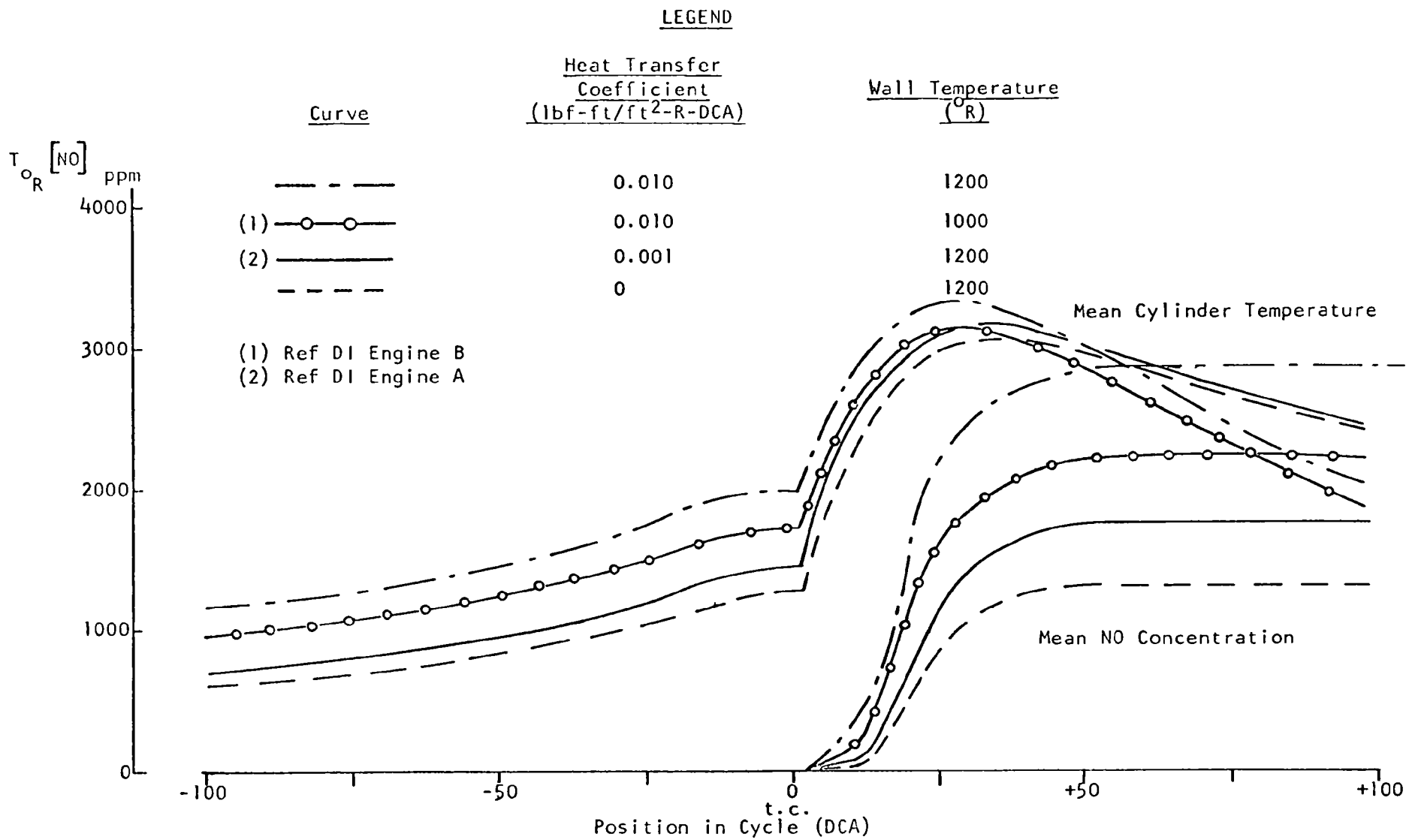


FIGURE 9 - SENSITIVITY OF PREDICTED NO EMISSION RATE TO HEAT TRANSFER PARAMETERS

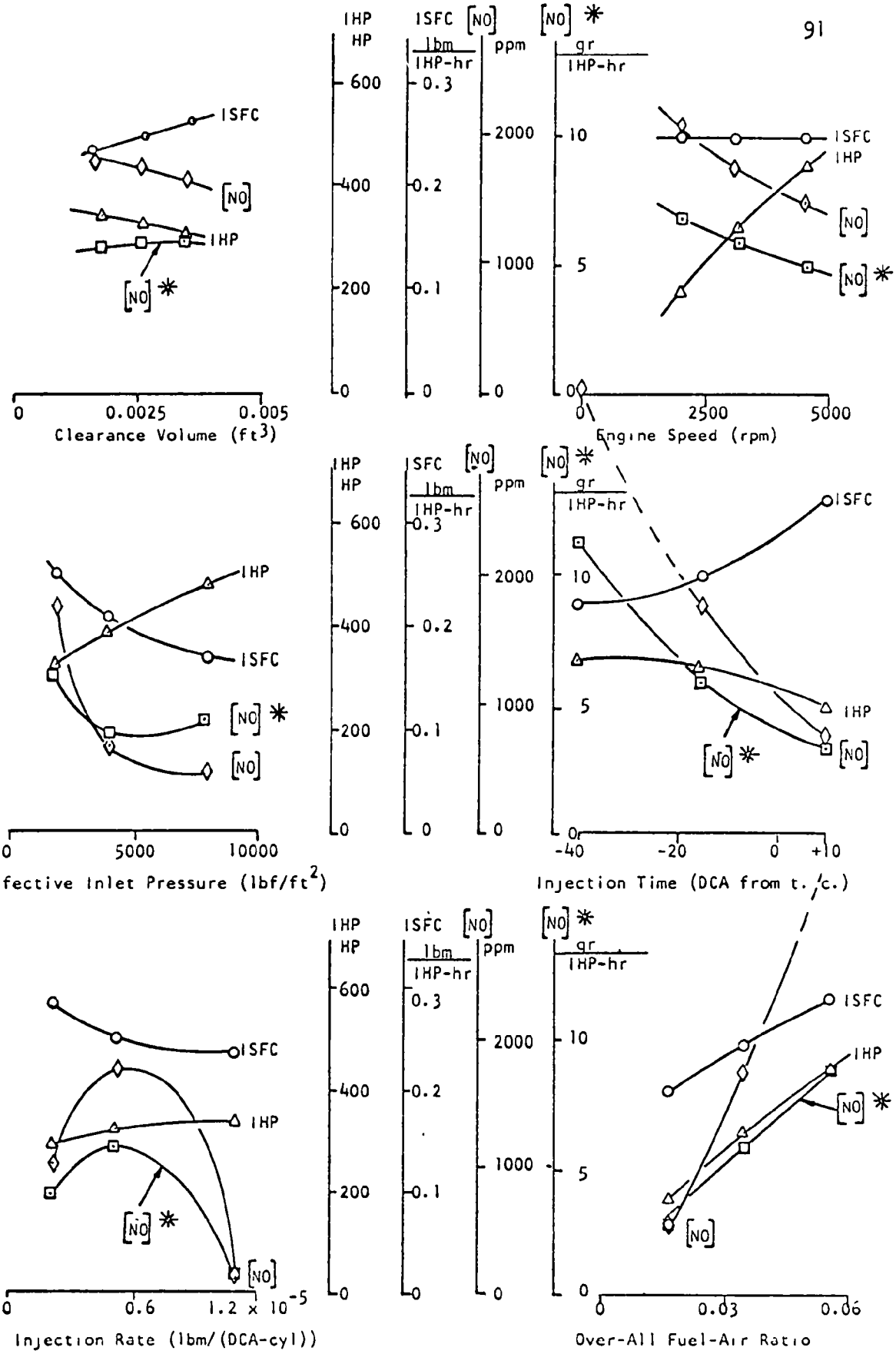


FIGURE 10 - SENSITIVITY OF PREDICTED DIRECT-INJECTION ENGINE PERFORMANCE TO DESIGN PARAMETERS

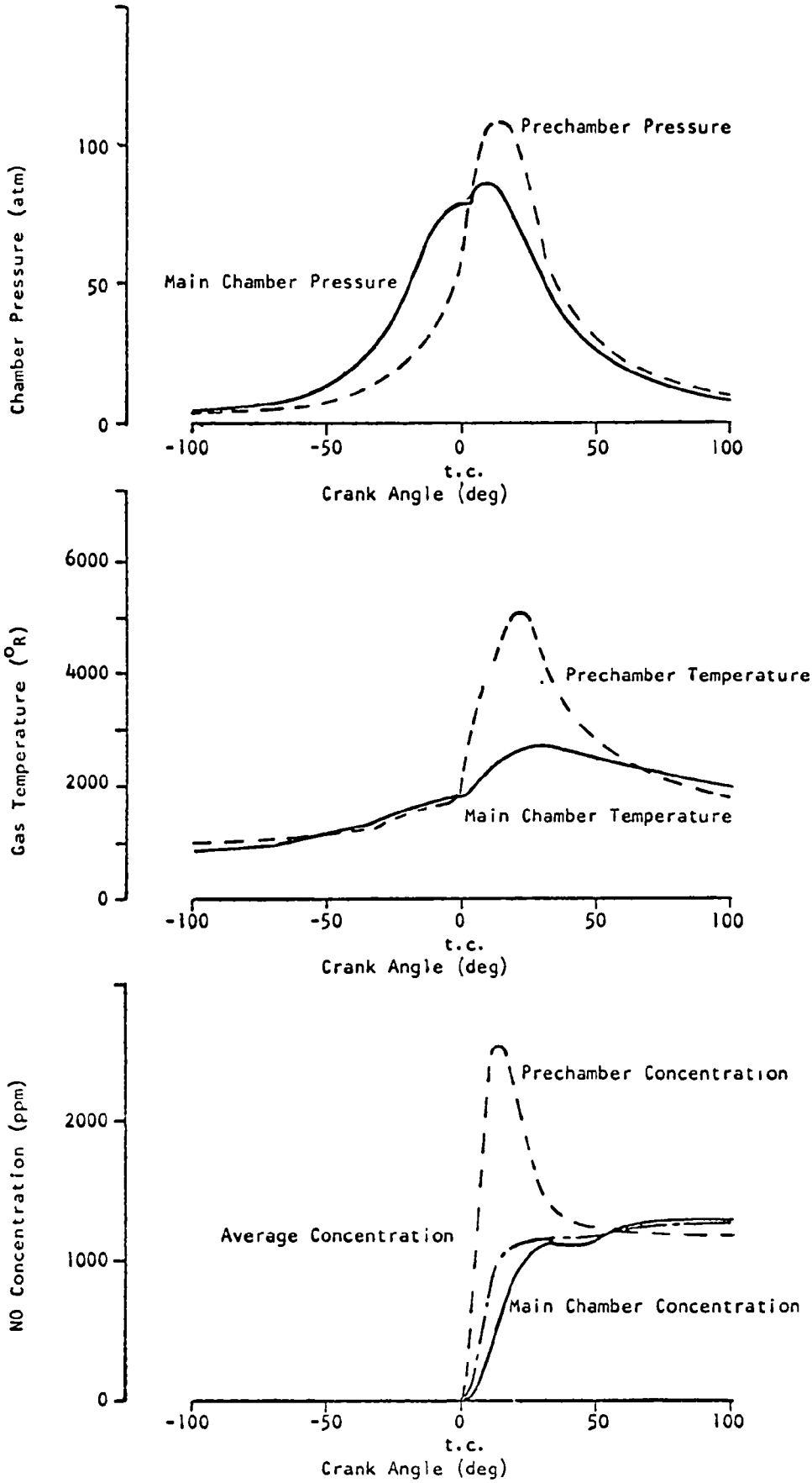
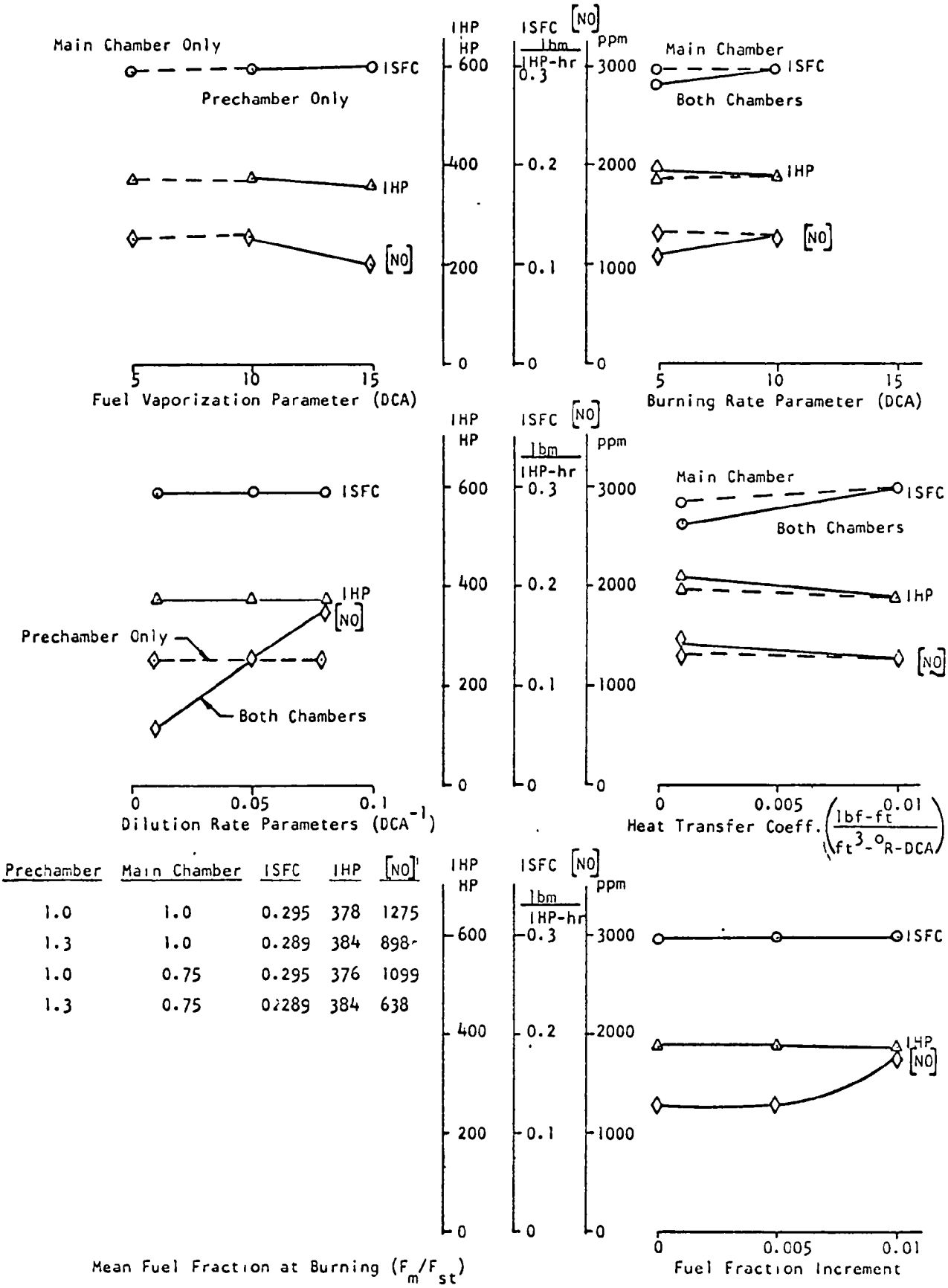


FIGURE 11 - PREDICTED PERFORMANCE OF THE REFERENCE INDIRECT-INJECTION ENGINE



Prechamber	Main Chamber	ISFC	IHP	[NO]
1.0	1.0	0.295	378	1275
1.3	1.0	0.289	384	898
1.0	0.75	0.295	376	1099
1.3	0.75	0.289	384	638

FIGURE 12 - SENSITIVITY OF PREDICTED INDIRECT-INJECTION ENGINE PERFORMANCE TO MODEL PARAMETERS

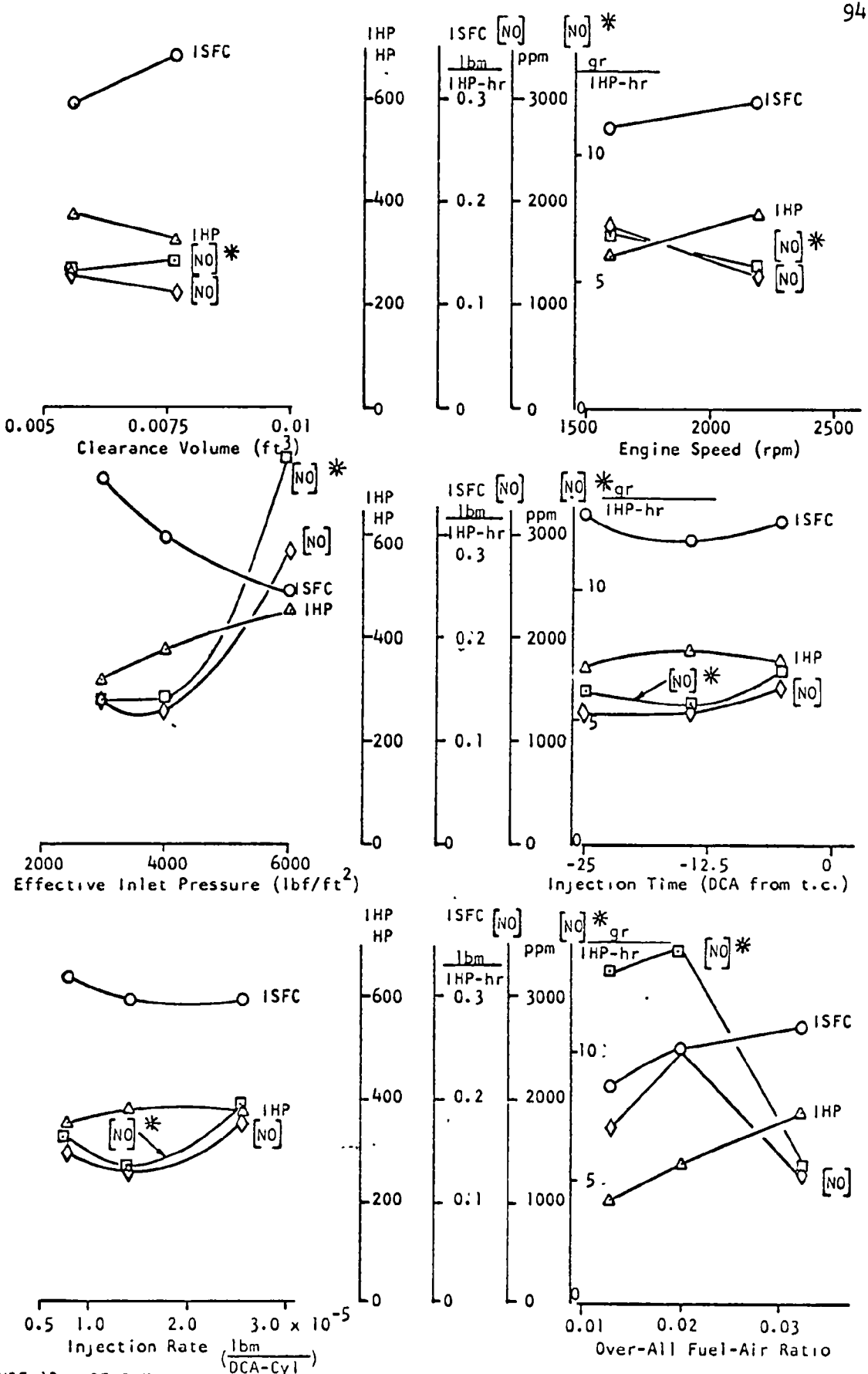


FIGURE 13 - SENSITIVITY OF PREDICTED INDIRECT-INJECTION ENGINE PERFORMANCE TO DESIGN PARAMETERS

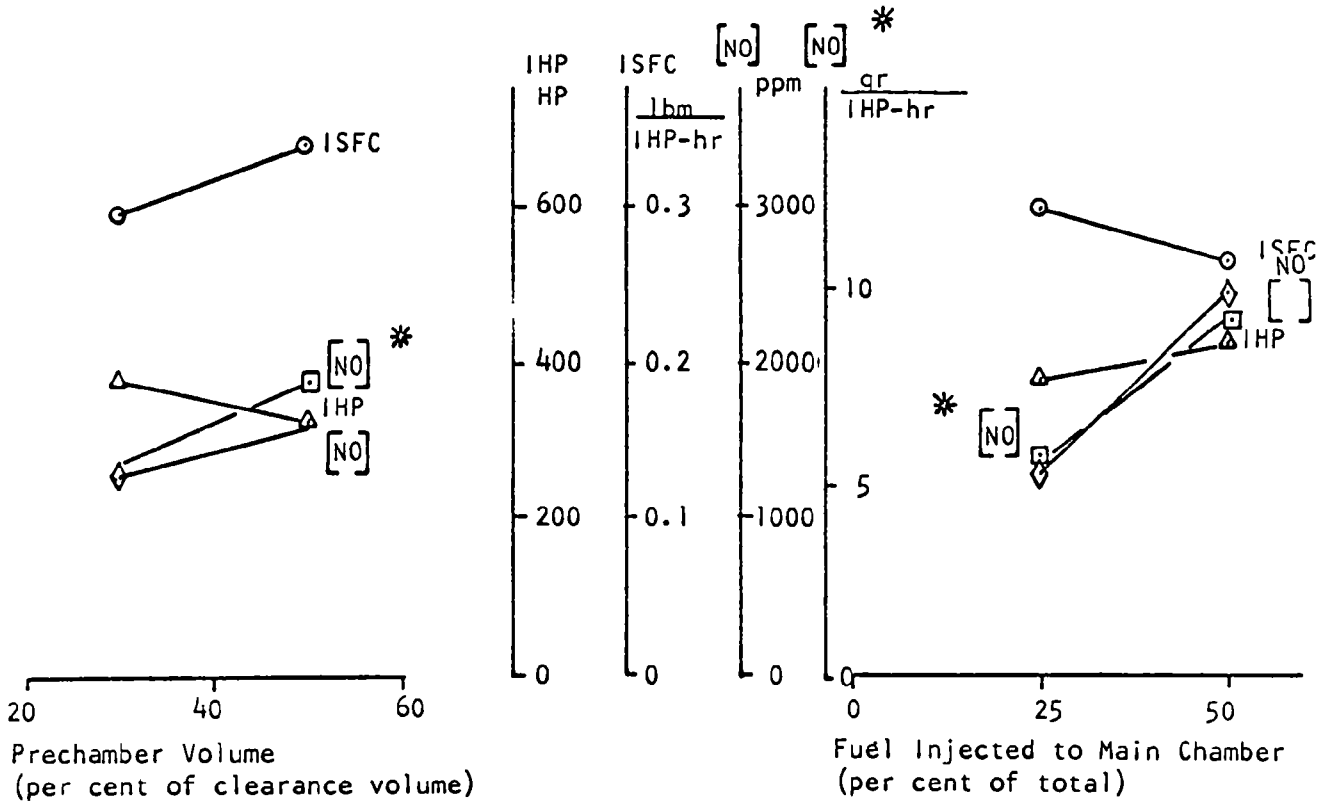


FIGURE 13 - SENSITIVITY OF PREDICTED INDIRECT-INJECTION ENGINE PERFORMANCE TO DESIGN PARAMETERS (CONTINUED)

NOMENCLATURE

NOMENCLATURE

Symbols	Description	Units
A	Area	sq ft
B	Cylinder bore	ft
C	Constant, specified model parameter	--
C_p	Specific heat at constant pressure	lbf-ft per slug deg R
F	Mass fraction of fuel	--
h	Enthalpy	lbf-ft per slug
IMEP	Indicated mean effective pressure	lbf per sq ft
ISFC	Indicated specific fuel consumption	lbm fuel per IHP hr
K	Polytropic index; reaction rate parameter	--
K_{f1}	Fraction of fuel injected into main chamber (IDI engine)	--
L	Connecting rod length	ft
M	Molecular weight	slug per slug mole
m	Mass	slug
$\dot{m}$	Instantaneous mass flow rate	slug per sec
N	Engine speed	rpm
n	Polytropic exponent	--
$[NO]$	NO concentration	Mass fraction
P	Pressure	lbf per sq ft
$\dot{Q}$	Heat transfer rate to wall	lbf-ft per deg crank angle (DCA)
R	Crank length; gas constant	ft; lbf-ft per slug deg R
$\dot{r}$	Rate of NO formation	slug per DCA
T	Temperature	deg R
V	Volume	cu ft
V_c	Clearance volume	cu ft
x	Number of revolutions per power stroke	--
α	Ratio of NO mass fraction to equilibrium NO mass fraction	--
ε	Internal energy	lbf-ft per slug

Symbols	Description	Units
θ	Crank angle position (θ=0 at TDC)	DCA
ρ	Fluid density	slug per cu ft
τ_{ig}	Ignition delay	msec
ϕ	Equivalence ratio	--

Subscripts

1	Precombustion chamber
2	Main chamber
a	Air-residual gas mixture
abm	Dilution air in burned mixture
bm	Burned mixture
eb	End of combustion
fb	Final burning; fuel burning
fbm	Fuel in burned mixture
fg	Gaseous fuel
fl	Liquid fuel
h	Homogeneous mixture
i	Number of crank angle increments; burned mass system
ig	Ignition
in	Fuel injection
i, j	Crank angle interval or system formed during interval
k, l	Chamber notation in indirect injection engine, k or l = 1 for precombustion chamber, k or l = 2 for main chamber
m	Mean value
s	Stoichiometric
vc	Valve closure
vo	Valve opening
w	Wall

Superscripts

o	Initial value
-	Mean value