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ISBN 0-315-56339-7

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Stochastic Model for Flame Propagation at Lean Ignition Limit and Partial Burn Limit of Spark Ignition Engines

by

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A Thesis presented to
the School of Graduate Studies at the University of Ottawa
in partial fulfillment of the requirements for the degree
of
Master of Applied Science
in
Mechanical Engineering

UNIVERSITÉ D'OTTAWA
UNIVERSITY OF OTTAWA

Stochastic Model for Flame Propagation at Lean Ignition Limit and Partial Burn Limit of Spark Ignition Engines

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ABSTRACT

A phenomenological model with stratification of temperature and species concentration was developed to simulate engine misfire. The fuel mixture in the combustion chamber is divided into equal mass particles, each of which has its own temperature and species concentration. The model incorporates the coalescence dispersion model for finite rate mixing and the mass entrainment model for flame propagation. The chemical rate of the first order reaction for the combustion of propane in air is used to formulate a set of ordinary differential equations for the evolution of temperature and species concentration. An ODE solver of the predictor corrector method was developed to solve the equations.

Two types of engine misfire limits were simulated : the ignition limit and partial burn limit. The model was tested extensively for the ignition limit, including the effect of turbulence intensity, intake temperature and pressure, equivalence ratio, ignition energy, spark gap distance, and engine RPM. The turbulence intensity, intake temperature and equivalence ratio were observed to have the strongest effect on ignition limit. Examples of partial burn cycles were also obtained. The concept of age mixing was implemented as an attempt to simulate partial burn more adequately, but more studies are required for the age mixing model to predict partial burn. Computation of a complete cycle has not been performed in any of the tests due to limited computing time. However, conclusion can still be reached with about 20 degree crank angles of result after ignition for the case of ignition limited misfire, and about 40 degree crank angles of result after ignition for the case of partial burn. The model in its present form has not been calibrated with actual engine experiments due to the lack of complete engine specifications in available literature. Such calibration has to be performed for model applications on any specific engine.

ACKNOWLEDGEMENT

The auther would like to express his deepest appreciation and gratitude to Professor Roger Milane of the Department of Mechanical Engineering at the University of Ottawa, for his help and support throughout the project and the preparation of this thesis.

NOMENCLATURE

A	Pre-exponential constant
A_e	Flame front area
a	Exponent of fuel
b	Exponent of oxygen
C	Constant of mixing frequency
C_m	Mean molecular speed of chain carriers
C_v	Specific heat at constant volume
D	Velocity divergence
d	Electrode diameter
E	Activation energy
E_b	Internal energy of the burned gas
E_{ign}	Ignition energy
E_T	Dissipation of turbulent kinetic energy
E_u	Internal energy of the unbuened gas
F_1, F_2, F_3	Fuel fraction of a particle
$F(r_e)$	Function of iteration for the flame radius
$g_i(t)$	Derivative of the dependent variable
H_{last}	Last time step
H_{new}	Current time step
h	Chamber height
K	Dimenionless parameter of pressure
K_T	Turbulent kinetic energy
L	Integral length scale
l	Spark gap distance
M_r	Mean molecular weight

M_x	Molecular weight of species x
m	Mass of a particle
m_e	Entrained mass
N	Number of particles in the chamber
N_i	Number of moles per gram of mixture in particle i
N_m	Number of mixing pairs
N_t	Number of particles in the reactor
n	Number of moles of mixture
P	Pressure
P_{in}	Pressure at the closing of the intake valve
P_r	Reference pressure
Q	Heat transfer to the systen
q	Specific heat transfer to the system
R	Universal gas constant
R_b	Gas constant of the burned gas
R_c	Bore radius of the chamber
R_u	Gas constant of the unburned gas
r_e	Entrainment radius
r_s	Spark location offset
S	Error to tolerance ratio
S_l	Laminar flame speed
T_b	Burned gas temperature
T_i	Temperature of particle i
T_{in}	Temperature at the closing of the intake valve
T_m	Mean temperature of the reaction zone
T_u	Unburned gas temperature
Δt	Time interval
U	Internal energy

U_1, U_2, U_3	Internal energy of a particle
U_{mi}	Internal energy per mole of mixture for particle i
u	Specific internal energy
u_e	Entrainment velocity
u'	Turbulence intensity
V	Chamber volume
V_b	Burned gas volume
V_e	Entrained volume
V_{in}	Chamber volume at the closing of the intake valve
Vol_1, Vol_2, Vol_3	Volume of a particle
V_p	Total volume of the particles
V_T	Actual chamber volume
v	Specific volume of a particle
W	Work done by the system
w	Moles of water per gram of mixture
X	Moles of fuel per cc of mixture
x	Moles of fuel per gram of mixture
$x_i(t)$	Dependent variable of an ordinary differential equation
Y	Moles of oxygen per cc of mixture
Y_f	Mole fraction of fuel
Y_{O_2}	Mole fraction of oxygen
y	Moles of oxygen per gram of mixture
z	Moles of carbon dioxide per gram of mixture
α	Exponet of pressure ratio
ϵ	Error bound
γ	Ratio of specific heats
ν	Moles of nitrogen per gram of mixture
ρ	Density

τ_i	Equilibration time
ω	Mixing frequency

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CHAPTER 1
INTRODUCTION

1.1 GENERAL OVERVIEW

Lean combustion improves specific fuel consumption and reduces emissions of carbon monoxide (CO) and oxides of nitrogen (NOx) in spark ignition engines (Shiomoto et al, 1978). However, misfire and cycle to cycle variation in lean burning engines cause rough operation and higher hydrocarbon (HC) emissions. Misfire limit is usually defined as the equivalence ratio at which a small percentage of cycles fail to ignite or burn completely for given operating conditions, namely, temperature, turbulence, spark advance etc.. A percentage of cycles is used because cyclic variation causes some cycles to misfire, and the others to burn completely. Different experimental methods have been used to determine if a cycle misfires. There is no agreement among researchers as to what percentage of cycles per minute misfires in the limit or on the specific method used to identify these cycles. Quader (1974) assumed that at the misfire limit, 0.5 to 0.8 % of the cycles misfired. He identified them by observing the pressure curve, the flame front position using an ionization probe and the exhaust HC level. Anderson and Lim (1985) used 0.4 to 2% of the cycles misfiring as the limit. They identified them by observing that the pressures at 40 degrees before and after top dead center in the same cycle are equal. Quader (1976) described two misfire limits: the ignition limit and the partial-burn limit. The ignition limit is reached if the spark fails to ignite a sufficiently large flame kernel to sustain flame propagation by the heat release of combustion. On the other hand, the partial burn limit is reached when the flame has not traversed the entire combustion chamber when the exhaust valve opens.

1.2 LITERATURE SURVEY

Germane et al (1983) provided an extensive review on the research works of lean mixture in spark ignition engines. They included over one hundred references dated from 1908 to 1983. The following literature survey does not intend to cover all available literature. Instead, the literature relevant to the present study will be reviewed.

As early as 1971, Tanuma et al (1971) investigated ways to improve lean combustion in spark ignition engines. They performed engine experiments with a modified ignition system, intake valve seat and combustion chamber geometry. The results showed that the lean limit can be extended using a larger spark gap, longer spark gap projection, higher ignition energy, and by using a valve seat with six inclined vanes. It was found that a compact combustion chamber and heated intake mixture improved fuel consumption and smoothness of operation. The engine speed was set at 1600 RPM for the testing of the lean limit. The authors defined the lean limit as the largest air to fuel ratio without misfire in 300 cycles. This definition was considered to be ambiguous by later researchers (Germane et al, 1983). The lean limit defined this way depended on the number of cycles observed. Tanuma et al (1971) were one of the earliest to investigate the lean limit of spark ignition engines. Their work did not provide insight in understanding the mechanism of lean misfire. Quader (1974) has done extensive experimental studies on lean misfire limit with propane and air and isooctane and air mixtures. The effects of varying different engine operating variables were investigated. His results indicated that the lean misfire limit was extended by increasing compression ratio and temperature, improving mixture homogeneity, decreasing charge dilution and engine speed. Quader (1976) also studied two types of misfire :. misfire at ignition and partial burn. He investigated whether the lean limit occurred at ignition or during flame propagation. His study showed that at early spark timing, misfire occurred at ignition and that misfire at ignition can be avoided by retarding the spark advance. However, at

late spark timing, misfire occurred during flame propagation and the partial burn limit was reached. The two papers by Quader (1974, 1976) have stimulated great interest in understanding misfire. The author defined misfire using experimental measurements. The combined effects of engine operating variables on misfire were presented. Several questions concerning misfire remained unanswered. In fact, the measurement technique to distinguish ignition misfire from partial burn did not suggest that they were two different phenomena.

Smith et al (1977) analyzed the bulk quenching of flame in an expanding chamber using schlieren photographs. Their study showed that bulk quenching depended on the amount of volume expansion rather than the rate of volume expansion. Therefore, the unburned gas density was critical when bulk quenching occurred. The authors also correlated the lean limit with the Karlovitz number for different ignition timing. They concluded that bulk quenching contributed to flame extinguishment when ignition timing was retarded. Their results were in agreement with the results of Quader (1976) that partial burn occurred at late ignition timing. On the other hand, Peters (1979) investigated some cases of partial burn. He obtained pressure traces for a large ensemble of partially burned cycles, and deduced the mass burn fraction using the two zone heat release model of Krieger and Borman (1967). Their results showed few cases of flame quenching before the exhaust valve opened. The majority of the partial burn cycles were still burning when the exhaust valve opened due to slow burning rate. Peters also observed that the calculated flame temperature at quenching was between 1650 to 1880^0K, but the slow burning cycles had a flame temperature above this range. The works of Smith et al (1977) and Peters (1979) have contributed to the understanding of partial burn. However, the question left open by Quader's studies remained unanswered.

The limitation of experimental works in understanding the physical mechanism behind misfire is mainly due to nature of engine experiments. All engines operate at a set of inter-related operating variables. For instance, if the speed of

the engine is changed, the turbulence intensity, residual fraction and other variables will also be affected. The effect of varying one operating parameter alone is very difficult to obtain. Engine experiments can only yield results of combined effects. Numerical models, on the other hand, can demonstrate the effect of varying any selected engine operating parameter, while perfectly isolating all other variables. Therefore, modelling provides information that is not available from experiments.

To date, attempts to model ignition limits have been made. Arici et al (1983) postulated that at the ignition limit, the energy production from combustion in the flame kernel was equal to the amount of heat dissipated to the unburned surrounding by turbulence. The burned mass was obtained using a mass entrainment model following the work of Tabaczynski et al (1977). The entrainment velocity was the sum of laminar flame speed and turbulence intensity. The effects of varying compression ratio, engine speed, intake temperature and exhaust gas recirculation were investigated. Comparison of model results with experimental results showed good agreement. Anderson and Lim (1985) determined experimentally the critical spark gap distance at which the leanest mixture could be ignited for a given spark advance. They called it the minimum energy condition. The critical spark gap distance was called the quench distance. At the minimum energy condition, reducing the spark gap would increase heat loss through the spark plug electrode and the flame would be quenched. On the other hand, increasing the spark gap would increase heat loss to the unburned gas and the flame would be quenched. The authors used a model by Ballal and Lefebvre (1977) to relate the quench distance to the effective (turbulent) flame thickness. The model failed to predict the effect of engine speed changes.

These two models for ignition limit provided some insights into the physics behind misfire at ignition. However, complete understanding of ignition misfire and partial burn is not obtained yet. As Quader(1976) stated in his paper in studying the constraint limits of lean operation, that 'this would require modelling the

thermochemical interactions near the spark gap to establish flame initiation during compression, and modelling the flame quenching process during expansion.' Since the thermochemical interaction at the spark and the flame quenching (partial burn) process are strongly influenced by local temperature and species concentration, a model incorporating temperature and species stratification coupled with finite rate chemistry and finite rate turbulent mixing is essential to predict the ignition limit and partial burn limit.

1.3 OBJECTIVE

The objective of this study is to formulate a model for flame propagation in a lean mixture to predict both ignition limit and at partial burn limit. At the present time, models for partial burn are not available in the literature. Both the misfire at ignition and partial burn are affected by the same type of engine operating variables, namely inlet flow condition, inlet condition of fuel mixture, ignition system, ignition timing, engine speed, and compression ratio. Therefore a model predicting both the ignition limit and partial burn limit will be useful in understanding the mechanism of engine misfire.

The model should be sensitive to the variation of all parameters that are believed to affect the misfire limits. These parameters have been used by Quader (1974) and Anderson and Lim (1985) in their extensive experimental works. They included the equivalence ratio, intake temperature, pressure, turbulence, engine speed, spark advance, spark gap and ignition energy. The model is expected to predict experimental trends when the parameters are varied. It should also predict the exact ignition limit and partial burn limit if complete engine data are available for precise model validation. However, this cannot be accomplished at the present stage due to the lack of complete engine data.

It should be noted that the model does not replace any engine experiments. The purpose is to assist researchers in understanding the results of engine experiments, and to direct future experiments. At the lean limit, misfire and cycle to cycle variation are coupled. Due to cyclic variation, the misfire limit predicted by the model represents some cycles of an engine operating at the lean limit. The percentage of misfiring cycles is an important consideration from the practical point of view. It cannot be obtained without knowing the cyclic distribution of mixture conditions from experiment. Therefore, experiment and modelling should always complement one another.

1.4 MODEL APPROACH

Combustion models for spark ignition engines are classified as either multi-dimensional or phenomenological. In multi-dimensional models, the conservation of mass, momentum, species and energy are solved numerically, and spatial variations of velocity, temperature and species concentration are calculated. These models require fine grids and excessive computing time. They are still in the development phase, and have not been used to calculate lean misfire limit. Phenomenological models assume a spatial average for the thermodynamic state of the mixture. They require less computing time, and can be used with engine development. A detailed classification is discussed by Heywood (1978).

In this study, a phenomenological model employing the coalescence dispersion approach by Curl (1963) is developed. The fuel mixture in the combustion chamber is divided into a number of equal mass particles, each having a homogeneous species concentration and temperature. Initially, a number of particles having a volume equal to the volume of the spark plug gap are selected and ignited to a fully burned state. The ignition energy released by the spark is equally distributed to those few particles. Then the thermodynamic state of the burned and unburned par-

ticles is calculated using the first law of thermodynamics and the volume constraint of the combustion chamber.

After ignition, the burned particles constitute the flame kernel. The flame front propagates by entraining unburned particles in the burned volume behind the flame front. This volume is assumed to be a partially stirred reactor. A turbulent entrainment model similar to Blizard and Keck (1974) is used to describe the rate of entrainment. The entrainment speed is a function of turbulence intensity (Tabaczynski et al, 1977). The particles in the partially stirred reactor mix in a binary fashion at a frequency determined by the turbulence intensity. The turbulence intensity is calculated assuming the rapid distortion theory for a spherical eddy in a homogeneous turbulent field (Morel and Mansour, 1982). The turbulence intensity in this simplified model depends on the unburned density. The binary mixing of particles are assumed to occur instantaneously, and separation occurs immediately after mixing. The resulting two particles have identical species concentration, temperature and volume. The burning of particles will take place when a burned particle is mixed with an unburned, or a burning with other particles. All three types of particles: unburned, burned, and burning particles can co-exist in the partially stirred reactor. This is consistent with the experimental observation by Namazian et al (1980).

The evolution of species and temperature of the burning particles is described by a set of chemical rate equations for all species applied to each burning particle. Using the first law and assuming a perfect gas, an expression for the rate of temperature rise is derived. An expression describing the rate of pressure rise is also obtained by applying the perfect gas law to the ensemble of particles and using the chamber volume constraint. These equations are solved simultaneously. The results give the species concentration and temperature of each burning particle, and the pressure of the system at each instant of time.

This model incorporates a turbulent flame front, finite rate turbulent mixing

and finite rate chemistry. It differs from other phenomenological models by incorporating temperature and species stratification. It is more accurate than using an average value of temperature, since the specific reaction rate given by Arrhenius is extremely sensitive to temperature, as demonstrated by Pratt (1976). The inclusion of the chemical rate in the model is an important feature. As shown in the literature survey, other models studying misfire do not include chemical rate explicitly; they use the laminar flame speed correlation. However, the comparison of chemical time with turbulent mixing (diffusion) time is important in the study of lean misfire. Peters (1979) stated that 'if the time required to complete the chemical reactions is longer than the time it takes for chemical species and energy to be transported away from the reaction zone, the flame will go out.' Explicit chemical rate in the model facilitates such a comparison.

CHAPTER 2
SUPPORTING MODELS

2.1 IGNITION

The ignition is modeled by burning completely the mixture within the spark gap during the specified ignition duration. The ignition energy is equally distributed among the burned particles. The thermodynamic states of the burned and unburned gases are calculated using the first law . The first law applied to the unburned gas outside the spark gap is expressed as,

$$E_u - E_{u,o} = Q - W_u \tag{1a}$$

where $E_{u,o}$ and E_u are respectively the internal energy of unburned gas before and after ignition, Q is the heat transferred to the unburned gas and W_u is the work done by the unburned gas. Assuming that the process is adiabatic, and that the ignition energy is delivered to the burned gas only, then the heat transfer term Q is zero and the first law applied to the unburned is rewritten as

$$E_u = E_{u,o} - W_u \tag{1b}$$

The first law applied to the burned gas is

$$E_b - E_{b,o} = Q - W_b \tag{2a}$$

where $E_{b,o}$ and E_b are respectively the internal energy of the burned gas before and after ignition, Q is the heat transferred to the burned gas, and W_b is the work done by the burned gas. Here, the heat transfer is equal to the ignition energy. Therefore the first law becomes

$$E_b = E_{b,o} + E_{ign} - W_b \tag{2b}$$

where E_{ign} is the ignition energy transferred to the burned gas. It is to be noted that E_{ign} represents the amount of energy transferred to the ignited gas rather than the total amount that the spark plug produces. In reality the energy supplied by ignition system is partially lost by heat transfer through the spark plug electrodes. This treatment is beyond the scope of the present study.

The work terms W_u and W_b in equations (1b) and (2b) are determined by the change in pressure and volume of the unburned and burned gases during the spark duration; they are

$$W_u = -\int P dV_u \tag{3a}$$

$$W_b = -\int P dV_b \tag{4a}$$

Since the spark duration is short, the variation of pressure can be assumed linear. The integrals are approximated using the trapezoidal rule, and equation (3a) and (4a) become,

$$W_u = \frac{P+P_o}{2}(V_u - V_{u,o}) \tag{3b}$$

$$W_b = \frac{P+P_o}{2}(V_b - V_{b,o}) \tag{4b}$$

where subscript o denotes properties before ignition, and P is the pressure after ignition. The unburned gas undergoes an isentropic compression from its initial pressure P_o to the pressure P. Therefore the unburned volume is given by

$$V_u = V_{u,o}(\frac{P_o}{P})^{1/\gamma} \tag{5}$$

where γ is the ratio of specific heat. The volume of the burned gas is expressed using the perfect gas law,

$$V_b = \frac{N_b R_b T_b}{P} \tag{6}$$

where T_b is the burned temperature.

Substituting the unburned volume V_u in equation (3b) using equation (5) and replacing the work term in equation (1b), the first law applied to the unburned gas is rewritten as

$$E_u = E_{u,o} - \frac{P+P_o}{2}(V_{u,o}(\frac{P_o}{P})^{1/\gamma} - V_{u,o}) \tag{7}$$

Substituting the burned gas volume V_b in equation (4b) using equation (6) and replacing the work term in equation (2b), the first law applied to the burned gas is expressed as

$$E_b = E_{b,o} + E_{ign} - \frac{P+P_o}{2}(\frac{N_b R_b T_b}{P} - V_{b,o}) \tag{8}$$

The volume of the combustion chamber can be expressed as,

$$V = V_u + V_b \tag{9a}$$

Replacing the unburned and burned gas volumes (V_u and V_b) in equation (9a) using equation (5) and (6),

$$V = V_{u,o}(\frac{P_o}{P})^{1/\gamma} + \frac{N_b R_b T_b}{P} \tag{9}$$

The three unknowns in equations (7), (8), (9) are the temperatures of the burned and unburned gases, and the pressure. The system of equations is closed since there are three unknowns in three equations.

The input variables to the ignition model are the initial temperature and pressure and equivalence ratio, spark timing, spark duration, spark gap distance, ignition energy, and the number of equal mass particles corresponding to the volume of the ignited gas. The volume of the ignited gas is assumed to be equal to the spark gap volume. This volume is estimated to be either a cylindrical volume $\frac{1}{4}\pi d^2 l$ or a spherical volume $\frac{1}{6}\pi l^3$, where d, the electrode diameter, is equal to 2.5 mm, and l is the spark gap distance. The total number of particles in the chamber is calculated as

$$N = \frac{N_b}{V_b} V \tag{10}$$

where N is the calculated number of particles in the combustion chamber, V is the volume of the combustion chamber and N_b is the number of particles ignited. The computer program for the ignition model is included in the main program listed in appendix (A). The solution requires calculation of the internal energies of burned (E_b) and unburned (E_u). The calculations of the internal energies are discussed in appendix (B).

2.2 TURBULENT ENTRAINMENT

After ignition, the unburned mass will be entrained into the flame zone at a rate determined by (Blizard and Keck, 1974)

$$\frac{dm_e}{dt} = \rho_u A_e u_e \tag{11}$$

where m_e is the entrained mass, ρ_u is the unburned density, A_e is the flame front area, u_e is the entrainment velocity. Models for the flame front area and entrainment velocity are required. The flame front is assumed to grow spherically from the spark plug located at the top of the disk shape combustion chamber (Figure 1). The model for entrainment velocity is taken from Tabaczynski et al (1977). The authors extended the model for entrainment velocity given by Blizard and Keck (1974) by assuming that the entrainment velocity u_e is equal to the sum of the turbulence intensity u' (root mean square of the velocity fluctuation component) and the laminar flame speed S_l.

$$u_e = u' + S_l \tag{12a}$$

However, Daneshyar and Hill (1988) estimated the entrainment velocity using the following relation,

$$u_e = \sqrt{\frac{2\rho_u}{3\rho_b}}u' + S_l \qquad (12b)$$

where ρ_u is the unburned density and ρ_b is the burned density. Milane and Hill (1988) confirmed the validity of this relationship with extensive experimental work, and suggested that equation (12b) is a better model than equation(12a). Therefore, the present study uses equation(12b) for the entrainment velocity. The laminar flame speed model of van Tiggelen (1957) is used,

$$S_l = KC_m[Y_f^a Y_{O_2}^b exp(-\frac{E}{RT_m})]^{1/2} \qquad (13)$$

$$C_m = \sqrt{\frac{8RT_m}{\pi M_r}}$$

$$K = \frac{2T_u}{\sqrt{3\pi T_m}}(\frac{P}{P_r})^\alpha$$

$$T_m = T_u + 0.74(T_b^o - T_u)$$

where C_m is the mean molecular speed of chain carriers whose mean molecular weight is M_r. Y_f is the mole fraction of fuel molecules in the unburned mixture, Y_{O_2} is the mole fraction of oxygen molecules in unburned mixture, a and b are reaction orders with respect to fuel and oxygen respectively, and E is the activation energy. T_m is the mean temperature of the reaction zone as proposed by van Tiggelen and Duval (1967). K is a dimensionless parameter dependent on pressure P and P_r is equal to 1 atm. The kinetic parameters for propane proposed by van Tiggelen (1957) are

$$M_r = 31\ g/mole \qquad \alpha = -0.06$$
$$a = -0.46 \qquad b = 1.46$$
$$E = 37.7\ Kcal/mole$$

The turbulence intensity in equation (12b) is described by the rapid distor-

tion theory for compression of spherical eddies as discussed in Morel and Mansour (1982),

$$\frac{1}{K}\frac{dK}{dt} = -\frac{2}{3}D \tag{14}$$

where the turbulent kinetic energy K is $\frac{3}{2}u'^2$ and D is the velocity divergence. The conservation of mass is

$$\frac{1}{\rho}\frac{d\rho}{dt} = -D \tag{15}$$

where ρ is the density. Replacing D in equation (14) by equation (15),

$$\frac{1}{K}\frac{dK}{dt} = \frac{2}{3}\frac{1}{\rho}\frac{d\rho}{dt} \tag{16}$$

Here the turbulence is assumed homogeneous in the combustion chamber. At any time after intake valve closing, the turbulence intensity is calculated by integrating equation (16),

$$u' = u'_o\left(\frac{\rho_{u,o}}{\rho_u}\right)^{1/3} \tag{17}$$

where u'_o is the turbulence intensity at intake valve closing, $\rho_{u,o}$ is the unburned density at intake valve closing, and ρ_u is the instantaneous unburned density.

At any instant of time, the turbulence intensity, the laminar flame speed and entrainment velocity are calculated by subroutine SPEED listed in appendix (C).

2.3 TURBULENT MIXING

The entrained volume behind the flame front is considered to be a partially stirred reactor, where binary mixing of particles is assumed (Pratt,1976). The number of mixing pairs in a given period of time Δt is determined by the mixing frequency and the total number of particles in the reactor,

$$N_m = \omega N_t \Delta t \tag{18}$$

where N_m is the number of mixing pairs, N_t is the total number of particles in reactor, and ω is the mixing frequency.

2.3.1 MIXING FREQUENCY

The mixing frequency is related to the turbulent kinetic energy K_T, and dissipation of the turbulent kinetic energy E_T (see Milane et al, 1983) as,

$$\omega \sim \frac{E_T}{K_T} \tag{19}$$

The dissipation is expressed as,

$$E_T \sim \frac{K_T^{3/2}}{L} \tag{20a}$$

where L is the integral length scale.

The conservation of angular momentum of large eddies gives;

$$K_T^{1/2} L \sim constant \tag{21}$$

Substituting for L in equation (20a) using equation (21), the dissipation is expressed as,

$$E_T \sim K_T^2 \tag{20b}$$

Replacing for E_T in equation (19) using equation (20b),

$$\omega = C u'^2 \tag{22}$$

where C is an empirical constant to be determined using experimental data.

2.3.2 RANDOM SELECTION OF MIXING PAIRS

Each particle in the partially stirred reactor is assigned a number according to the order in which it enters the reactor. A random number generator is used to select the N_m pairs which will mix. The random number generator is described in subroutine GGUD, whose listing is in the IMSL library of the main frame computer of University of Ottawa. Subroutine GGUD selects a desired number of integers between one and the total number of particles (N_t) in the entrained volume. Subroutine GGUD is called N_m times. Two integers representing the mixing pair are selected each time. If any one of the two particles has already been selected in the same period of time, subroutine GGUD is called again until a new pair of particles is selected.

2.3.3 BINARY MIXING

The mixing process assumes that two particles mix and separate instantaneously. They become identical after mixing. During the mixing process, the composition is assumed 'frozen'. Therefore, the conservation of species applied to the system of two particles yields that the fuel fraction (ratio of mass of fuel to total mass) after mixing is the arithmetic average fuel fraction of the two particles before mixing,

$$F_3 = \frac{F_1+F_2}{2} \tag{23}$$

where F_1 and F_2 are the fuel fraction of the two particles before mixing and F_3 is their fuel fraction after mixing. The total volume does not change during mixing because the composition is frozen and mixing takes place instantaneously,

$$Vol_3 = \frac{Vol_1+Vol_2}{2} \tag{24}$$

where Vol_1, Vol_2 are the volume of the two particles before mixing and Vol_3 is the volume of each particle after mixing.

The temperature after mixing is calculated using the first law written for the pair of mixing particles,

$$dU = dQ - PdV$$

Since frozen composition is assumed, heat release by combustion and heat transfer to neighbouring particles is nil ($dQ = 0$), and the total volume does not change, ($dV = 0$). The first law becomes

$$dU = 0$$

therefore,

$$U_1 + U_2 = 2U_3 \qquad (25)$$

where U_1 and U_2 are the internal energies of two particles before mixing and U_3 is the internal energy of each particle after mixing .

The internal energies are calculated as a function of temperature and species composition (see appendix (B)). Equation (25) is solved by iterating on the temperature after mixing until the calculated internal energy converges to $2U_3$. These calculations are performed by subroutine MIXFRO listed in appendix (D).

The turbulent mixing is performed by subroutine RANMIX listed in appendix (E). The subroutine RANMIX calls subroutines GGUD and MIXFRO. The results of MIXFRO are the initial conditions of the thermodynamic states of particles for the time interval.

2.4 GOVERNING EQUATIONS FOR THERMODYNAMIC STATES

2.4.1 CHEMICAL RATE EQUATIONS

The global reaction equation for the combustion of propane and air is assumed for each burning particle,

$$C_3H_8 + \frac{5}{\phi}O_2 + \frac{5\times3.76}{\phi}N_2 \rightarrow (\frac{5}{\phi} - 5)O_2 + 3CO_2 + 4H_2O + \frac{5\times3.76}{\phi}N_2 \tag{26}$$

where ϕ is the equivalence ratio defined as

$$\phi = \frac{actual\ air\ fuel\ ratio}{stoichiometric\ air\ fuel\ ratio}$$

The reaction rate is described by the single step reaction mechanism of Westbrook and Dryer (1981),

$$\frac{dX_i}{dt} = -Aexp(-E/RT_i)X_i^aY_i^b \tag{27}$$

where X_i is the concentration of propane in moles/cc and subscript i denotes the ith burning particle, T_i is the temperature of the mixture, Y_i is the concentration of oxygen in moles/cc, A is the pre-exponential constant, E is the activation energy, and a, b are empirical constants. The authors suggested the following values of the constants for a single step propane in air reaction.

$$E = 30.0\ Kcal/mole \quad A = 8.6 \times 10^{11}\ Kcal/mole$$
$$a = 0.1 \qquad\qquad b = 1.65$$

(27) can be rewritten as

$$\frac{dx_i}{dt} = -Av_iexp(-E/RT_i)x_i^ay_i^b \tag{28}$$

where x_i, y_i are respectively the moles of fuel and oxygen per gram of mixture, and v_i is the specific volume of mixture. The rates of change of the number of moles of species per gram of mixture for oxygen y_i, carbon dioxide z_i, water w_i and nitrogen ν_i are related to that of propane x_i by the stoichiometric coefficients of the reaction equation (26),

$$\frac{dy_i}{dt} = 5\frac{dx_i}{dt} \tag{29}$$

$$\frac{dz_i}{dt} = -3\frac{dx_i}{dt} \tag{30}$$

$$\frac{dw_i}{dt} = -4\frac{dx_i}{dt} \tag{31}$$

$$\frac{d\nu_i}{dt} = 0 \tag{32}$$

2.4.2-RATE OF TEMPERATURE RISE OF A BURNING PARTICLE

The temperature of a burning particle which is required in (28) is calculated using the first law of thermodynamics applied to the individual particle i,

$$\frac{du_i}{dt} = q_i - P\frac{dv_i}{dt} \tag{33}$$

where u_i, q_i and v_i are specific quantities. In an adiabatic process the heat transfer is zero ($q = 0$). The specific internal energy is,

$$u_i = M_x x_i u_x + M_y y_i u_y + M_\nu \nu_i u_\nu + M_z z_i u_z + M_w w_i u_w \tag{34}$$

where $x_i, y_i, \nu_i, z_i, w_i$ are respectively the moles of species per gram of mixture for C_3H_8, O_2, N_2, CO_2 and H_2O for particle i, $M_x, M_y, M_\nu, M_z, M_w$ are molecular weight of species, in gram/mole of species and $u_x, u_y, u_\nu, u_z, u_w$ are specific internal energies of species in cal/gram of species. The derivative of equation (34) is

$$\begin{aligned} du_i =& M_x x_i du_x + M_y y_i du_y + M_\nu \nu_i du_\nu + M_w w_i du_w \\ &+ M_x u_x dx_i + M_y u_y dy_i + M_\nu u_\nu d\nu_i + M_z u_z dz_i + M_w u_w dw_i \end{aligned} \tag{35}$$

The change of internal energy of each species is expressed in terms of the specific heat at constant volume C_v.

$$du_x = C_{v_x} dT_i$$

$$du_y = C_{v_y} dT_i$$

$$du_\nu = C_{v_\nu} dT_i$$

$$du_z = C_{v_z} dT_i$$

$$du_w = C_{v_w} dT_i$$

Replacing the above terms as well as dy_i, $d\nu_i, dz_i, dw_i$ in equations (35) using equations (29), (30), (31), (32), and rearranging,

$$\begin{aligned}\frac{du_i}{dt} =& (M_x x_i C_{v_x} + M_y y_i C_{v_y} + M_\nu \nu_i C_{v_\nu} + M_z z_i C_{v_z} + M_w w_i C_{v_w}) \frac{dT_i}{dt} \\ &+ (M_x u_x + 5M_y u_y - 3M_z u_z - 4M_w u_w) \frac{dx_i}{dt}\end{aligned} \tag{36}$$

Eliminating the derivative of internal energy by equating equation (33) and equation (36) and rearranging,

$$\frac{dT_i}{dt} = \frac{-\frac{dx_i}{dt}(M_x u_x + 5M_y u_y - 3M_z u_z - 4M_w u_w) - P\frac{dv_i}{dt}}{M_x x_i C_{v_x} + M_y y_i C_{v_y} + M_\nu \nu_i C_{v_\nu} + M_z z_i C_{v_z} + M_w w_i C_{v_w}} \tag{37}$$

The derivative of specific volume ($\frac{dv_i}{dt}$) is required in equation (37). The perfect gas law applied to particle i,

$$Pv_i = \frac{n_i}{m} RT_i$$

where m is the mass of the particle, R is the universal gas constant and n_i is the

$$n_i = m(x_i + y_i + \nu_i + z_i + w_i)$$

Therefore, the specific volume v_i is expressed as,

$$v_i = \frac{(x_i+y_i+\nu_i+z_i+w_i)RT_i}{P}$$

The derivative of specific volume is

$$\frac{dv_i}{dt} = \left(\frac{dx_i}{dt} + \frac{dy_i}{dt} + \frac{d\nu_i}{dt} + \frac{dy_i}{dt} + \frac{dw_i}{dt}\right)\frac{RT_i}{P} + (x_i + y_i + \nu_i + z_i + w_i)\frac{R}{P}\frac{dT_i}{dt} - (x_i + y_i + \nu_i + z_i + w_i)\frac{RT_i}{P^2}\frac{dP}{dt} \tag{38}$$

Substituting $\frac{dv_i}{dt}$ (equation (38)) in equation (37), and simplifying using equations (29) to (32),

$$\frac{dT_i}{dt} = \frac{\frac{dx_i}{dt}[RT_i - (M_x u_x + 5M_y u_y - 3M_z u_z - 4M_w u_w)] + (x_i+y_i+\nu_i+z_i+w_i)\frac{RT_i}{P}\frac{dP}{dt}}{(M_x x_i C_{v_x} + M_y y_i C_{v_y} + M_\nu \nu_i C_{v_\nu} + M_z z_i C_{v_z} + M_w w_i C_{v_w}) + (x_i+y_i+\nu_i+z_i+w_i)R} \tag{39a}$$

Equation (39a) is composed of several terms. The internal energy per mole of mixture for particle i is,

$$Um_i = M_x u_x + 5M_y u_y - 3M_z u_z - 4M_w u_w$$

The specific heat at constant volume of particle i is,

$$C_{v_i} = M_x x_i C_{v_x} + M_y y_i C_{v_y} + M_\nu \nu_i C_{v_\nu} + M_z z_i C_{v_z} + M_w w_i C_{v_w}$$

The number of moles per gram of mixture in particle i is,

$$N_i = x_i + y_i + \nu_i + z_i + w_i$$

Equation (39a) is rewritten as

$$\frac{dT_i}{dt} = \frac{\frac{dx_i}{dt}(RT_i - Um_i) + N_i(\frac{RT_i}{P})\frac{dP}{dt}}{C_{v_i} + (N_i)(R)} \tag{39b}$$

2.4.3 RATE OF PRESSURE RISE OF THE SYSTEM

The rate of change of temperature of a burning particle depends on the value of pressure, the rate of change of pressure, and the concentrations of different species. The rate of change of pressure in the system is derived using the perfect gas law applied to the ensemble of particles in the chamber, composed of N_1 burning, N_2 unburned and N_3 burned particles. The perfect gas law applied to each burning particle is

$$PV_i = n_i RT_i \tag{40a}$$

where R is the universal gas constant. The perfect gas law applied to N_1 burning particles is

$$P\sum_{i=1}^{N_1} V_i = R\sum_{i=1}^{N_1} n_i T_i \tag{40b}$$

The perfect gas law applied to each unburned particle is

$$PV_u = n_u RT_u \tag{41a}$$

where

$$n_u = m(X_u + Y_u + \nu_u)$$

The perfect gas law applied to N_2 identical unburned particles is

$$N_2 PV_u = N_2 n_u RT_u \tag{41b}$$

The perfect gas law applied to each burned particle is

$$PV_j = n_j R T_j \tag{42a}$$

where $$n_j = m(Y_j + Z_j + \nu_j + W_j)$$

The perfect gas law applied to N_3 burned particles is

$$P \sum_{j=1}^{N_3} V_j = R \sum_{j=1}^{N_3} n_j T_j \tag{42b}$$

Therefore, the perfect gas law applied to the ensemble of particles is obtained by summing equations (40b), (41b), (42b),

$$P(\sum_{i=1}^{N_1} V_i + N_2 V_u + \sum_{j=1}^{N_3} V_j) = R(\sum_{i=1}^{N_1} n_i T_i + N_2 n_u T_u + \sum_{j=1}^{N_3} n_j T_j) \tag{43a}$$

The volume of the chamber V is expressed as,

$$V = (\sum_{i=1}^{N_1} V_i + N_2 V_u + \sum_{j=1}^{N_3} V_j)$$

Therefore, equation (43a) is written as,

$$PV = R(\sum_{i=1}^{N_1} n_i T_i + N_2 n_u T_u + \sum_{j=1}^{N_3} n_j T_j) \tag{43b}$$

The expression for the rate of pressure rise is calculated by taking the derivative of equation (43b),

$$\begin{aligned} V\frac{dP}{dt} + P\frac{dV}{dt} &= R[\sum_{i=1}^{N_1}(T_i\frac{dn_i}{dt} + n_i\frac{dT_i}{dt}) + N_2(T_u\frac{dn_u}{dt} + n_u\frac{dT_u}{dt}) \\ &\quad + \sum_{j=1}^{N_3}(T_j\frac{dn_j}{dt} + n_j\frac{dT_j}{dt})] \end{aligned} \tag{44}$$

The composition of the unburned and burned particles does not change, therefore the number of moles remains constant,

$$\frac{dn_u}{dt} = \frac{dn_j}{dt} = 0 \tag{45}$$

Also, the rate of change of the number of moles for each burning particle is

$$\frac{dn_i}{dt} = m(\frac{dx_i}{dt} + \frac{dy_i}{dt} + \frac{dv_i}{dt} + \frac{dz_i}{dt} + \frac{dw_i}{dt})$$

Replacing $\frac{dy_i}{dt}$, $\frac{dv_i}{dt}$, $\frac{dz_i}{dt}$ and $\frac{dw_i}{dt}$ using equations (29) to (32),

$$\frac{dn_i}{dt} = -m\frac{dx_i}{dt} \tag{46}$$

Therefore equation (44) is rewritten as,

$$V\frac{dP}{dt} + P\frac{dV}{dt} = R[\sum_{i=1}^{N_1}(-mT_i\frac{dx_i}{dt} + n_i\frac{dT_i}{dt}) + N_2 n_u\frac{dT_u}{dt} + \sum_{j=1}^{N_3} n_j\frac{dT_j}{dt}]$$

(47)

The derivatives of the temperature of burned and unburned are calculated assuming isentropic relations. The temperature of the unburned particle is,

$$T_u = T_{u,o}(\frac{P}{P_o})^{\frac{\gamma_u - 1}{\gamma_u}} \tag{48}$$

where $T_{u,o}$ and P_o are initial unburned temperature and pressure, and γ_u is the ratio of specific heat for unburned gas at T_u and P. The temperature of a burned particle is,

$$T_j = T_{j,o}(\frac{P}{P_o})^{\frac{\gamma_j - 1}{\gamma_j}} \tag{49}$$

where $T_{j,o}$ is the initial temperature of burned particle j and γ_j is the ratio of specific heat of particle j at T_j and P.

Therefore, the rates of change of unburned and burned temperatures are respectively,

$$\frac{dT_u}{dt} = T_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u - 1}{\gamma_u}}(\frac{\gamma_u - 1}{\gamma_u})P^{-\frac{1}{\gamma_u}}\frac{dP}{dt} \tag{50}$$

and

$$\frac{dT_j}{dt} = T_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j - 1}{\gamma_j}}(\frac{\gamma_j - 1}{\gamma_j})P^{-\frac{1}{\gamma_j}}\frac{dP}{dt} \tag{51}$$

Replacing $\frac{dT_u}{dt}$ and $\frac{dT_j}{dt}$ in equation (44) by equation (50) and (51),

$$V\frac{dP}{dt} + P\frac{dV}{dt} = R\Big\{\sum_{i=1}^{N_1}(-mT_i\frac{dx_i}{dt} + n_i\frac{dT_i}{dt}) + N_2 n_u T_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u-1}{\gamma_u}}(\frac{\gamma_u-1}{\gamma_u})P^{-\frac{1}{\gamma_u}}\frac{dP}{dt} + \sum_{j=1}^{N_3}[n_j T_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j-1}{\gamma_j}}(\frac{\gamma_j-1}{\gamma_j})P^{-\frac{1}{\gamma_j}}\frac{dP}{dt}]\Big\} \tag{52}$$

Now, the term $\frac{dT_i}{dt}$ is eliminated from equation (52) using equation (39b),

$$V\frac{dP}{dt} + P\frac{dV}{dt} = R\Big\{\sum_{i=1}^{N_1}\Big(-mT_i\frac{dx_i}{dt} + n_i\frac{\frac{dx_i}{dt}(RT_i - Um_i) + N_i(\frac{RT_i}{P})\frac{dP}{dt}}{C_{v_i} + (N_i)(R)}\Big) + N_2 n_u T_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u-1}{\gamma_u}}(\frac{\gamma_u-1}{\gamma_u})P^{-\frac{1}{\gamma_u}}\frac{dP}{dt} + \sum_{j=1}^{N_3}[n_j T_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j-1}{\gamma_j}}(\frac{\gamma_j-1}{\gamma_j})P^{-\frac{1}{\gamma_j}}\frac{dP}{dt}]\Big\}$$

Rearranging,

$$\frac{dP}{dt} = \frac{R\sum_{i=1}^{N_1}\Big\{\frac{dx_i}{dt}[-mT_i + \frac{n_i(RT_i - Um_i)}{C_{v_i} + N_i(R)}]\Big\} - P\frac{dV}{dt}}{\Big\{V - \sum_{i=1}^{N_1}[\frac{n_i N_i \frac{RT_i}{P}}{C_{v_i} + N_i(R)}] - N_2 n_u T_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u-1}{\gamma_u}}(\frac{\gamma_u-1}{\gamma_u})P^{-\frac{1}{\gamma_u}} - \sum_{j=1}^{N_3}[n_j T_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j-1}{\gamma_j}}(\frac{\gamma_j-1}{\gamma_j})P^{-\frac{1}{\gamma_j}}\Big\}} \tag{53}$$

The set of ordinary differential equations describing the evolution of thermodynamic properties during a time interval is equation (28), (29), (30), (31), (32), (39b) for each burning particle and equation (53) for the entire ensemble of particles. Therefore, the number of equations is $6N_1 + 1$, for N_1 burning particles. The unknowns are the number of moles of the five species (C_3H_8, O_2, N_2, CO_2, H_2O) per gram of mixture in each burning particle ($5N_1$ unknowns), the temperature of each burning particle (another N_1 unknowns), and the pressure in the chamber. Therefore, a total of $6N_1 + 1$ unknowns are to be solved. This set of equations is

handled by subroutine KINET in appendix (F).

CHAPTER 3
METHODS OF SOLUTION

After ignition, the flame propagation, turbulent mixing and chemical reaction take place simultaneously. The governing equations are solved numerically by discretizing the continuous phenomena of flame propagation and turbulent mixing. The solution procedure of ignition, turbulent entrainment, binary mixing, and the thermodynamic states of particles are discussed in the following sections.

3.1 IGNITION

As discussed in section 2.1, ignition is described by three equations, equations (7), (8), and (9). The three unknowns are the temperatures of the burned particles T_b and unburned particles T_u, and the pressure of the system P. The mixture conditions before ignition are calculated assuming isentropic compression from the closing of the intake valve to the time of ignition,

$$P_o = P_{in}(\frac{V_o}{V_{in}})^{\gamma} \tag{54}$$

$$T_o = Tin(\frac{P_o}{P_{in}})^{\frac{\gamma-1}{\gamma}} \tag{55}$$

where P_{in} and T_{in} are pressure and temperature at the closing of the intake valve, V_{in} is the chamber volume at closing of the intake valve, P_o and T_o are respectively the pressure and temperature after the spark event when the chamber volume is V_o, and γ is the specific heat ratio of the unburned mixture.

The volumes V_{in} and V_o corresponding to given crank angles are calculated by function subroutine VTO(CA). This function calculates the volume of the com-

bustion chamber as a function of crank angle, given the cylinder dimensions (see Table 1). The listing of VTO(CA) is in appendix (G)

The ratio of specific heat γ is obtained from subroutine UPROP in appendix (II). Since γ is dependent on temperature, its value is updated for new temperature every 0.5 crank angle using equations (54) and (55).

Now that the mixture conditions before ignition are obtained, the governing equations of ignition, equations (7),(8) and (9), can be solved,

$$E_u = E_{u,o} - \frac{P+P_o}{2}(V_{u,o}(\frac{P_o}{P})^{1/\gamma} - V_{u,o}) \tag{7}$$

$$E_b = E_{b,o} + E_{ign} - \frac{P+P_o}{2}(\frac{N_b R_b T_b}{P} - V_{b,o}) \tag{8}$$

$$V = V_u + V_b \tag{9}$$

An iteration method is used :

1. The initial guess of pressure P is taken as the pressure before ignition.

2. This pressure is used to calculate the volume and temperature of unburned gas assuming isentropic relations,

$$V_u = V_{u,o}(\frac{P_o}{P})^{\frac{1}{\gamma}} \tag{56}$$

$$T_u = T_o(\frac{P_o}{P_{in}})^{\frac{\gamma-1}{\gamma}} \tag{57}$$

3. The volume of burned gas is calculated using (9),

$$V_b = V - V_u$$

4. The temperature of burned gas is given by the perfect gas law,

$$T_b = \frac{V_b P}{n_b R_b}$$

5. The internal energies of burned and unburned after ignition, E_b and E_u, are obtained by subroutines CLDPRD and UPROP in appendix (H). The method of calculation is explained in appendix (B).

6. The internal energies before ignition for the unburned gas within the spark gap $E'_{b,o}$ and the rest of the chamber $E'_{u,0}$ are calculated by equations (7) and (8).

7. If the calculated values of $E'_{u,o}$ and $E'_{b,o}$ are close to the actual values $E_{u,o}$ and $E_{b,o}$ corresponding to the temperatures before ignition, the solution has converged.

$$\frac{|E'_{u,o}-E_{u,o}|}{E_{u,o}} < \epsilon$$

and

$$\frac{|E'_{b,o}-E_{b,o}|}{E_{b,o}} < \epsilon$$

where ϵ is a small positive number.

8. If their calculated values are either greater or smaller than the actual values,

$$\frac{|E'_{u,o}-E_{u,o}|}{E_{u,o}} > \epsilon$$

or

$$\frac{|E'_{b,o}-E_{b,o}|}{E_{b,o}} > \epsilon$$

then the pressure is guessed using the Half Interval Method (Carnahan et al, 1969), and the solution is iterated again from step (2).

3.2 TURBULENT ENTRAINMENT

Mass entrainment is calculated by integrating equation (11) using Euler's rule

$$m_e(t+\Delta t) - m_e(t) = \rho_u A_e u_e \Delta t \tag{58}$$

where $m_e(t+\Delta t)-m_e(t)$ is the mass to be entrained in the time interval Δt. This mass $m_e(t+\Delta t)-m_e(t)$ may not correspond to an integer number of particles. Any fraction in excess of the integer is counted in the next time interval. Now, the flame front area A_e is calculated assuming that the flame propagates hemispherically from the spark plug (see Figure 1). In general, the volume of this hemisphere can be written as

$$V_e = \int_0^h (\alpha r^2 + \beta {R_c}^2 - r_s R sin\beta) dz \tag{59a}$$

where,

$$cos\alpha = (r_s^2 + r^2 - {R_c}^2)/2r_s r \tag{59b}$$

$$cos\beta = (r_s^2 + {R_c}^2 - r^2)/2r_s R_c \tag{59c}$$

$$r^2 = r_e^2 - z^2 \tag{59d}$$

α,β,r and z are shown in Figure 1, R_c is half the bore of the cylinder, h is the chamber height, and r_e is the entrainment radius. Before the flame reaches the piston and the side wall, α is equal to π and β is equal to 0. Therefore, (59a) is simplified to

$$V_e = \frac{2}{3}\pi r_e^3 \tag{60}$$

and the flame front area is

$$A_e = 2\pi r_e^2 \tag{61}$$

After the flame reaches the piston or the side wall, a Newton Raphson iteration

method is required to calculate the flame front area. (59a) is rewritten as

$$F(r_e) = \int_0^h (\alpha r^2 + \beta {R_c}^2 - r_s R sin\beta) dz - V_e \tag{62}$$

The derivative of $F(r_e)$ with respect to the entrained radius r_e is also required in the Newton Raphson method,

$$\frac{dF(r_e)}{dr_e} = A_e(r_e) = 2r_e \int_0^h \alpha dz \tag{63}$$

An initial guess of r_e is needed to start the iteration. The $(K+1)_{th}$ iterated value of r_e in terms of its K_{th} iterated value, according to the Newton Raphson method, is

$$r_{e,k+1} = r_{e,k} - \frac{F(r_{e,k})}{A(r_{e,k})} \tag{64}$$

The solution converges when the following is satisfied,

$$|r_{e,k+1} - r_{e,k}| < \varepsilon$$

where ε is a small positive number. This method essentially iterates on $F(r_e)$ until it is equal to a small number. Once the solution for r_e is calculated, the flame front area $A_e(r_e)$ is obtained from equation (63). The above calculation of the flame front area is performed by the subroutine SHAPE; the listing is found in appendix (I).

3.3 BINARY MIXING

The thermodynamic states of the mixing pairs are calculated for burning and burned particles. In order to recognize whether a particle is unburned, burning or burned, an index is assigned to each of them according to the fuel fraction. If a particle's fuel fraction is equal to that of an unburned particle, the index is assigned to be 2. If the fuel fraction is zero, it is fully burned, and the index is 3. Otherwise, the index is 1, indicating a burning particle. The mass of fuel is related to the

concentration. The fuel fraction of an unburned particle can be determined by the stoichiometic coefficients of the chemical reaction equation.

The thermodynamic state of a particle is determined by its composition, volume and temperature. The composition and volume of particles after mixing are their average values before mixing. The temperature after mixing is given by the first law (equation (25)),

$$U_1 + U_2 = 2U_3$$

An iteration procedure is used to obtain the final temperature corresponding to the internal energy U_3.

1. The initial guessed temperature T_{guess} is the average temperature of the pair before mixing.

2. The total internal energy U_{guess} is calculated from T_{guess} using polynomial curve fitting of thermodynamic properties in the JANAF Tables (1971). The method of calculation is decribed in appendix (B).

3. If the calculated internal energy $U_{guess}$is close to the actual value $2U_3$, the solution of the temperature is adequate.

$$\frac{|2U_3 - U_{guess}|}{2U_3} < \epsilon$$

4. Otherwise, the temperature is adjusted to T_{next} as follows, and iteration repeated from step (2).

$$2U_3 - U_{guess} = mC_v(T_{next} - T_{guess}) \tag{65}$$

C_v is the heat capacity at constant volume. Rearranging equation (65),

$$T_{next} = \frac{U_{exact} - U_{guess}}{mC_v} + T_{guess} \tag{66}$$

3.4 GOVERNING EQUATIONS FOR THERMODYNAMIC STATES

The thermodynamic state of a burning particle is determined by the species concentrations, temperature and volume. These properties are calculated using the chemical rate equations for propane, oxygen, carbon dioxide, water, nitrogen and the equation for the rate of temperature rise of a burning particle.

$$\frac{dx_i}{dt} = -Av_i exp(-E/RT_i) x_i^a y_i^b \tag{28}$$

$$\frac{dy_i}{dt} = 5\frac{dx_i}{dt} \tag{29}$$

$$\frac{dz_i}{dt} = -3\frac{dx_i}{dt} \tag{30}$$

$$\frac{dw_i}{dt} = -4\frac{dx_i}{dt} \tag{31}$$

$$\frac{d\nu_i}{dt} = 0 \tag{32}$$

$$\frac{dT_i}{dt} = \frac{\frac{dx_i}{dt}(RT_i - Um_i) + N_i(\frac{RT_i}{P})\frac{dP}{dt}}{C_{v_i} + (N_i)(R)} \tag{39b}$$

Equations (29) to (32) can be replaced by algebraic relationships,

$$y_i = y_{i,o} + 5(x_i - x_{i,o}) \tag{67}$$

$$z_i = z_{i,o} - 3(x_i - x_{i,o}) \tag{68}$$

$$w_i = w_{i,o} - 4(x_i - x_{i,o}) \tag{69}$$

$$\nu_i = \nu_{i,o} \tag{70}$$

where the initial moles of species per grams of mixture are $y_{i,o}, z_{i,o}, w_{i,o}, \nu_{i,o}$ respectively.

The thermodynamic properties of burned and unburned particles are calcu-

lated using the isentropic relations provided by the equation for the rate of pressures rise,

$$\frac{dP}{dt} = \frac{R\sum_{i=1}^{N_1}\left\{\frac{dx_i}{dt}[-mT_i+\frac{n_i(RT_i-Um_i)}{C_{v_i}+N_i(R)}]\right\}-P\frac{dV}{dt}}{\left\{V-\sum_{i=1}^{N_1}[\frac{n_iN_i\frac{RT_i}{P}}{C_{v_i}+N_i(R)}]-N_2n_uT_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u-1}{\gamma_u}}(\frac{\gamma_u-1}{\gamma_u})P^{-\frac{1}{\gamma_u}}-\sum_{j=1}^{N_3}[n_jT_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j-1}{\gamma_j}}(\frac{\gamma_j-1}{\gamma_j})P^{-\frac{1}{\gamma_j}}]\right\}} \tag{53}$$

where the following terms in equation (53) calculate the rate of temperature rise for the unburned and burned particles respectively.

$$T_{u,o}(\frac{1}{P_o})^{\frac{\gamma_u-1}{\gamma_u}}(\frac{\gamma_u-1}{\gamma_u})P^{-\frac{1}{\gamma_u}}\frac{dP}{dt} = \frac{dT_u}{dt}$$

$$T_{j,o}(\frac{1}{P_o})^{\frac{\gamma_j-1}{\gamma_j}}(\frac{\gamma_j-1}{\gamma_j})P^{-\frac{1}{\gamma_j}}\frac{dP}{dt} = \frac{dT_j}{dt}$$

The ordinary differential equations (ODE), to be solved are the rate equation of propane (equation (28)), temperature of each burning particle (equation (39b)) given by the first law, and the pressure derivative (equation (53)). If the number of burning particles in a time step is N_1, then the ODE system consists of N_1 rate equations, N_1 temperature equations and one pressure equation, a total of $2N_1 + 1$ equations.

Several methods to solve the set of (ODE) are attempted, and the one with least computing time and moderate accuracy is selected. If no burning particles are present in the time interval, subroutine ISCOMP in appendix (J) is used to perform isentropic compression calculations.

3.4.1 ORDINARY DIFFERENTIAL EQUATION SOLVERS

The first method considered was DGEAR. This subroutine is in the IMSL

library of the main frame computer at the University of Ottawa. DGEAR is capable of dealing with a wide variety of ODE's. It uses the variable order Adams predictor corrector method if the user specifies that the ODE system is non-stiff, or the Gears backward differential formula if a stiff system is specified. The method of DGEAR was appealing because of its capability to solve a stiff system, which is typically the case for chemical rate equations. The program is accessible and ready to be used. The user specifies either one of the two basic methods (Adams or Gears), and the desired tolerance for error, the initial step size, and one of six methods of corrector iteration. DGEAR automatically selects the step size to minimize computing time. The algorithm is adapted from a package designed by Hindmarsh (1974) based on Gear's subroutine DIFSUB (1971). A similar method by Hindmarsh called LSODE (1980) was evaluated by Radhakrishnan (1985) for a batch reactor, and it was found to be very efficient for the test problem. However, upon testing DGEAR with the present model, DGEAR was found to be very sensitive to the specified tolerance, initial step size and corrector iteration method used, but relatively insensitive to whether the stiff method of Gear or the non-stiff method of Adams is used. Most importantly, the computing time was excessively long. The results constantly indicated that a large number of steps were taken. If the tolerance and initial step size is increased in order to reduce the number of steps, warning and error messages indicate that the step size was reduced more than once and the error bound was exceeded. After experimenting with different values of tolerance, initial step size and different corrector iteration methods, it was found that small tolerance and initial step size yielded most stable computation at the expense of longer computing time. The user attempted to obtain the listing of DGEAR in order to understand its detail algorithm, but did not succeed due to the copyright protection policy of IMSL. Both the Adams predictor corrector method and Gear backward differentiation formula are implicit linear multistep methods. Since DGEAR did not yield satisfactory results, an explicit one step method was considered.

The Runge-Kutta fourth order method is often used among explicit one step methods. Among the different Runge-Kutta methods, the one derived by England (1969) is a fourth order six stage method having an error estimate valid for a system of non-linear equations. The error estimate at each step is used to control step size and minimize the number of steps required, hence minimizing computing time. The initial step size and tolerance are required in this method. It was found that the solution is sensitive to the values of initial step size and tolerance. The iteration in each step requires excessive computing time, and the method was not as efficient as DGEAR. If the initial step size and tolerance are very small, England's method is even slower than DGEAR. However this method accepts large values of initial step size and tolerance but DGEAR does not. This study shows that DGEAR is more efficient than England for the same level of accuracy.

Since DGEAR and Runge-Kutta methods are designed for general systems of ODE, it was then decided to test a method specifically designed for chemical rate equations. A method developed by Young and Boris (1977) (called CHEMEQ) uses a second order predictor-corrector method. It determines the stiff equations among the system equations, and applies an asymptotic integration method. The other normal equations (non-stiff) are treated using Euler's predictor and the trapezoidal rule as the corrector. The user specifies the error tolerance. The initial step is automatically determined. The step size control is based on the number of iterations required to achieve convergence. If the step converges in a small number of iterations, the step size is increased. If the step does not converge within a specified number of iterations, the step size is reduced and the calculation of the step is repeated. The algorithm is simpler than the Runge-Kutta method, and most importantly, requires fewer iterations at each step.

3.4.2 THE ADOPTED METHOD

The method by Young and Boris (1977) is designed to solve chemical rate equation in the form of,

$$\frac{dx_i}{dt} = Q_i - \frac{x_i}{\tau_i} \tag{71}$$

where Q is the production rate and τ_i is the equilibration time. Rewriting equation (71),

$$\frac{dx_i(t)}{dt} = g_i(t) \tag{72}$$

where $$g_i(t) = Q_i(t) - \frac{x_i(t)}{\tau_i(t)} \tag{73}$$

The initial step size is taken as proportional to the minimum of the characteristic time $\frac{x_i(0)}{g_i(0)}$ among all the equations,

$$\delta t = \epsilon \; min\{\frac{x_i(0)}{g_i(0)}\} \tag{74}$$

where ϵ is a scale factor typically of order 10^{-3}. An equation is considered stiff if the production term Q_i and the dissipation term n_i/τ_i are large and nearly equal. This is determined by, $$\frac{\delta t}{\tau_i(0)} > 1 \tag{75}$$

For normal equations, Euler's method is used as predictor,

$$x_i(1) = x_i(0) + \delta t g_i(0) \text{ for normal equations.} \tag{76}$$

and the trapezoidal rule is used as the corrector,

$$x_i(m+1) = x_i(0) + \frac{\delta t}{2}[g_i(m) + g_i(0)] \tag{77}$$

For stiff equations, an asymptotic integration method is used. The predictor is,

$$x_i(1) = \frac{x_i(0)[2\tau_i(0) - \delta t] + 2\delta t \tau_i(0) Q_i(0)}{2\tau_i(0) + \delta t} \tag{78}$$

and the corrector is,

$$x_i(m+1) = \frac{\{\frac{\delta t}{2}[\tau_i(m) + \tau_i(0)]\}[Q_i(m) + Q_i(0)] + x_i(0)[\tau_i(m) + \tau_i(0) - \delta t]}{[\tau_i(m) + \tau_i(0) + \delta t]} \tag{79}$$

A step converges when consecutive corrector iterations yield nearly equal results, indicated by the local error being smaller than the specified tolerance,

$$\frac{|x_i(m+1)-x_i(m)|}{min[x_i(m+1),x_i(m)]} < \epsilon_3 \qquad (80)$$

where ϵ_3 is of order 10^{-3}. If convergence is not achieved in two to four iterations, the step size is reduced by a factor of two to three and the calculation of the step is repeated. This was found to be more efficient than reducing the step size by a factor of less than two. If convergence is achieved in one or two iterations, the step size is increased by 5-10% for the next step. It was found that increasing the step size by more than 10% would be less efficient due to the need to reduce the step size again in the next step.

Upon applying this method to the present problem, it was found that none of the equations met the criterion for stiffness. Therefore, only the predictor and corrector for normal equations are used. The fact that the chemical rate equations in this model are non-stiff may be explained by Radhakrishnan (1985), who stated that 'The problem of stiffness in chemical kinetics is the result of widely varying rates of change in different species'. Since there is only one rate equation for propane in the model, widely varying rates of change in different species are not present in the model. Also the initial step size is determined by equation (74) can sometimes be an order of magnitude smaller than the last step size used in the previous time interval. In order to prevent an excessively small initial step size, equation (74) is extended as,

$$\delta t = max[\epsilon \; min\{\frac{n_i(0)}{g_i(0)}\}, H_{last}, \triangle t/10] \qquad (81)$$

where H_{last} is the last step size used in the previous time interval and $\triangle t$ is the length of the present time interval.

It was found that five corrector iterations should be allowed before reducing step size and repeating the step in order to minimize the required number of steps

and avoid an excessive reduction of step size. If more than five corrector iterations are required, step size is reduced by a factor of two to five.

$$H_{new} = max\{min(\delta t/2, \delta t/S), \delta t/5\} \tag{82}$$

where H_{new} is the new step size, δt is the step size to be reduced, and

$$S = \frac{\frac{|x_i(m+1)-x_i(m)|}{min|x_i(m+1),x_i(m)|}}{\epsilon_3}$$

S is the ratio of local error to the specified tolerance ϵ_3. It is greater than one when convergence has not been achieved. S measures the difference between the actual error and its desired value (ϵ_3). If this ratio S is less than two, the step size is reduced by a factor of two. If S is between two and five, the step size is reduced by a factor of S. If S is greater than five, the step size is reduced by a factor of five. Reducing the step size by a factor of two to five is more efficient than reducing it by a factor of two to three as used by Young and Boris (1977). The step size is allowed to be reduced up to three times, after which computation is stopped. If a step converges within two corrector iterations, the next step size is increased by 50% to minimize the number of steps. The total number of steps allowed is one hundred; however, warning messages are issued when the number of steps exceeds fifty. Computation is stopped when the number of steps exceeds one hundred. The method being adopted is more efficient than DGEAR and Runge-Kutta when moderate accuracy is required. The listing of this ODE solver subroutine CODE is in appendix (K).

3.5 OVERALL SOLUTION PROCEDURE

The solutions for ignition, entrainment, mixing and thermodynamic states of particles are calculated using the following procedure.

1. Specify the input parameters at the closing of the intake valve, namely

the crank angle at which the intake valve closes, the turbulence intensity, mixture temperature, pressure, equivalence ratio, spark advance, spark duration, ignition energy, spark gap, number of particles to be ignited, engine RPM, time interval (see section 3.6), and the timing for the opening of the exhaust valve.

2. Calculate temperature and pressure before ignition, using the isentropic relations as discussed in the solution procedure for ignition (section 3.1).

3. Calculate temperature and pressure of burned and unburned gases after ignition, using the first law and volume constraint as discussed in the solution procedure for ignition (section 3.1).

4. The volume of the burned particles after ignition is considered to be the partially stirred reactor.

5. The surface area of the reactor is calculated using subroutine SHAPE. The entrainment velocity is calculated using subroutine SPEED. The number of unburned particles entering the reactor is calculated using the entrainment model as discussed in the solution procedure for turbulent entrainment (section 3.2).

6. The mixing frequency is calculated as a function of turbulence intensity. The number of mixing pairs is calculated as a function of the mixing frequency and the number of particles in the reactor.

7. The random number generator GGUD is called to select pairs of particles to be mixed. The results of each binary mixing is calculated using subroutine MIXFRO, as discussed in the solution procedure for binary mixing (section 3.3). The results of binary mixings are the initial thermodynamic states of particles at the beginning of the time interval.

8. The thermodynamic states of particles are calculated using the chemical rate equations, rate equations of temperature rise for each burning particle, and the rate equation of pressure rise for the system, which includes the isentropic relations for the compression of burned and unburned particles. The solution procedure for these equations is discussed in section 3.4.

9. The thermodynamic states of particles at the end of the time interval are used to calculate the volume and surface area of the partially stirred reactor for the next time interval.

10. Step (5) to (9) are repeated for the calculations of the next time interval, until misfire occurs or the exhaust valve opens.

3.6 APPROXIMATION OF PRESSURE DERIVATIVE

The computing time spent on the iteration of the rate of pressure rise (equation (53)) was found excessive regardless of the method used. The thermodynamic state of each particle, including the unburned particle outside the partially stirred reactor is updated in each iteration, consuming a large amount of computing time. The result showed that the pressure rise is smooth and increases slightly in for the time interval used in the study. Therefore, a linear pressure rise approximation in the time interval is adequate, and significant computing time is saved. The pressure rise is estimated using an iteration procedure.

1. The initial guessed pressure derivative is assumed to be the same as in the previous time interval.

$$\frac{dP}{dt} = \frac{P(t) - P(t-\Delta t)}{\Delta t}$$

2. The pressure during the time interval Δt is calculated using the guessed

pressure derivative,

$$P(t + \Delta t) = P(t) + \frac{dP}{dt}\Delta t$$

3. The system of ODE without the pressure equation is solved in the time interval.

4. Thermodynamic states of all particles are updated at the end of the time interval.

5. The volume constraint is used as the criterion of convergence. If the total volume is close to the chamber volume, then the solution is converged.

$$|V_p - V_t| < \epsilon$$

where ϵ is a small positive number.

6. Otherwise, the pressure derivative is adjusted using the perfect gas law applied to the chamber volume,

$$P_{next} = P(\frac{V_p}{V_t}) \tag{83}$$

$$\frac{dP}{dt} = \frac{(P_{next} - P_o)}{\Delta t} \tag{84}$$

where P_{next} is the next guessed pressure at the end of time interval, P is the pressure at the end of the time interval obtained from the present guessed pressure rise, V_p is the total volume of particles with the present guessed pressure rise, V_t is the chamber volume at the end of time interval, $\frac{dP}{dt}$ is the next guessed pressure rise, P_o is the pressure at the beginning of the time interval. The iteration is repeated from step (2).

A maximum of three iterations is allowed, after which computation is stopped.

This procedure eliminates the need of the rate of pressure rise equation, so that the number of equations to be solved by CODE is $2N_1$ where N_1 is the number of burning particles. This procedure is performed by subroutine KINET listed in appendix (F).

3.7 SELECTION OF TIME INTERVAL

As discussed in section 3.1, the flame propagation, turbulent mixing and chemical reaction take place simultaneously. Therefore, the time interval should be as short as possible for accurate simulation. However, computing time generally increases as the number of time intervals increases. On the other hand, if the time interval is long, all the burning particles will have sufficient time to become fully burned before being mixed with other particles, since all mixing occurs only at the beginning of each time interval. The quenching of the burning particles is not realistically modeled in this case, no matter how high the mixing frequency is. The balance between realistic simulation and computational efficiency should be considered.

In the early stage of the development of the model, a time interval corresponding to one crank angle degree at 1500 RPM was used. It was observed from the result that some of the burning particles remain burning if the pre-exponential constant in the rate equation is taken as 4.3×10^{11}, which is half of the value given in Westbrook and Dryer (1981). This constant is empirical and can be adjusted as suggested by Westbrook and Dryer. It affects the time scale in which a burning becomes a fully burned. The sensitivity to the selection of time interval was studied using one degree crank angle, one half degree crank angle and one quarter degree crank angle. The study showed that the use of different time intervals yielded the same solution. The use of a half degree crank angle resulted in less computing time than using one degree. This is due to the nature of the rate equations being

solved and the method of solution. When one crank angle interval was selected, the adopted method determined an initial step size, and proceeded with calculation until the portion of the solution where the rate of change was high, then the step size was reduced to follow the solution. In the case of half a degree crank angle interval, the slope of the solution did not vary as much, and computing time was saved since there was no need to reduce the step size. One quarter of a degree crank angle was also attempted, but no improvement was found. Therefore, one half crank angle degree was used for an engine speed of 1500 RPM. When engine speed is increased to 3000 RPM, one crank angle degree is selected.

CHAPTER 4
RESULTS AND DISCUSSION

The model was tested for the ignition limit and partial burn limit. The sensitivity of the model to turbulence, intake pressure and temperature, fuel equivalence ratio, spark advance, ignition energy, spark gap and engine speed were investigated for the ignition limit. Furthermore, the sensitivity of the model to the number of particles ignited and to the activation energy was also studied. For the partial burned limit, two cases of flame quenching at the expansion stroke were obtained. To determine if the cycle misfires, the mass burn fraction is calculated against the engine crank angle. The mass burn fraction is defined as the ratio of the mass of combustion product to the total mass of mixture in the combustion chamber. Misfire occurs when the mass burn fraction does not increase with respect to crank angle.

4.1 EMPIRICAL CONSTANTS IN MODEL

The empirical constants of the model should be adjusted using experimental data from an actual engine. However, since experimental investigation is beyond the scope of this study, typical values are used. Experimental results from other researchers have been considered. However, incomplete engine specifications prohibited precise comparison of data. The empirical constants are the constants in the mixing frequency expression and chemical rate equations.

The constant C (ω/u') in the mixing frequency expression was selected such that when the turbulent intensity u' is about 200 cm/sec, the mixing frequency ω will be about 700 Hz. The value of C is $0.017 sec/cm^2$. Figure 2 shows the sensitivity of the model to constant C for the engine operating conditions shown in Table 2. (

All results shown in graphs have a resolution of one crank angle degree.)

There are four constants in the chemical rate equation,

$$\frac{dX_i}{dt} = -AT_i exp(\frac{-E}{RT}) X_i^a Y_i^b \qquad (27)$$

Westbrook and Dryer (1981) proposed that the pre-exponential A was 8.6×10^{11} $Kcal/mole$, the activation energy E was 30.0 $Kcal/mole$, the concentration exponents for fuel and oxygen, a and b, were respectively 0.1 and 1.65. In their study, the authors adjusted the pre-exponetial and activation energy to predict the laminar flame speed. However, the values of these constants are not certain due to the absence of experimental data for the laminar flame thickness. In their work, the authors adjusted the value of the pre-exponential while keeping the activation energy at 30.0 $Kcal/mole$. In the present study, when the pre-exponential was 8.6×10^{11} and activation energy was 30.0 $Kcal/mole$, all the burning particles become fully burned in half a degree crank angle even at the equivalence ratio of 0.5. The pre-exponential constant was lowered to 50% of the suggested value. The result shows some burning particles remained burning in the same condition. Radhakrishnan and Pratt (1984) adjusted this constant to 60% of the value proposed by Westbrook and Dryer (1981). The activation energy E may also have to be adjusted (Hallett, 1988). The sensitivity of the present model to the pre-exponential and activation energy was investigated. The value for the activation energy E was varied from 25.0 to 40.0 $Kcal/mole$ and the pre-exponential constant was 8.3×10^{11}. Testing conditions are shown in Table 2. The results are shown in Figure 3. The burning rate is sensitive to the activation energy. It decreases with increasing activation energy, and misfire occurred when the activation energy was equal to 40.0 $Kcal/mole$. The activation energy represents the energy required to initiate chemical reaction. Therefore, it is reasonable to assume that burning rate decreases with increasing activation energy. The prediction of the model (Figure 3) confirms this trend.

The pre-exponential A was varied from 2.0×10^{11} to 8.6×10^{11} $Kcal/mole$.

The activation energy was kept at 30.0 $Kcal/mole$. The model is sensitive to the variation of the pre-exponential (Figure 4). However, the burning rate is more sensitive to the variation of activation energy than the pre-exponential. It varies exponentially with activation energy and linearly with the pre-exponential. Radhakrishnan and Pratt (1984) followed Westbrook and Dryer (1981), keeping the activation energy constant, and adjusting the pre-exponential. This approach is adopted in the present study. The following constants are used for chemical kinetics in the the present study.

$$E = 30.0\ Kcal/mole \quad A = 4.6 \times 10^{11}\ Kcal/mole$$
$$a = 0.1 \qquad\qquad b = 1.65$$

4.2 TURBULENCE INTENSITY

The sensitivity to turbulence intensity of the model was investigated. In these tests, the intake temperature and pressure respectively were $300°K$ and 0.5 atm. The mass per cycle was about 0.24 grams. The engine speed was set at 1500 RPM, and ignition at 60 degrees before top dead center. The ignition energy was 6 mJ and deposited to 10 particles in 2 crank angle degrees, corresponding to the ignition duration of 0.2 msec. The fuel equivalence ratio was 0.5. The turbulence intensity at the closing of the intake valve was varied from 1 m/sec to 2 m/sec, then varied again to 3 m/sec. The engine specification for all tests is shown in Table 1. The complete testing conditions are listed in Table 3. Each computer experiment took about 30 minutes of CPU time, which yielded about 20 crank angle degrees of results.

A comparison of the mass burned fraction of the three cases is shown in Figure 5. The model is sensitive to the changes in turbulence intensity. As turbulence intensity was increased from 1 m/sec to 2 m/sec, the mass burned fraction rate increased. This was due to the higher rate of mass entrainment and mixing frequency

when turbulence intensity was increased. When the turbulence intensity was further increased to 3 m/sec, the mass burn fraction increased even faster initially, but became constant after about 10 degrees. The flat portion of the curve shows that no burning took place after about 10 degrees after ignition. In other words, misfire occurred. At a high turbulence intensity, the rate of mixing was high. The burning particles were quenched by being mixed with unburned before having enough time to become fully burned. A mixing time can be defined as a characteristic time inversely proportional to the mixing frequency. It measures the duration between consecutive mixing events. When turbulence intensity is increased, the mixing frequency increases. As a result, the mixing time decreases. Therefore, the time available for undisturbed chemical reaction, which is the duration between consecutive mixings, is shorter at higher turbulence intensity.

At low turbulence intensity (1 m/sec), the mixing time is longer, and the mass burning rate is controlled by flame propagation and mixing rate. Therefore, higher turbulence intensity increases mass burning rate. At higher turbulence intensity (3 m/sec), the mixing time is shorter, and the mass burning rate is controlled by the chemical rate. Consequently, higher mixing frequency decreases mass burning rate. There is an optimum level of turbulence intensity at which the mass burning rate is highest. The result shows that 2 m/sec can be the optimum turbulence level for the given operating condition. The existence of an optimum turbulence intensity is consistent with the finding of Ho and Santavicca (1987) : the authors stated that wrinkling of the flame front by turbulence increases burning rate, while a very high level of turbulence extinguishes the flame.

The pressure traces for different turbulence intensities are essentially identical (see Figure 6). This is due to the small fraction of the mixture being burned. The pressure rise was mostly due to the compression by the piston, since the burned mass was less than 0.05 % . Such results were also observed in other tests in this study, except when mentioned otherwise.

Turbulence intensity in engines is a function of the design of the intake system. The level of turbulence at the closing of intake valve is a fraction of the volumetric flow velocity passing through the intake valve (see for example R.E. Milane et al, 1983). Therefore the turbulence intensity can be increased by reducing the valve lift and increasing the flow velocity. However, this will also affect the intake pressure and mass flow. On the other hand, increasing throttle or load to the engine also increases turbulence intensity due to the increased mass flow, but this will also increase the pressure. The previous results on the variation in turbulence intensity while keeping other variables constant are not applicable. The effect of pressure variation will be discussed in the following section, and the combined effect of turbulence intensity and pressure variation will also be investigated.

4.3 INTAKE PRESSURE

The change of pressure leads to a change in mass flow if temperature stays constant. Any change in mass flow rate affects the flow velocity across the intake valve, and in turn affect the turbulence intensity of the flow field. If the change of pressure is the result of changing the throttle position, the variation in turbulence intensity is linearly proportional to that of the pressure in the combustion chamber. The turbulence intensity, pressure and mass flow are functions of the valve geometry. The change of pressure can result from changing the valve lift. But the valve geometry is not known in this study, therefore only the case of constant intake valve area will be used in the testing.

The model was first tested for the variation of pressure while the turbulence intensity was kept constant. Complete testing conditions are listed in Table 4. The result shows that the mass burning rate decreased with increasing pressure, when the pressure was varied from 0.2 atm to 0.8 atm. (see Figure 7). This is the result of (39b) describing the temperature rate of the combustion of propane and

air mixture. This equation shows that temperature rate increases with decreasing pressure. The increase of temperature rate then causes an increase in mass burning rate. It is to be noticed that such an effect of variation of pressure alone does not usually occur in real engines, because any variation of pressure will also affect other variable such as the turbulence intensity as discussed above.

The model was tested for the effect of variation of pressure and turbulence intensity. The turbulence intensity is assumed to be linearly proportional to the intake pressure. Four different sets of pressure and turbulence intensity combinations were used. They were 0.4 atm with 1.6 m/s, 0.5 atm with 2.0 m/s, 0.65 atm with 2.6 m/s and 0.8 atm with 3.2 m/s, all taken at the closing of the intake valve. Spark advance was set at 60 degrees before top dead center, and intake temperature at 300 degrees Kelvin. Table 5 lists the complete testing conditions. The mass flow rates under these conditions varied from about 0.2 grams/cycle to 0.4 grams/cycle at an engine speed of 1500 RPM. The results show that the mass burning rates were higher for the case of higher pressure and turbulence intensity for the first 10 degrees crank angle after ignition (see Figure 8) , but the trend was reversed afterwards. The mass burning rate stayed at a constant level in the case of 0.8 atm with 3.2 m/s of turbulence, indicating that misfire has occurred. This is the result of flame quenching caused by high turbulence intensity and high rate of mixing between the burning and unburned particles. The overall effect of variation of pressure and turbulence intensity is very similar to that of the variation of turbulence intensity alone. In other words, turbulence intensity has a stronger influence on mass burning rate than the pressure has.

4.4 INTAKE TEMPERATURE

The model was tested for the sensitivity to the variation of intake temperature. The intake temperature is the temperature of fuel mixture in the combustion

chamber at the closing of the intake valve. This temperature is not necessarily the same as the temperature of the flow in the intake manifold or the ambient temperature. The relationship of these different temperatures are functions of the design of the particular intake system, which is beyond the scope of the present study.The model was tested with intake temperatures of $200°K$, $250°K$, $300°K$, $350°K$, and $400°K$. The intake pressure was 0.5 atm with the turbulence intensity at 2 m/s. The engine ran at 1500 RPM with the spark advance at 60 degrees before top dead center. Complete testing conditions are shown in Table 6. The mass flow rates of the three temperature settings ranged from 0.18 grams/cycle to 0.24 grams/cycle. The result of the variation of temperature indicates that the mass burning rate increases with increasing temperature (see Figure 9). Misfire occurs at $200°K$.

The pressure traces of the three cases are shown in Figure 10. The three pressure traces are very close to each other, and approximately parallel to one another. As expected in the ignition period, the mass burned fractions are small. However, we observe that at the lower intake temperature, the pressure was higher. The pressure rise at the initial period of combustion was not due to combustion itself, since the mass burned fraction was very small. Therefore, the pressure rise in this regime was the result of compression. The fuel mixture went through the same amount of change in volume for the three cases of different temperatures, but the ratio of specific heat for the mixture is a function of temperature. Its value decreases with increasing temperature for any given composition of the mixture. Therefore, the mixture at lower temperature will have a higher ratio of specific heat and a higher final pressure after compression. The resulted pressure traces show that the model is sensitive to the variation of the ratio of specific heat. A similar conclusion was also reached in the following section on the variation of the fuel equivalence ratio.

4.5 FUEL EQUIVALENCE RATIO

The model's sensitivity to the variation of equivalence ratio was one of the most important tests, since the most accepted definition of misfire limit is defined as the equivalence ratio at which combustion fails. The test was conducted with four different values of equivalence ratio, 0.3, 0.5, 0.7 and 0.9. The intake conditions were set at 300°K, 0.5 atm and a turbulence intensity of 2 m/s. The engine ran at 1500 RPM and the spark advance was set at 60 degrees before top dead center. Complete testing conditions are shown in Table 7. Results of Figure 11 indicate that burning rate increased with equivalence ratio. For an equivalence ratio of 0.3, misfire occurred after about 12 degrees from ignition. Although the result shows no misfire for the case of 0.5 equivalence ratio, it does not contradict with the result of other researches which suggested that the lean misfire limit was generally in the range of 0.6, because the testing result does not correspond to any actual engines. The model needs to be calibrated in order to generate more solid data instead of showing general trends.

The pressure traces in Figure 12 for the different fuel-air ratios also show trends similar to that of the variation of intake temperature. Again, the pressure traces are close together and approximately parallel because of the very small mass burned and heat release, but the one with the lower equivalence ratio is always higher than that with the higher equivalence ratio. The pressure rise was the result of compression since burned mass is small. The ratio of specific heat of the fuel mixture is now a function of composition. Its value increases with decreasing equivalence ratio. Therefore, the leaner mixture has a higher final pressure than the richer mixture for the same amount of change in volume due to compression.

4.6 SPARK ADVANCE

The spark advance was varied from 90 degrees before top dead center to 60 and 30 degrees before top dead center. The model was tested at 1500 RPM, with the fuel equivalence ratio of 0.5, and intake temperature and pressure as $350°K$ and 0.5 atm respectively. The turbulence intensity was 2 m/s at the closing of the intake valve. Table 8 shows the complete testing conditions. The variation of spark advance affects the temperature, pressure and turbulence intensity at ignition, whose values increase when spark timing is retarded. The results show that the mass burning rate increased when spark advance was retarded (see Figure 13). For the earliest spark advance (90 degrees BTDC), the burning was slow just after ignition, and misfire occurred after about 17 degrees. The volume in the spark gap which was ignited was the same for the three cases, but the mass was slightly higher when the spark timing was retarded (to 30 degrees before top dead center) because of higher density. This effect combined with the higher temperature and turbulence intensity at ignition resulted in an increase in the burning rate when spark timing was retarded to 30 degrees BTDC. The higher pressure at ignition, at 30 degrees BTDC, did not slow down the chemical reaction enough to affect the burning rate. Furthermore, the high turbulence intensity did not produce a quenching effect on the burning particles at high temperature, because the chemical time at high temperature was relatively short. Therefore the combined effect of higher temperature, pressure and turbulence intensity increases the mass burning rate.

The trend of misfiring when spark timing is advanced also agrees with the experiments of Anderson and Lim (1985). The ignition energy and spark gap used in this study were respectively 6 mJ and 1 mm. The spark duration during which the selected 10 particles became fully burned was 2 degrees, or about 0.2 msec at 1500 RPM. The influence of these ignition variables will be discussed in the following sections.

4.7 IGNITION ENERGY

Ignition energy refers to the energy deposited in the ignited particles from the spark, as described in Chapter 2. The amount of energy required to initiate combustion is not investigated in this study. The objective of this study is to investigate flame propagation after ignition. The influence of the ignition energy on the flame propagation was investigated using several ignition energies : 3 mJ, 6 mJ and 9 mJ. The engine speed was 1500 RPM and spark advance was 60 degrees before top dead center. The fuel equivalence ratio was 0.5, and the intake temperature and pressure were respectively $350°K$ and 0.5 atm. The turbulence intensity was 2 m/s at the closing of intake valve, and the spark gap was 1 mm. Table 9 lists the complete testing conditions. The result shows that the mass burning rate increased with increasing ignition energy (see Figure 14). The higher ignition energy caused the temperature of the ignited particles to increase, which in turn yielded a higher burning temperature when they mixed with other unburned particles. The adiabatic flame temperature increased from $2000°K$ to $2700°K$ as the ignition energy was increased from 3 mJ to 9 mJ. No misfire was observed even when the ignition energy was 3 mJ. This is not surprising. The model for ignition assumes that the mass within the spark gap is ignited, and initial flame propagation is supported by the heat release from the burned mass. In reality, heat is lost to the electrode, and a fraction of the mass within the spark may be ignited. Anderson and Lim (1985) related the minimum ignition energy to a quench distance, and stated that if the flame kernel grows to the size of the quench distance, propagation can be supported by the chemical heat release alone. Therefore, if the cases tested in the model had their initial flame kernel size at least as large as a theoretical quench distance, misfire due to insufficient ignition energy will not occur. The variation of spark gap size simulated by igniting a different initial volume represents another aspect of the effect of spark ignition on misfire.

4.8 SPARK GAP DISTANCE

The spark gap distances used were 0.5 mm, 1 mm and 2 mm. The ignition energy was held constant. In reality, heat loss to the spark plug electrode decreases when the gap distance is increased. However, the amount of energy being transferred to the ignited gas as a function of the gap distance is not established in this study. This energy depends on the specific design of the ignition system, which is beyond the scope of this study. The present tests were conducted with an ignition energy of 6 mJ and 2 degree spark duration. The engine ran at 1500 RPM and spark advance was set at 60 degrees before top dead center. Intake temperature and pressure were $350°K$ and 0.5 atm respectively, while the turbulence intensity at the closing of the intake valve was 2 m/s. Complete testing conditions are listed in Table 10. For the fuel equivalence ratio of 0.5, the result shows that the mass burning rate was not a strong function of spark gap. (see Figure 15). The burned particles of the smaller spark gap had a higher temperature ($3000°K$ for 0.5 mm), because the same amount of ignition energy was deposited to all three cases. However, the higher temperature at $3000°K$ was offset by the small burned volume of 0.5 mm spark gap. The present ignition model is not able to predict the effect of spark gap distance due to the lack of a model for the heat losses through electrode and the unburned surrounding. If the heat loss through the electrode is taken into account, the burned temperature at small spark gap of 0.5 mm will be lower than $3000°K$. If heat loss to the unburned surrounding is taken into account, the spark will not be able to ignite all the mass within the spark gap when the gap distance is large (2 mm). Therefore, a more realistic model should include the relationship between the spark gap, ignition energy and amount of mixture to be ignited.

4.9 ENGINE SPEED

The sensitivity of the model to the variation of engine speed was tested.

The change of engine speed alters the turbulence intensity at the closing of the intake valve. It is assumed that turbulence intensity varies linearly with RPM (Tabaczynski, 1976). The model was tested with 2 m/s of turbulence intensity at 1500 RPM and 4 m/s at 3000 RPM. Spark advance was set at 60 degrees before top dead center. The fuel equivalence ratio was 0.5, with the intake temperature and pressure of 350°K and 0.5 atm respectively. Table 11 lists the complete testing conditions. The results shown in Figure 16 indicated that the engine misfired right after ignition at 3000 RPM, while a fast burning rate was obtained at 1500 RPM. The large difference between the two cases was the result of the very high turbulence intensity generated at 3000 RPM. The turbulence intensity at the closing of the intake valve at 3000 RPM was assumed to be double that at 1500 RPM at the same intake temperature and pressure. In reality, the intake temperature and pressure is not necessarily the same as the engine speed increases from 1500 to 3000 RPM. Therefore the turbulence intensity will also be affected by the intake pressure. Nevertheless, the present result shows the trend toward misfire as engine speed and turbulence intensity increase.

4.10 NUMBER OF IGNITED PARTICLES

The number of particles to be ignited is an input variable in the model. The selection of its value is independent on the spark gap size, which determines the volume to be ignited. Therefore, it does not influence the amount of fuel mixture being burned initially, but it determines the size of each particle. One expects that the size of particle should be very small to closely simulate the actual phenomena, but an excessively small particle size and a large number of particles require longer computing time. The objective is to select a number of particles yielding reasonably accurate results with the least computing time. The model was tested by igniting 10, 25 and 50 particles, with the fuel equivalence ratio of 0.5. The intake temperature

and pressure were respectively 350°K and 0.5 atm. The turbulence intensity of 2 m/s was used, and the engine ran at 1500 RPM, with the spark advance set at 60 degrees before top dead center. Complete testing conditions are shown in Table 12. All three cases were computed using 5 minutes of CPU time. When 10 particles were ignited, 13 crank angle degrees of results were obtained, for 25 ignited particles, 11 degrees, and for 50 ignited particles, 8 degrees (see Figure 17). It is obvious that the smaller number of particles reduces computing time significantly. A comparison of the mass burning rate of the three cases shows that the case with larger number of particles burned slightly faster at the beginning, but the difference was reduced after a few crank angles. These results also reveal that the initial burning rate when 50 particles was used is smoother than the others. This is due to the more accurate modelling of the mass entrainment at the initial stage when the number of particles in the partially stirred reactor is large. However, after several particles are entrained into the reactor, the cases of 25 and 10 ignited particles also yield good accuracy. The slight difference in the results does not justify using a large number of particles because it uses a longer computing time. Therefore, all model testing was done using 10 ignited particles. The minimum number of ignited particles also depends on the turbulence intensity which controls both the entrainment and mixing of particles. A smaller number of ignited particles can be used for higher turbulence intensity since more particles will be entrained and mixed in a shorter period of time, eliminating the initial inaccuracy due to the small number of particles.

4.11 PARTIAL BURN LIMIT

The above model tests have demonstrated several cases of misfire at the ignition limit. Arici et al (1983) believed that the ignition limit occurred more often than the partial burn limit for actual engine conditions. Peters (1979) observed that partial burn corresponded to slow burning cycles still burning at the opening

of the exhaust valve, rather than being quenched before the exhaust valve opened. However, quenching during the expansion stroke still occurs. This has led to the experimental study of Smith et al (1977) in an expanding chamber. It was the purpose of this present model to simulate both the ignition and partial burn limited misfire. Therefore, the model will be tested for partial burn. Various attempts were made to create a partial burn cycle, but few were successful. This agrees with the observations of Peter (1979). The case of expansion stroke quenching is rare. However, two combinations of operating conditions shown in Table 13 were observed to create quenching during the expansion stroke. The engine displacement in these two cases was taken as about half the size of other tests, because much computing time can be saved with a smaller cylinder since it contains fewer particles. The specification of the engine is listed in Table 1. More efficient computation is neccessary for partial burn cycles because more crank angles of results are required for a conclusion. The two cases observed had the same inlet conditions, at $290° K$ and 0.5 atm, as well as a turbulence intensity of 3 m/s at 3000 RPM when the intake valve was closed. The first case deposited 1 mJ of energy to the ignited gas at the spark advance of 10 degrees before the top dead center, while the second case deposited 3 mJ of ignition energy at 30 degrees before top dead center. The flame was quenched at 25 degrees after top dead center in the first case (Figure 18), which was 35 degrees after ignition, while the quenching occurred at 15 degrees after top dead center in the second case, (Figure 19), about 45 degrees after ignition. The mass burned fractions in both cases were less than one percent, but the flame had entrained respectively 40 and 50 percent of the volume in the two cases. The results of ignition misfire indicate that about one percent of volume was entrained by the flame. The partial burned cycles are distinguished from the ignition misfire by the following conditions. Firstly, the volume entrained at partial burned limit is near 50%, while the ignition misfiring cycles entrained about 1% of the volume. Secondly, partial burn occurs in the expansion stroke, but the ignition misfire occurs in the

compression stroke. In the present study, the model could not reproduce the same data reported by Peters (1979). The two examples of partial burn in the present study have a mass burn fraction of less than 1%, but Peters (1979) reported that 20% of mass had burned in some cycles which were quenched during the expansion stroke. The small percentage of mass burn fraction predicted by the present model is possibly due to the lack of age mixing in the flame zone. In reality, only particles near each other can mix. However, the present model allows particles anywhere in the flame zone to mix. The lack of age mixing in the model affects the result of partial burn more severely than the ignition misfire, because the flame zone volume is large in the partially burned cycles. Therefore, introducing age mixing may prove to predict partial burn more adequately.

4.12 AGE MIXING

Age mixing allows only the neighbouring particles to mix. A particle close to the spark location cannot mix with one that is entrained later in time and therefore far away from the spark. The mixing of particles that are entrained at different time is controlled using the following procedure :

1. The burned particles from ignition are assigned to be at age 1.

2. For each time interval, unburned particles are entrained behind the flame front, creating a new age of particles. The ages of particles are assigned according to the order in which they are entrained. For example, the particles entrained one time interval after ignition are assigned to be at age 2, and those entrained in the next time interval are at age 3.

3. Particles with an age difference of one are allowed to mix. The mixing starts between age 1 and 2, followed by age 2 and 3 and so on. Mixing procedure is completed when all ages of particles have participated.

The procedure for age mixing is performed by subroutine AGEMIX (appendix L). Subroutine RANMIX is used when the volume behind the flame front is treated as a partially stirred reactor, without using the age mixing procedure. Tests for the ignition misfire regime and partial burn regime were performed. Results of the age mixing model are shown in Figures 20 to 22. Figure 20 shows that at early spark advance (60° BTDC), the burning rate predicted by the age mixing model is slower than that without age mixing. Age mixing allows fewer unburned particles to mix with burned ones, reducing the probability of creating burning particles. The result is a reduction in burning rate. This result is not expected to change the trend of the ignition limit although it predicts a higher equivalence ratio at the ignition limit. Figures 21 and 22 show that at late spark timings (at 10° and 30° BTDC), the age mixing model did not predict partial burn while the model without age mixing did. The burning rates predicted by the age mixing model are faster. At late spark timing, the turbulence intensity is high, and more unburned particles are entrained. The large number of unburned particles compared to burning and burned ones reduces the probability of mixing between unburned and burned or between unburned and burning particles (The highest probability of mixing two types of particles occurs when their numbers are about the same). Restricting mixing between neighbouring reaction zones by age mixing reduces the number of unburned allowed to mix with burned and burning. Therefore, age mixing increases burning rate. It is concluded that for the ignition limit, age mixing is not expected to alter the trend predicted by the model without age mixing. However, the age mixing model did not predict partial burn while the model without age mixing did. Further studies on the partial burn limit are required.

CHAPTER 5
CONCLUSION AND RECOMMENDATION

5.1 CONCLUSION

The model was developed to study misfire in lean combustion in spark ignition engines. It has the capability to simulate both the ignition limit and the partial burn limit. Tests have been performed extensively for the ignition limited cases. It usually requires no more than 20 degrees of crank angles after ignition to observe whether the ignition limit is reached, but the result after TDC is usually required to determine if the partial burn limit is reached. The results of partial burn cycles suggest that the concept of age mixing should be investigated. It was also observed that there was only a narrow range of combination of variables for which partial burn would occur when age mixing was not used.

5.1.1 IGNITION LIMIT

The testing on the effect of mixture, engine and ignition system variables on the ignition limit led to the following conclusions.

1. Turbulence intensity is a critical parameter for ignition limit.
2. Pressure does not have very strong effect on ignition limit, but it affects the flow rate into the cylinder, and the turbulence intensity is affected accordingly.
3. Temperature is another important parameter affecting the ignition limit.
4. Fuel equivalence ratio, the parameter often used to measure ignition limit, has great influence on ignition misfire.

5. Spark advance combines the effect of temperature, pressure and turbulence intensity. It shows the dominant effect of temperature, while turbulence intensity enhances flame propagation at higher temperature.

6. Ignition energy has an effect on the early burning rate, but does not influence the ignition limit as much as temperature and turbulence intensity.

7. Spark gap does not have direct influence on ignition limit, but the present ignition model lacks the detailed relations between ignition energy, gap distance and mass burned.

8. The model is not sensitive to the number of particles to be ignited initially, provided the number is sufficiently large, depending on the turbulence intensity.

9. Engine speed does not affect the ignition limit directly, but it changes turbulence intensity, and that has a strong effect on ignition limit.

The parameters affecting the ignition limit are the turbulence intensity, temperature and fuel equivalence ratio. The turbulence intensity controls flame propagation and particle mixing, while the temperature and fuel equivalence ratio control the chemical rate. Therefore, one can conclude that the balance of mixing and chemical rate is of great importance in engine misfire. High frequency of mixing enhances burning rate at high temperature and equivalence ratio. If the mixing frequency is further increased, it will adversely affect the burning rate, particularly at low temperature and equivalence ratio. In other words, the comparison of chemical time to mixing time determines the occurrence of misfire.

5.1.2 PARTIAL BURN AND AGE MIXING

Extensive parametric study on the partial burn limit was not performed due to the narrow range of combination of variables for which partial burn would

occur, and the longer computing time for the study. Therefore, it is not known how different parameters will influence the partial burn limit. However, cases of partial burn limited misfire have been obtained. The flame had propagated to 50 percent of the volume when it was quenched, but the mass burned fraction remained very small (less than 1 percent). The concept of age mixing was introduced in an attempt to improve the result of partial burn cycles. It was found that in the ignition misfire regime (early spark advance), the model of age mixing predicts a slower burning rate than that without age mixing. In the partial burn regime (late spark advance), the burning rate predicted by the age mixing model is faster than that without age mixing. The age mixing model did not predict partial burn when the model without age mixing did. More studies on partial burn cases are required. The difference in burning rate prediction between the model with age mixing and without age mixing is due to the probability of mixing between unburned and other particles.

5.2 RECOMMENDATION

The major difficulty encounted in the development of the model is the computing time required to yield a reasonable amount of results. There has not been a single run of the Fortran program giving results of a complete cycle. Only about 20 to 40 crank angle dehrees of results has been obtained in most tests. Therefore, a more efficient algorithm should be included in the future development of this model, particularly for the method of solving the ODE system of the chemical kinetics.

A more efficient computation will make possible a more extensive study of the partial burn limit. A parametric study similar to the one performed on the ignition limit described in the previous chapter will help to understand the behavior of partial burn in engines. The age mixing model was implemented and initial tests were performed. However, ignition limit and partial burn limit have not been studied using the age mixing model as extensively as the model without age mixing. In the

partial burn regime, the age mixing model has not shown any occurrence of partial burn. Therefore, it is recommended that more studies on age mixing, particularly for partial burn cases, are required.

The model presently assumes that ignition alway takes place regardless of the amount of ignition energy supplied to the unburned gas surrounding the spark plug. Therefore, it showed that the occurrence of misfire is not greatly influenced by the ignition energy. This is not true in reality. A more detailed ignition model including the relationship between the spark gap distance, ignition energy and the mass or volume ignited by the given energy should be considered in future development.

The rapid distortion theory without dissipation of kinetic energy is presently used to calculate turbulence intensity. A more accurate model should include the dissipation. The lean misfire limit is strongly influenced by the turbulence intensity; therefore, a turbulence model including dissipation may prove to be important, especially in the expansion stroke. The present model does not take into account the residual fraction or exhaust gas recirculation. If such parameters are of interest, they should also be incorporated into the model. Heat transfer is another aspect the present model does not include, and it is a possible future development.

The model constants have not been adjusted with any actual engine experiment due to the unavailability of complete data and engine specification. Therefore any future application of the model has to include constants validation with actual engine experiments.

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TABLE 1

ENGINE SPECIFICATIONS

(For Testings of Ignition Limit)

Bore	=	8.0 cm
Stroke	=	8.0 cm
Length of Connecting Rod	=	15.0 cm
Spark Plug Offset from Center	=	1.5 cm
Compression Ratio	=	9.9

(For Testings of Partial Burn, Age Mixing, and Empirical Constants)

Bore	=	4.0 cm
Stroke	=	4.0 cm
Length of Connecting Rod	=	7.5 cm
Spark Plug Offset from Center	=	0.75 cm
Compression Ratio	=	8.0

TABLE 2

TESTING CONDITIONS : VARIATIONS OF EMPIRICAL CONSTANTS

Constants	A	B	C
Engine Speed (RPM)	1500.	1500.	3000.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	3.0
Intake Pressure (atm)	0.5	0.5	0.7
Intake Temperature (K)	300.	300.	270.
Spark Advance (BTDC)	60.	60.	10.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	1.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	5.

Constants : A = Pre-exponential constant
B = Activation Energy
C = Constant for Mixing Frequency

TABLE 3

TESTING CONDITIONS : VARIATION OF TURBULENCE INTENSITY

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	1.0	2.0	3.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	300.	300.	300.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.
Result	Slower burning.	Fastest burning.	Misfire.

TABLE 4

TESTING CONDITIONS : VARIATION OF PRESSURE

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.2	0.5	0.8
Intake Temperature (K)	350.	350.	350.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.
Result	Burning rate decreased with increasing pressure.		

TABLE 5

TESTING CONDITIONS : VARIATION OF PRESSURE & TURBULENCE INTENSITY

Engine Speed (RPM)	1500.	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	1.6	2.0	2.6	3.2
Intake Pressure (atm)	0.4	0.5	0.65	0.8
Intake Temperature (K)	300.	300.	300.	300.
Spark Advance (BTDC)	60.	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.	10.
Result	Burning rate decreased with increasing turbulence intensity.			Misfire.

TABLE 6

TESTING CONDITIONS : VARIATION OF INTAKE TEMPERATURE

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	250.	300.	350.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.
Result	Burning rate increased with increasing temperature.		

TABLE 7

TESTING CONDITIONS: VARIATION OF EQUIVALENCE RATIO

Engine Speed (RPM)	1500.	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.	120.
Equivalence Ratio	0.3	0.5	0.7	0.9
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5	0.5
Intake Temperature (K)	350.	350.	350.	350.
Spark Advance (BTDC)	60.	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.	10.
Result	Misfire.	Burning rate increased with increasing equivalence ratio.		

TABLE 8

TESTING CONDITIONS : VARIATION OF SPARK ADVANCE

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	350.	350.	350.
Spark Advance (BTDC)	90.	60.	30.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.
Result	Misfire.	Burning rate increased with decreasing spark advance.	

TABLE 9

TESTING CONDITIONS.: VARIATION OF IGNITION ENERGY

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	350.	350.	350.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	3.0	6.0	9.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	10.	10.
Result	Burning rate increased with increasing ignition energy.		

TABLE 10

TESTING CONDITIONS : VARIATION OF SPARK GAP

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Rtaio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	350.	350.	350.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	0.5	1.0	2.0
Number of Particles Ignited	10.	10.	10.
Result	Burning rate is not a strong function of spark gap.		

TABLE 11

TESTING CONDITIONS : VARIATION OF ENGINE SPEED

Engine Speed (RPM)	1500.	3000.
Closing of Intake Valve (BTDC)	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.
Equivalence Ratio	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	4.0
Intake Pressure (atm)	0.5	0.5
Intake Temperature (K)	350.	350.
Spark Advance (BTDC)	60.	60.
Spark Duration (Crank Angles)	2.	2.
Ignition Energy (mJ)	6.0	6.0
Spark Gap (mm)	1.0	1.0
Number of Particles Ignited	10.	10.
Result	Normal combustion.	Misfire.

TABLE 12

TESTING CONDITIONS : VARIATION OF NO. OF IGNITED PARTICLES

Engine Speed (RPM)	1500.	1500.	1500.
Closing of Intake Valve (BTDC)	140.	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.	120.
Equivalence Ratio	0.5	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	2.0	2.0	2.0
Intake Pressure (atm)	0.5	0.5	0.5
Intake Temperature (K)	350.	350.	350.
Spark Advance (BTDC)	60.	60.	60.
Spark Duration (Crank Angles)	2.	2.	2.
Ignition Energy (mJ)	6.0	6.0	6.0
Spark Gap (mm)	1.0	1.0	1.0
Number of Particles Ignited	10.	25.	50.
Result	Burning rate increased slightly with increasing no. of ignited particles just after ignition. Difference decreased afterward.		

TABLE 13

TESTING CONDITIONS : PARTIAL BURN

Engine Speed (RPM)	3000.	3000.
Closing of Intake Valve (BTDC)	140.	140.
Opening of Exhaust Valve (ATDC)	120.	120.
Equivalence Ratio	0.5	0.5
Turbulence Intensity at Closing of Intake Valve (m/sec)	3.0	3.0
Intake Pressure (atm)	0:5	0.5
Intake Temperature (K)	290.	290.
Spark Advance (BTDC)	10.	30.
Spark Duration (Crank Angles)	2.	2.
Ignition Energy (mJ)	1.0	3.0
Spark Gap (mm)	1.0	1.0
Number of Particles Ignited	10.	10.
Result	Partial burn : Flame was quenched after travelling over 50 % of volume.	

Table 14

Coefficients for Polynomial Fit to Thermodynamic Properties

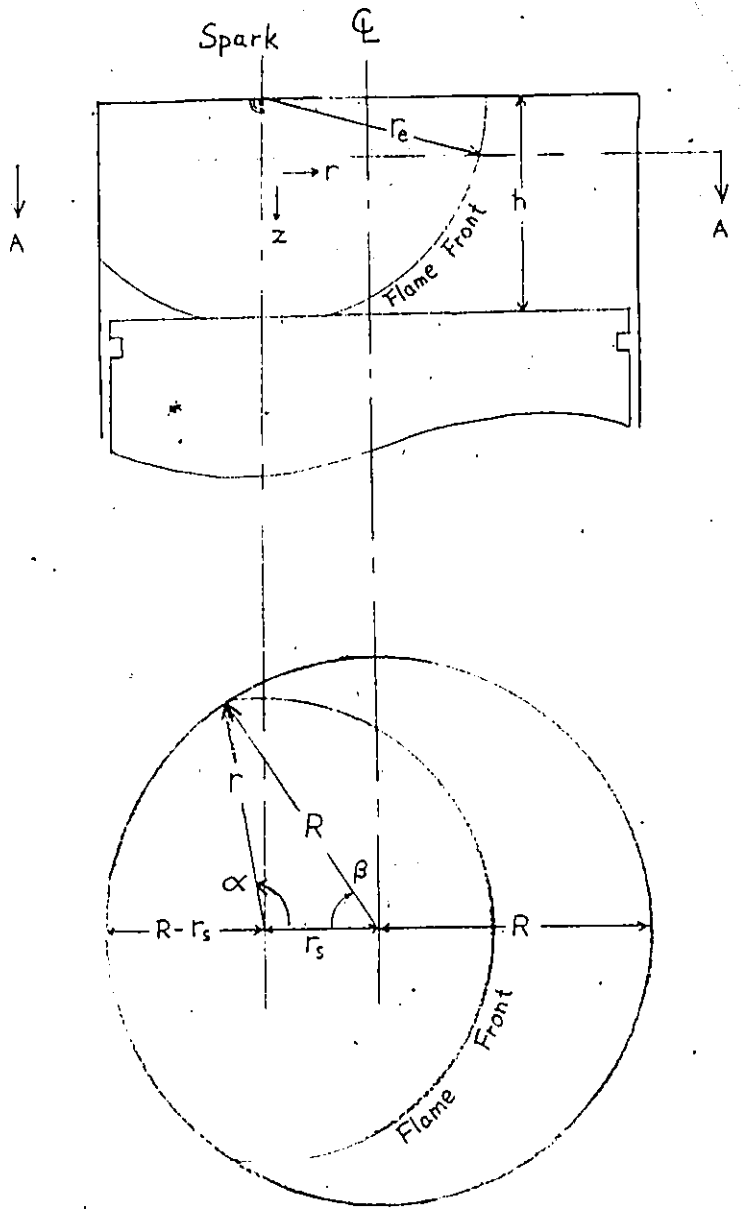
Coeffeicients for tempertaure between $100^o K$ to $500^o K$:

i	Species	a_{i1}	a_{i2}	a_{i3}	a_{i4}	$ai5$	a_{i6}
1	CO_2	11.94033	2.088581	-0.47029	0.037363	-0.589447	-97.1418
2	H_2O	6.139094	4.60783	-0.9356009	0.06669498	0.0335801	-56.62588
3	CO	7.099556	1.275957	-0.2877457	0.022356	-0.1598696	-27.73464
4	H_2	5.555680	1.787191	-0.2881342	0.01951547	0.1611828	0.76498
5	O_2	7.865847	0.6883719	-0.031944	-0.00268708	-0.2013873	-0.893455
6	N_2	6.807771	1.453404	-0.328985	0.02561035	-0.1189462	-0.331835

Coeffeicients for tempertaure between $500^o K$ to $6000^o K$:

i	Species	a_{i1}	a_{i2}	a_{i3}	a_{i4}	$ai5$	a_{i6}
1	CO_2	4.737305	16.65283	-11.23249	2.828001	0.00676702	-93.75793
2	H_2O	7.809672	-0.2023519	3.418708	-1.179013	0.00143629	-57.08004
3	CO_2	6.97393	-0.8238319	2.942042	-1.176239	0.0004132409	-27.19597
4	H_2	6.991878	0.1617044	-0.2182071	0.2968197	-0.01625234	-0.118189
5	O_2	6.295715	2.388387	-0.0314788	-0.3267433	0.00435925	0.103637
6	N_2	7.0922	-1.2958	3.2069	-1.2022	-0.0003458	-0.013967

Figure 1. Flame Front Geometry in the Combustion Chamber



Section A - A

Figure 2. Mass Burn Fraction versus Crank Angle for different Mixing Frequency constant (C)

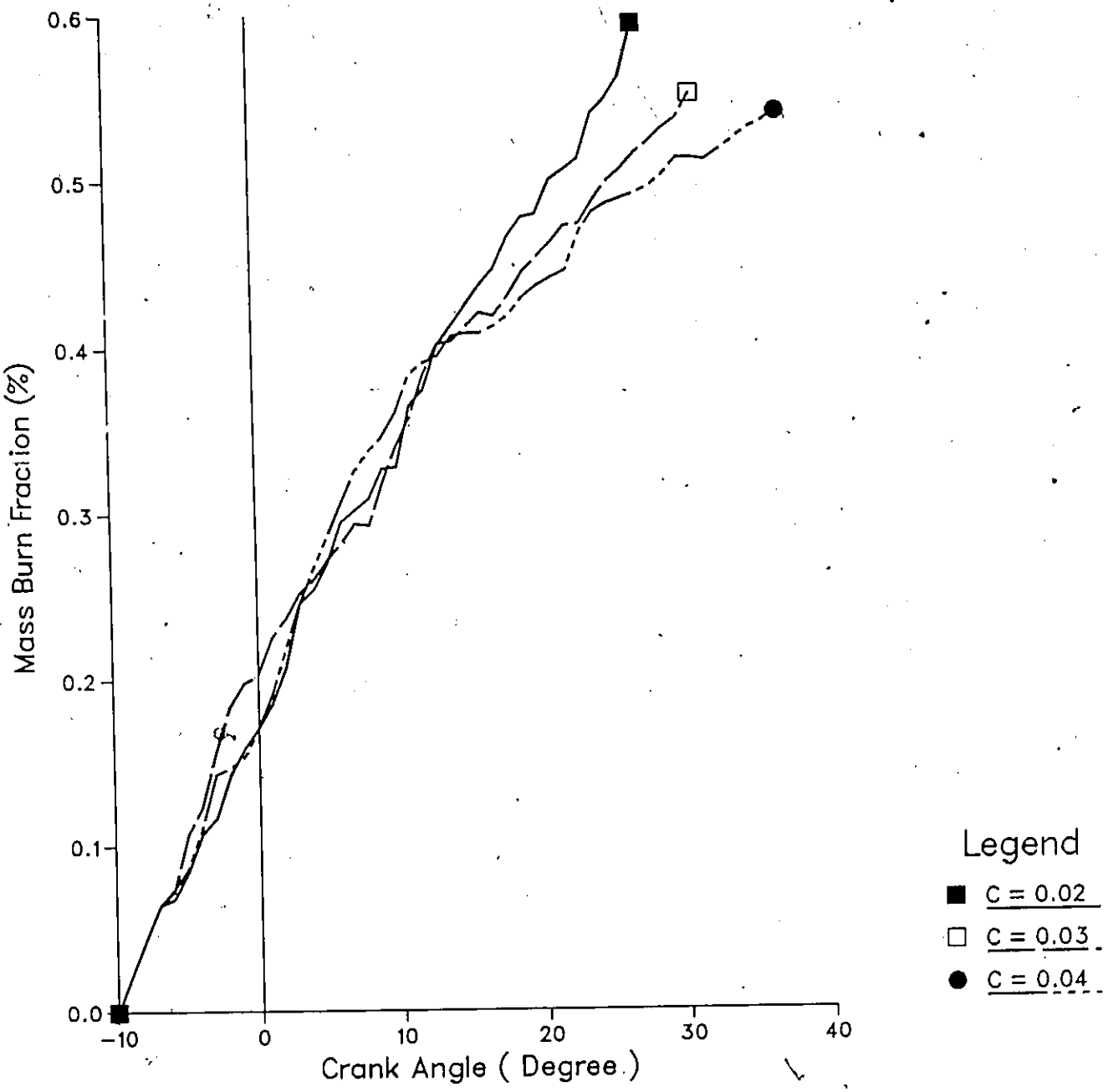


Figure 3. Mass Burn Fraction versus Crank Angle for different Activation Energy (B)

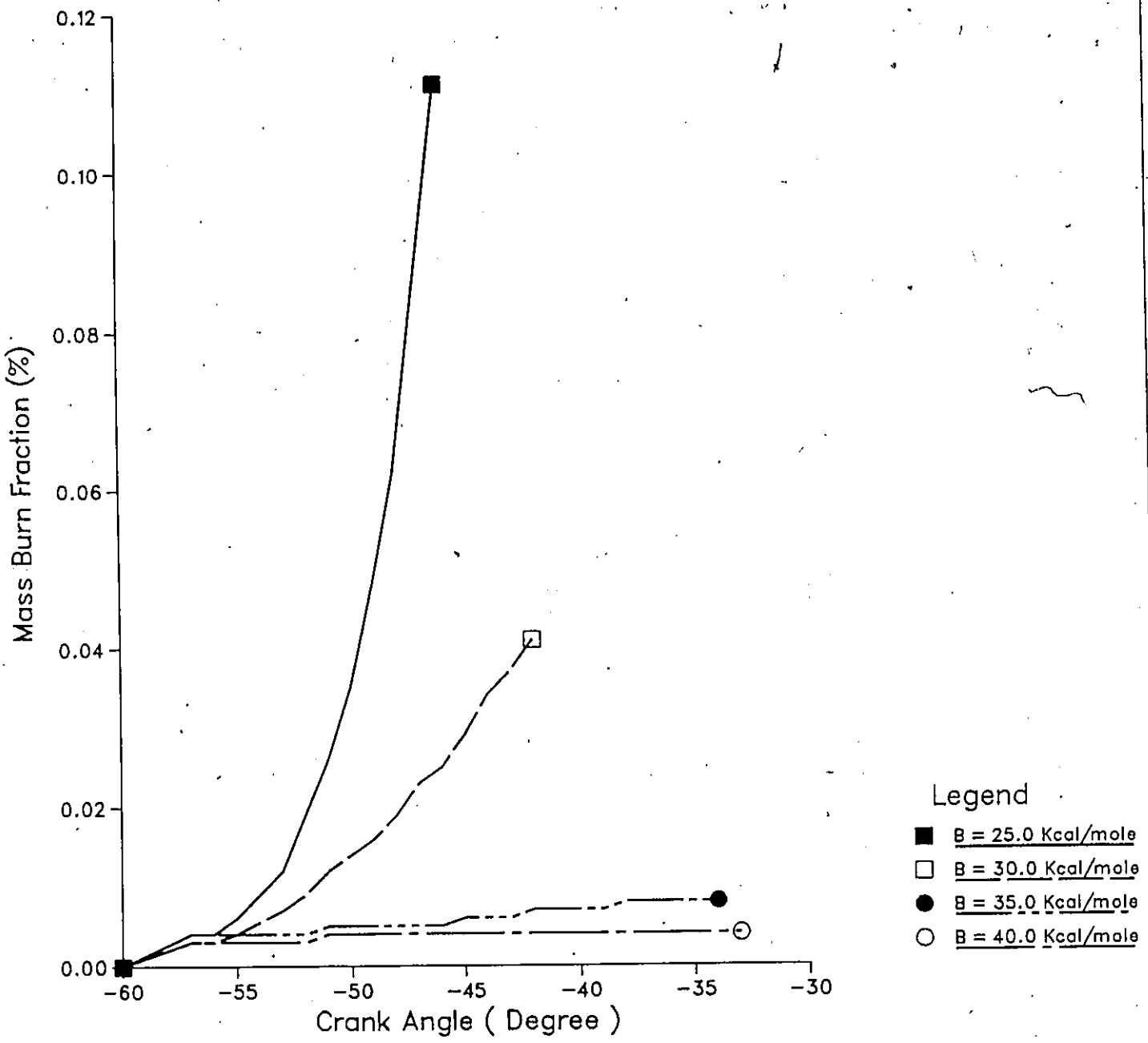


Figure 4. Mass Burn Fraction versus Crank Angle for different Pre-exponential Constant (A)

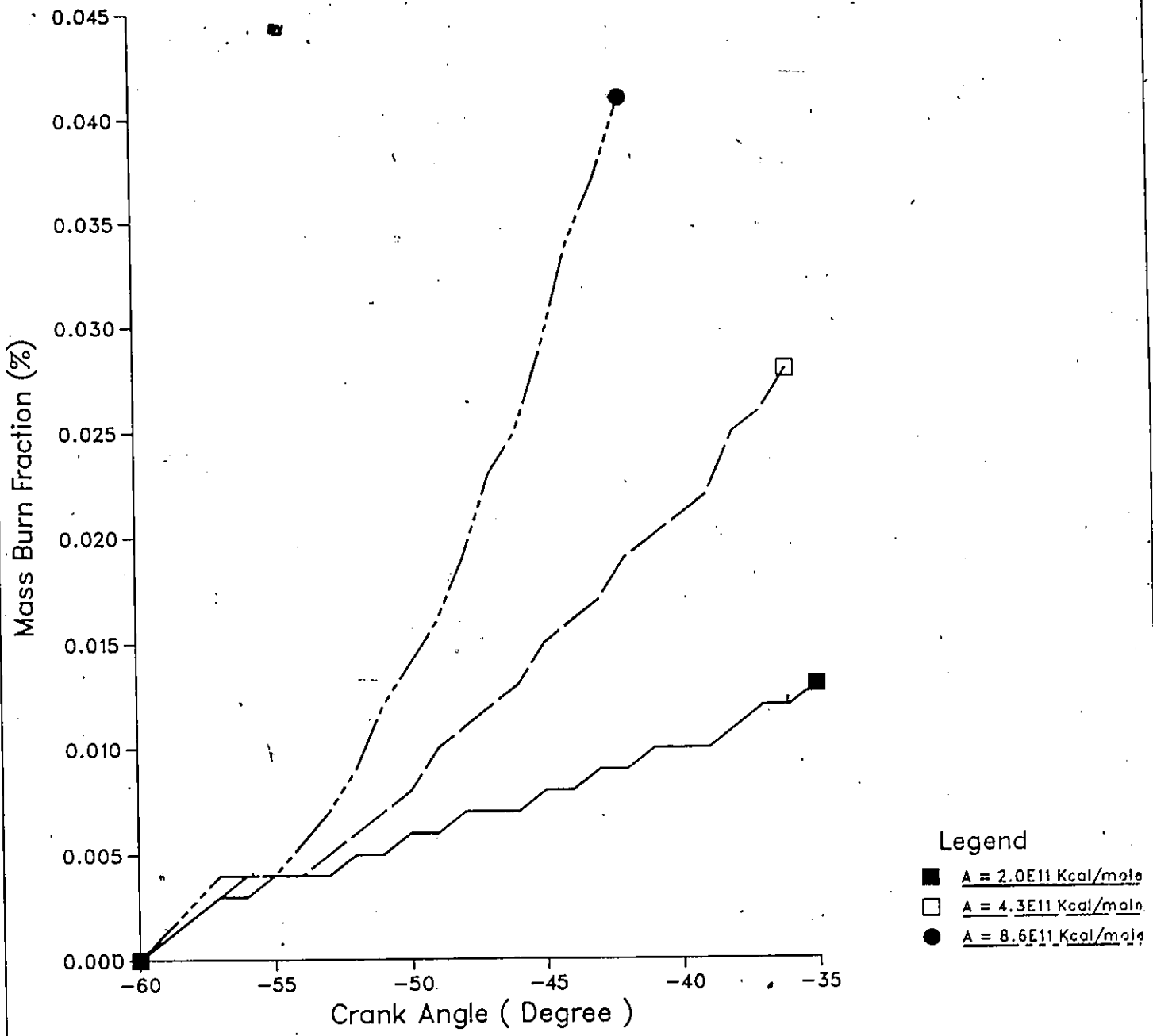


Figure 5. Mass Burn Fraction versus Crank Angle for different level of Turbulence Intensity

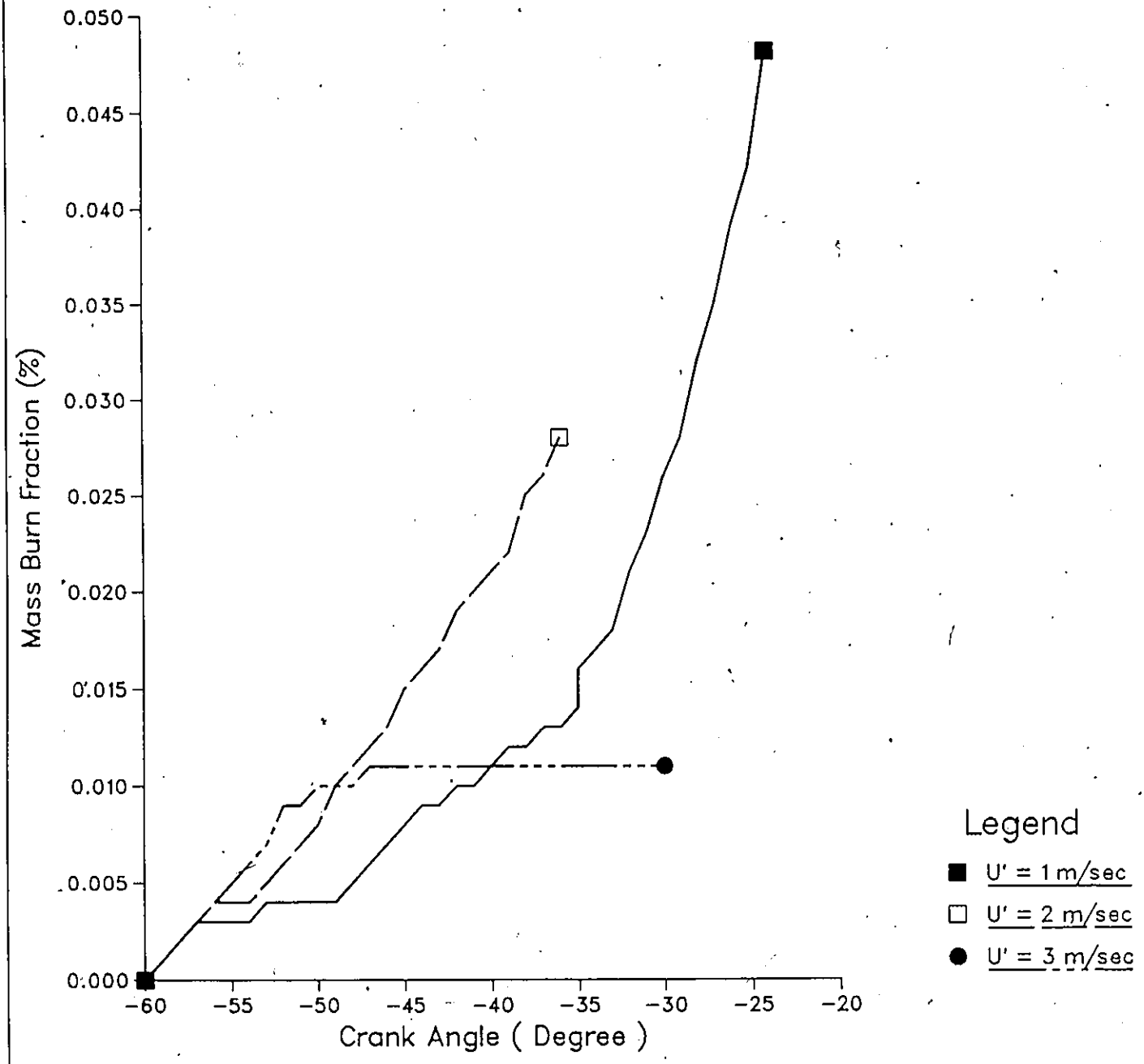


Figure 6. Pressure versus Crank Angle for different level of Turbulence Intensity

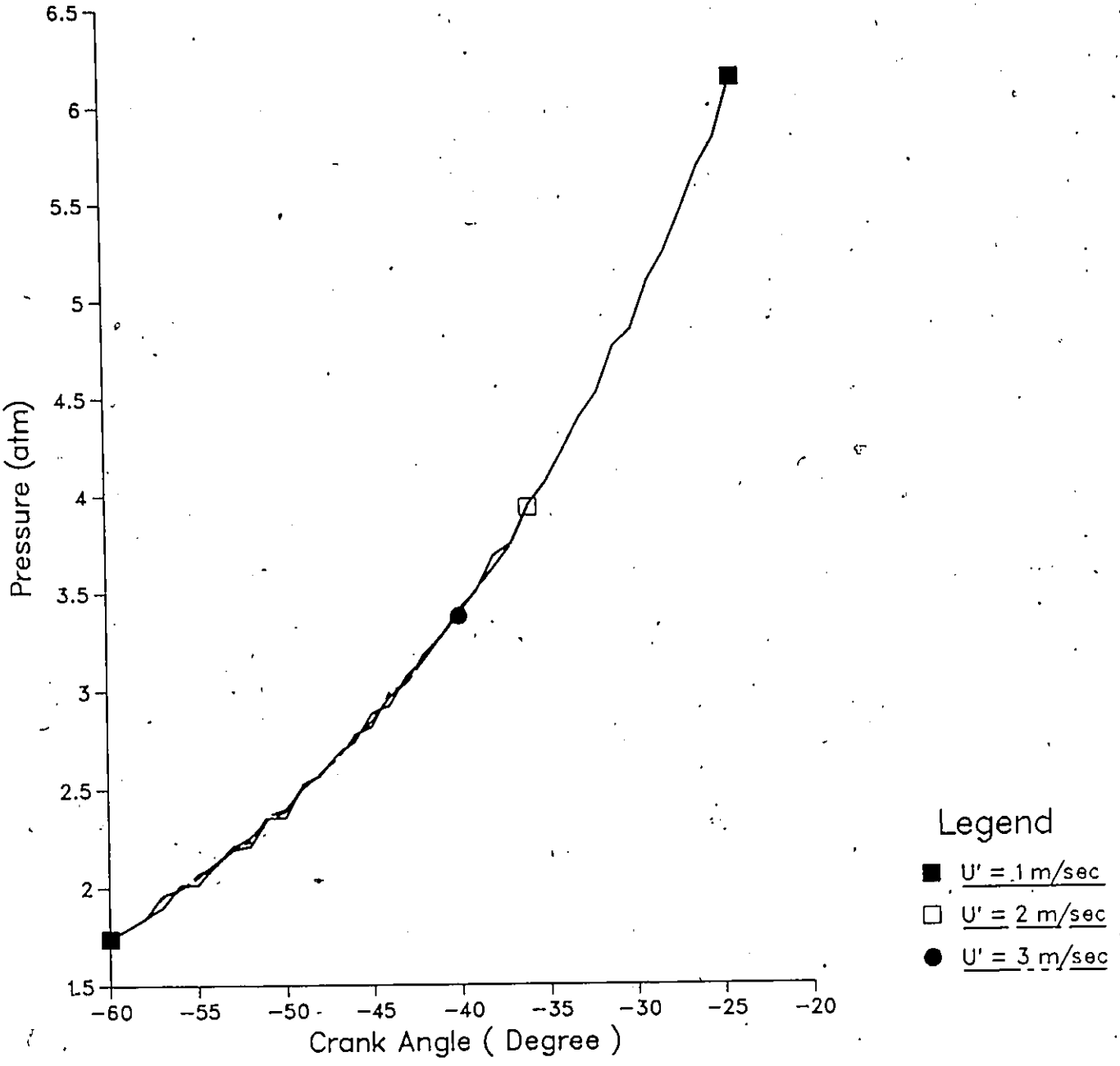


Figure 7. Mass Burn Fraction versus Crank Angle for different Intake Pressure

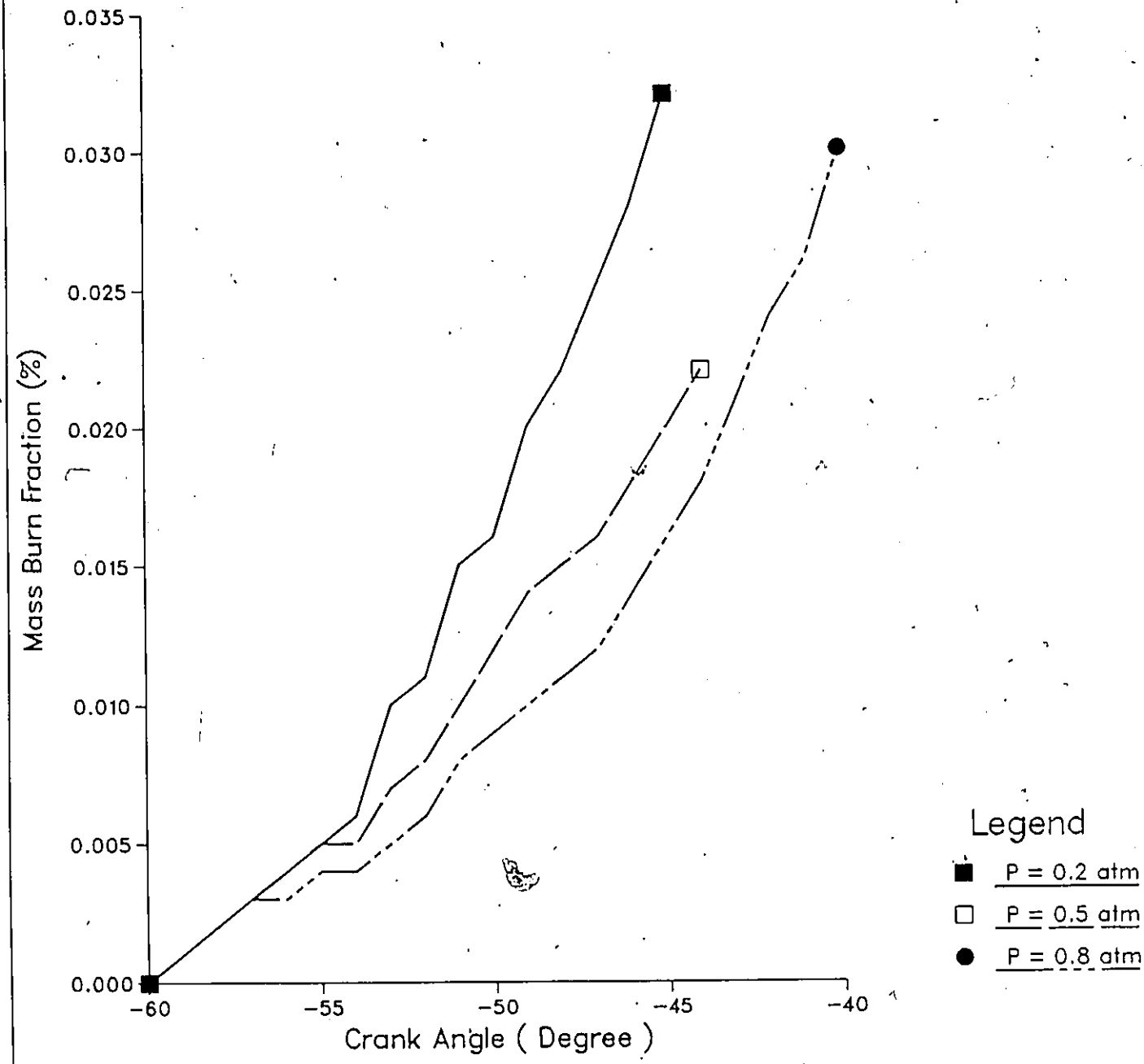


Figure 8. Mass Burn Fraction versus Crank Angle for different Intake Pressure and Turbulence Intensity

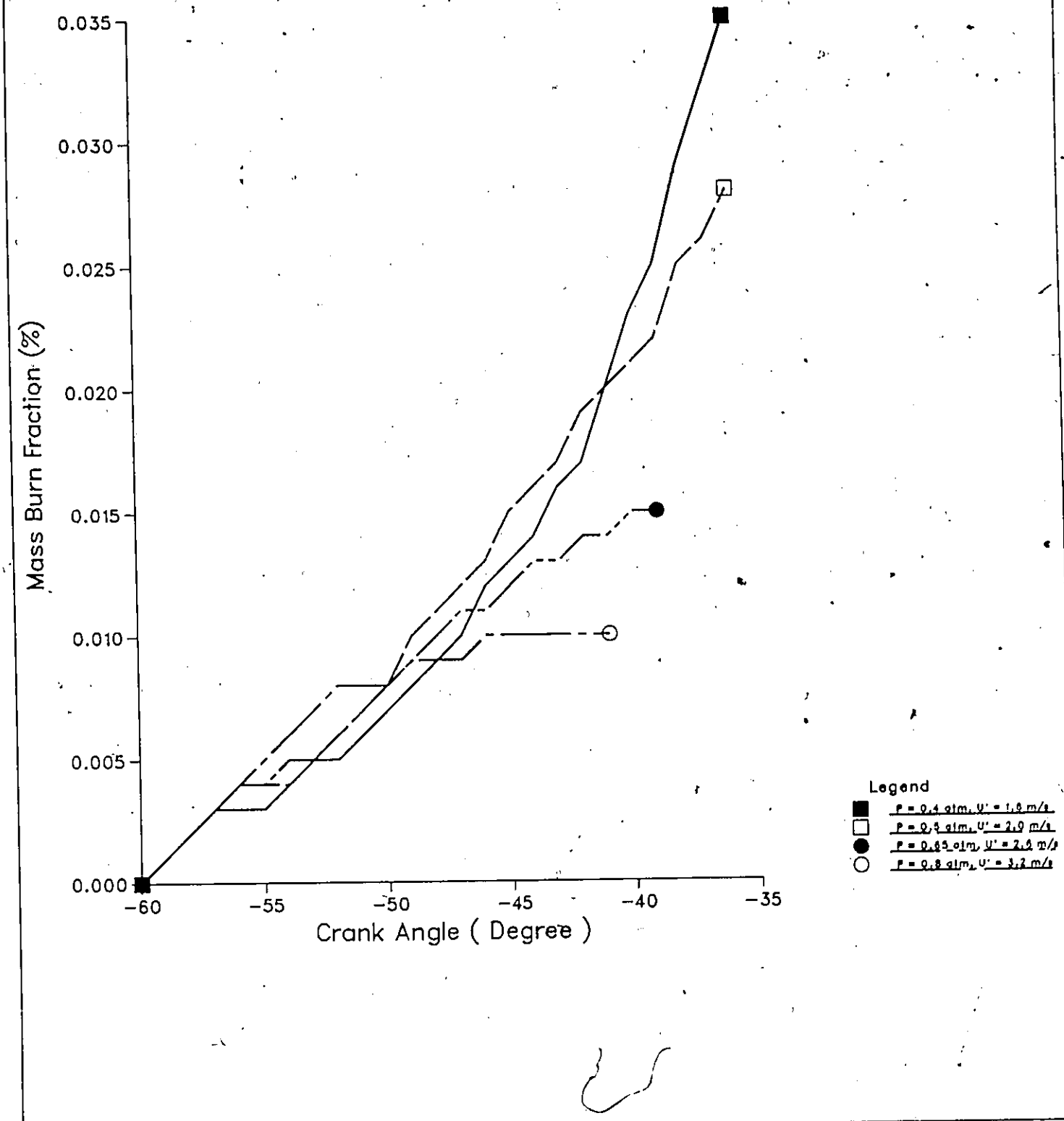


Figure 9. Mass Burn Fraction versus Crank Angle for different Intake Temperature

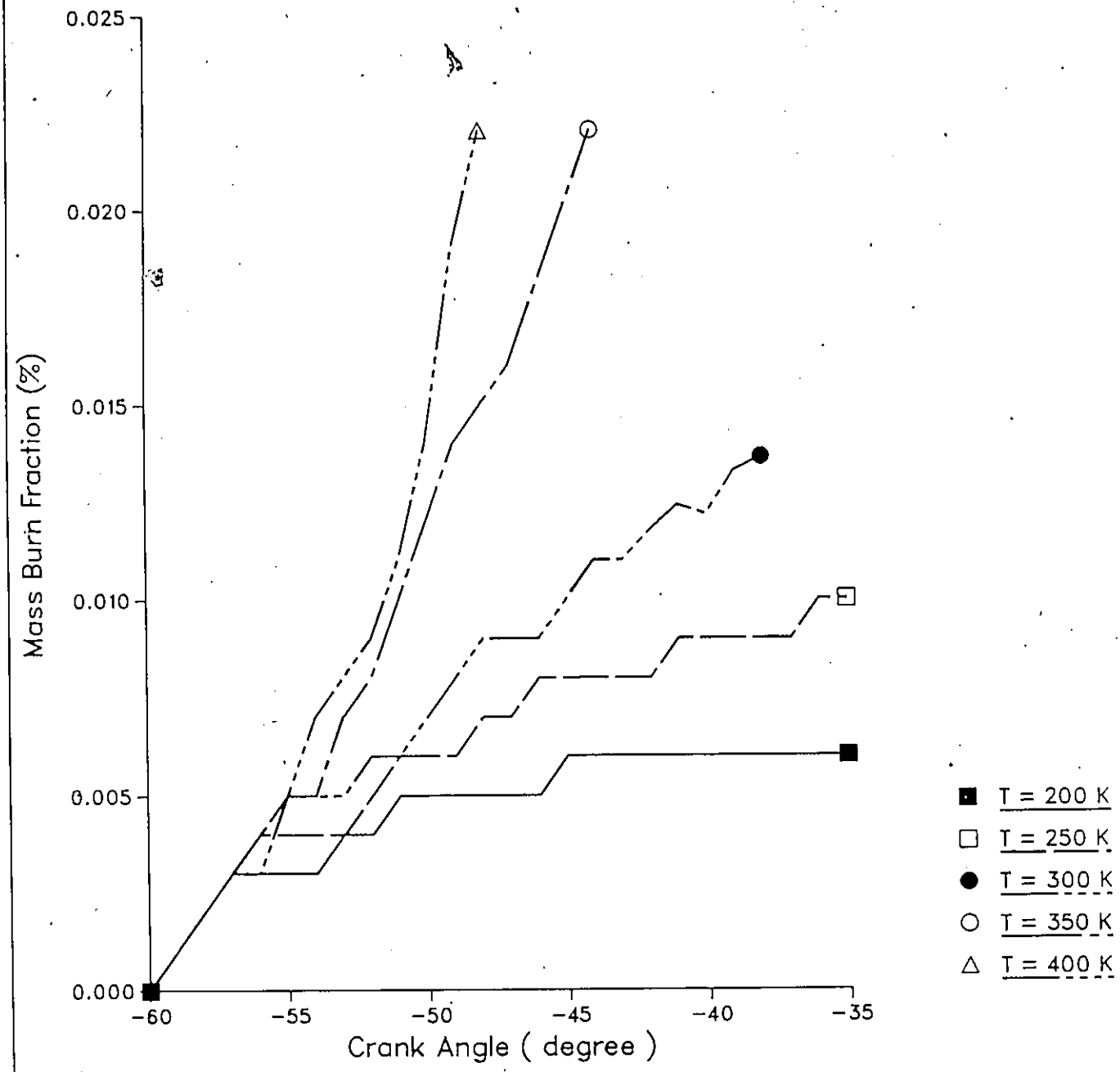


Figure 10. Pressure versus Crank Angle for different Intake Temperature

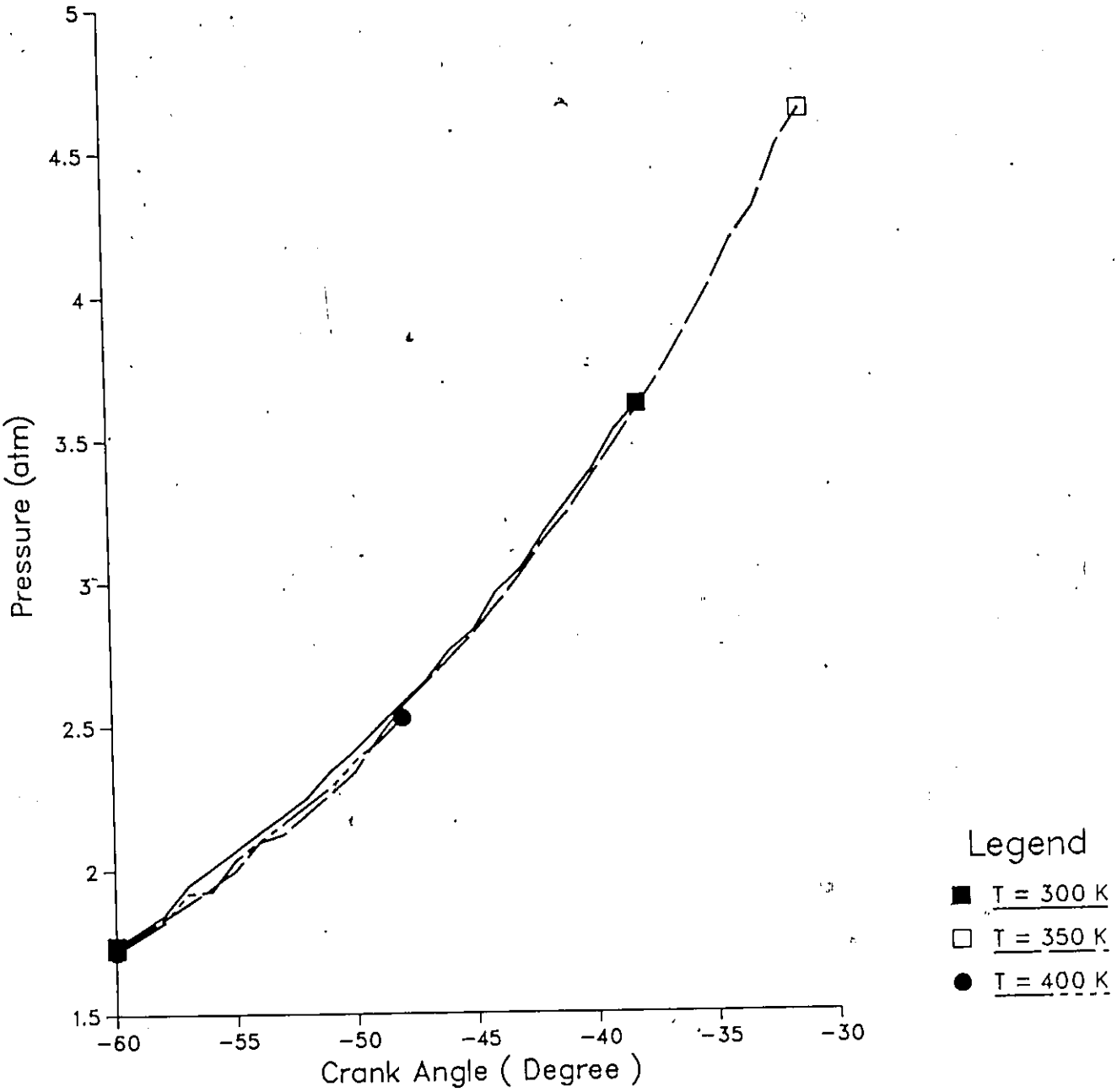


Figure 11. Mass Burn Fraction versus Crank Angle for different Equivalence Ratio

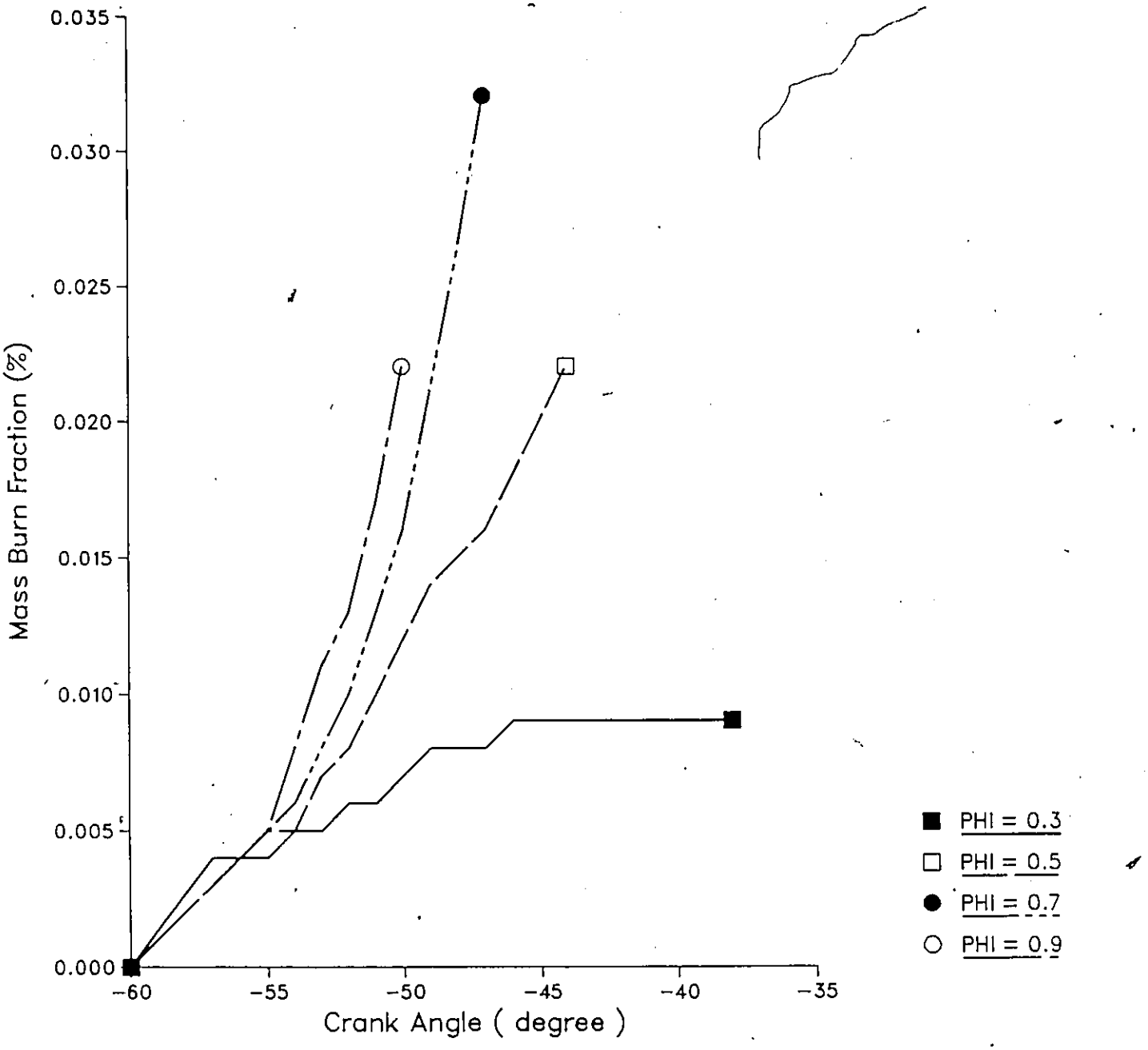


Figure 12. Pressure versus Crank Angle for different Equivalence Ratio

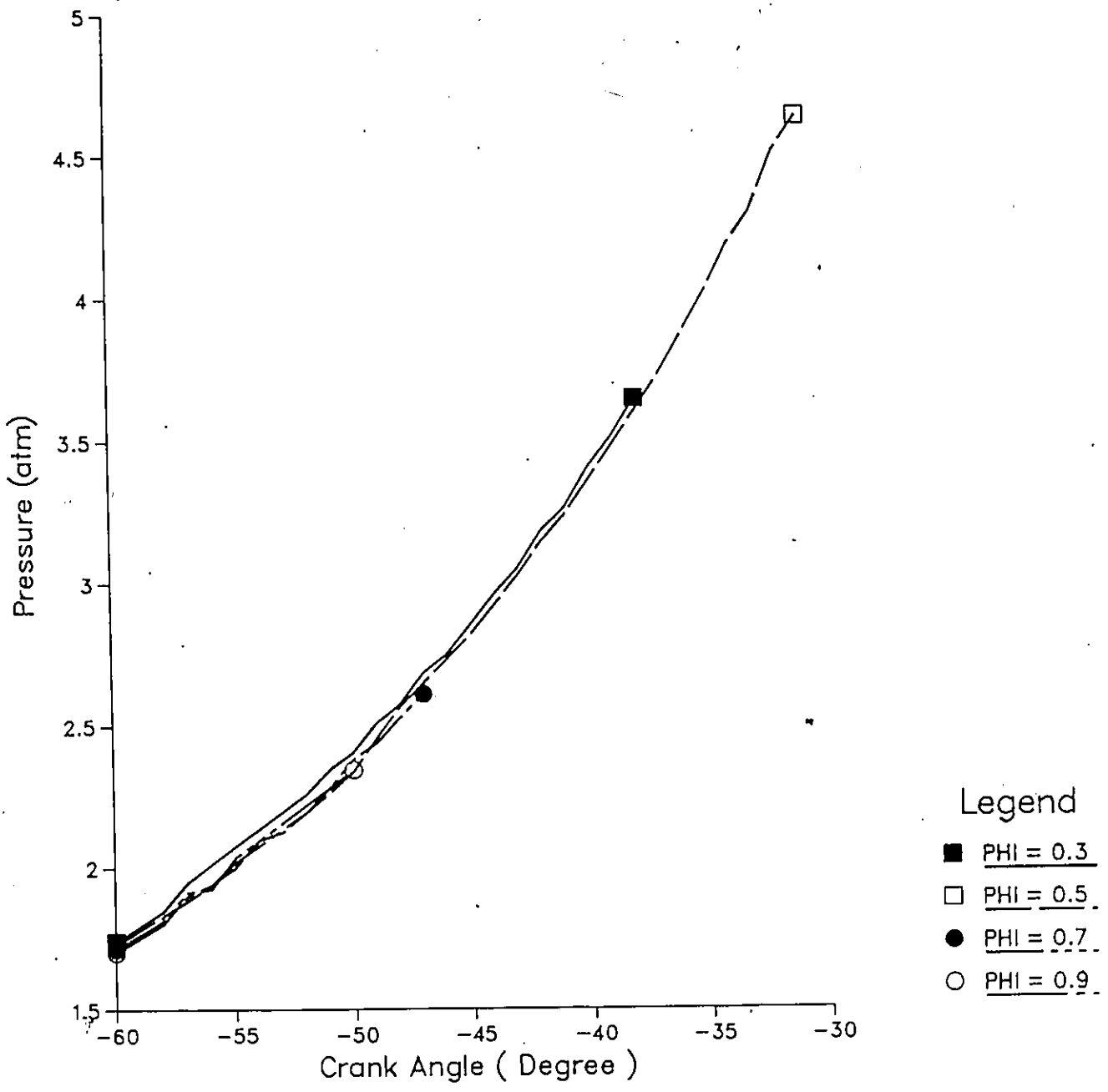


Figure 13. Mass Burn Fraction versus Crank Angle after Ignition for different Spark Advance

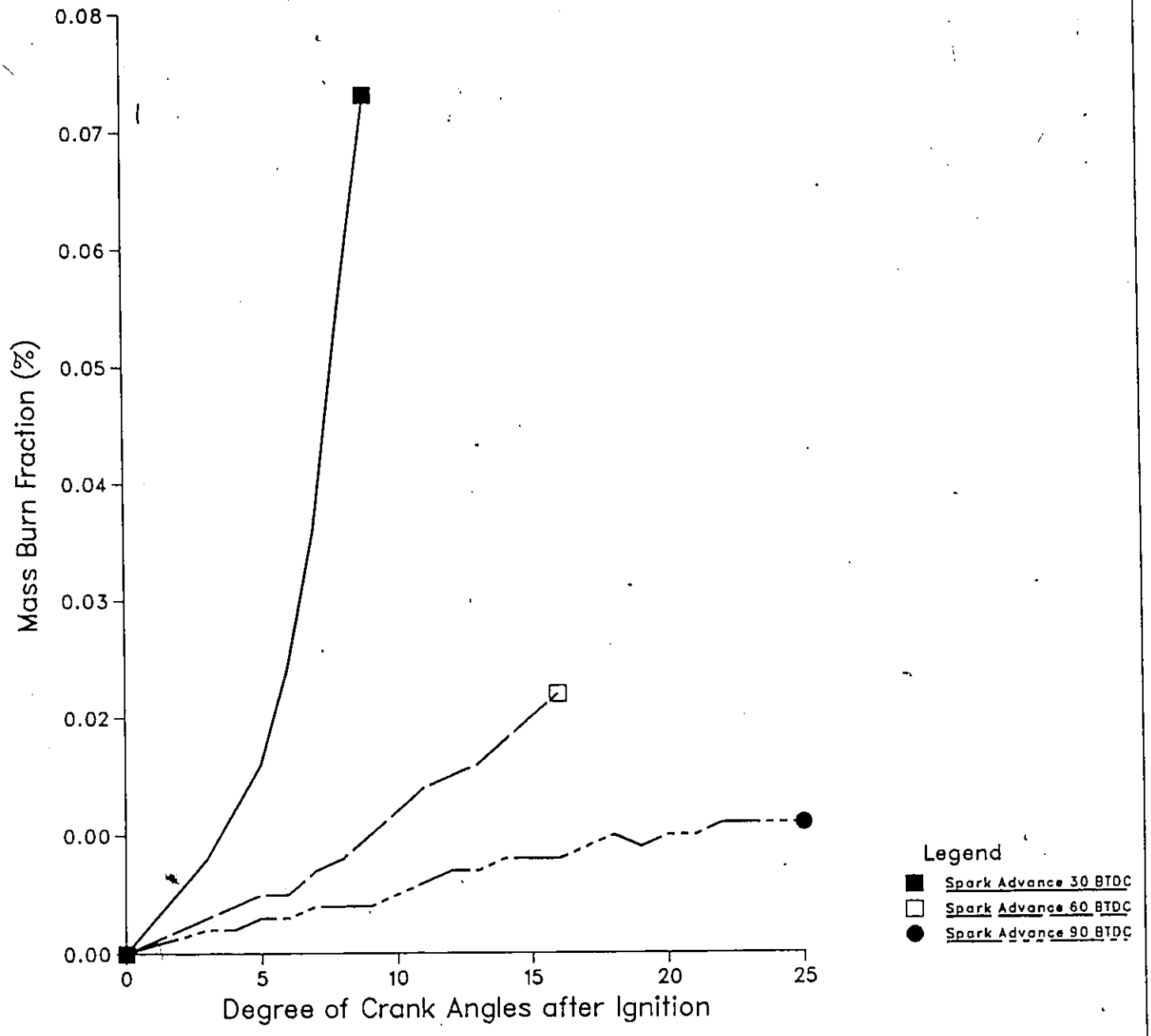


Figure 14. Mass Burn Fraction versus Crank Angle for different Ignition Energy

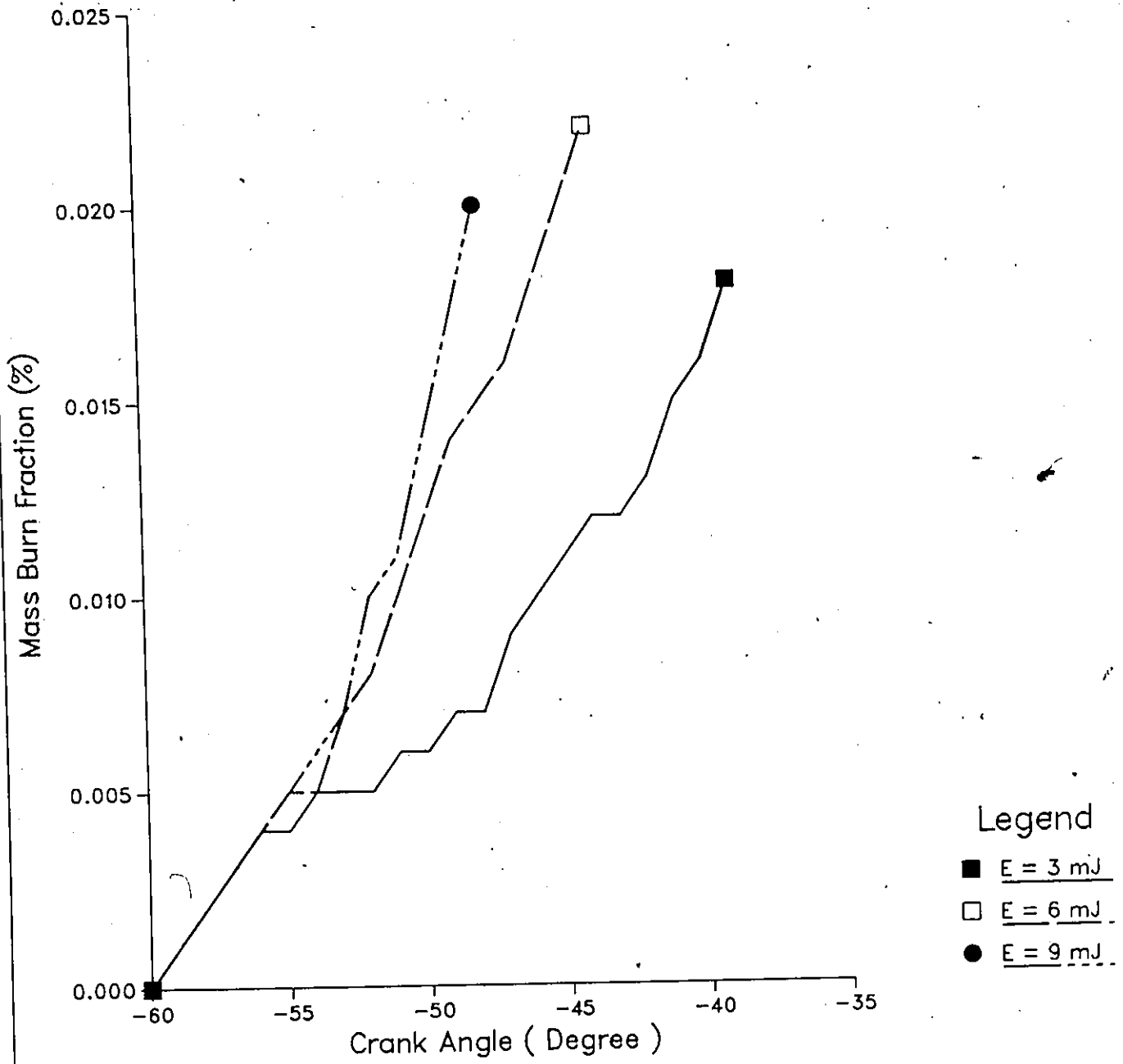


Figure 15. Mass Burn Fraction versus Crank Angle for different Spark Gap Size

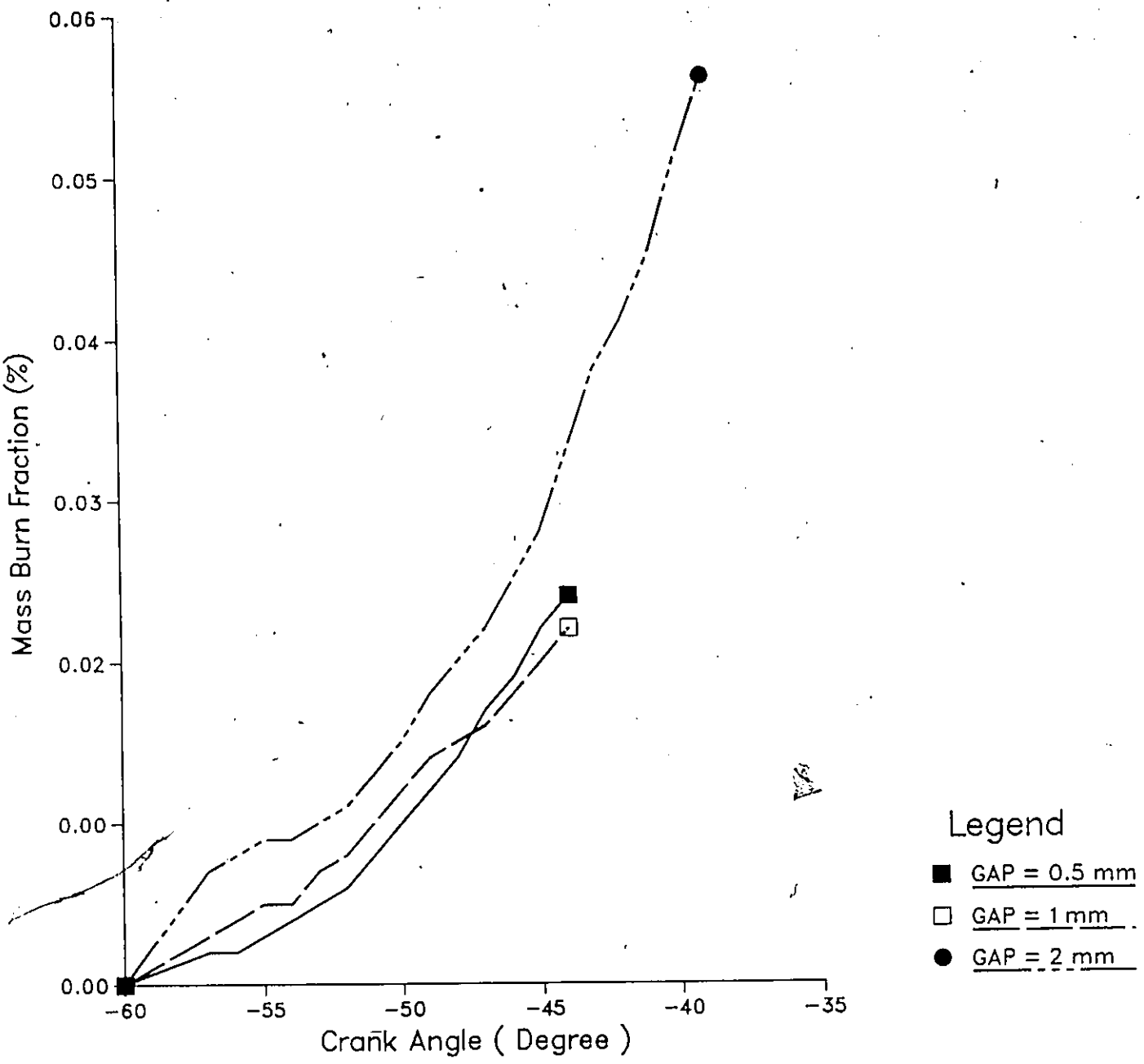


Figure 16. Mass Burn Fraction versus Crank Angle for different Engine Speed

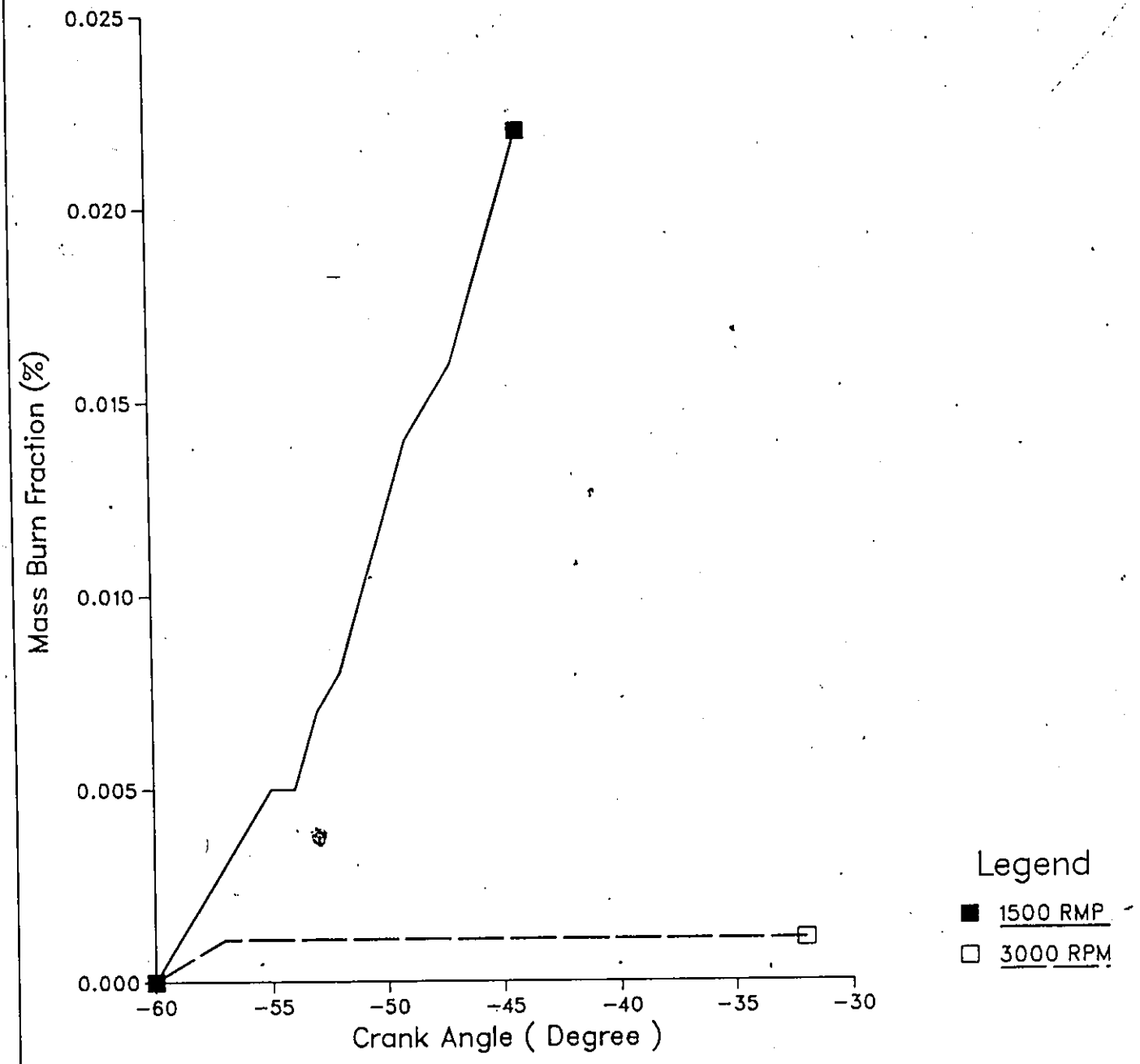


Figure 17. Mass Burn Fraction versus Crank Angle for different Number of Ignited Particles

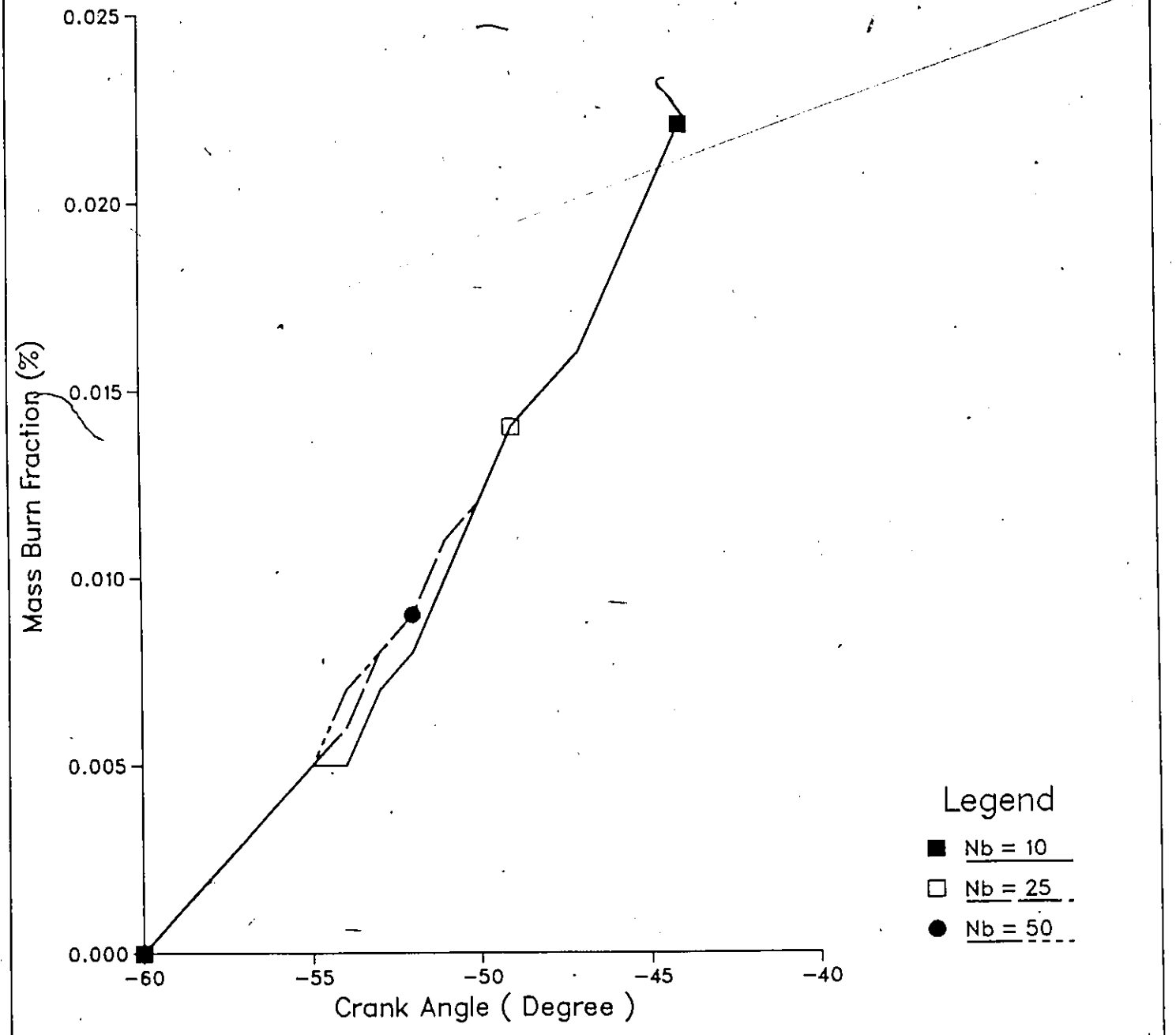


Figure 18. Mass Burn Fraction versus Crank Angle for a Partial Burn Cycle
Spark Advance : 10 degrees BTDC

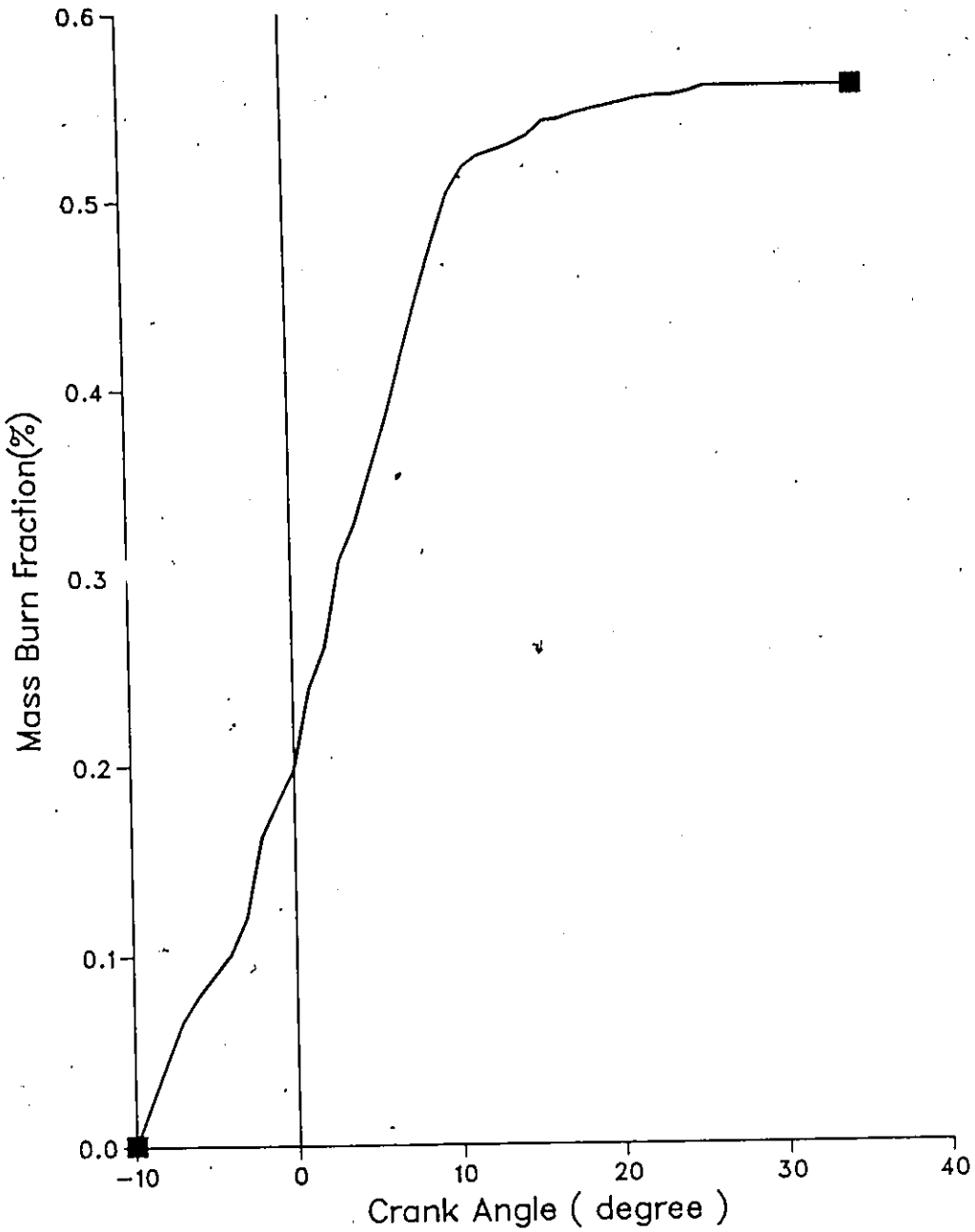


Figure 19. Mass Burn Fraction versus Crank Angle
for a Partial Burn Cycle
Spark Advance : 30 degrees BTDC

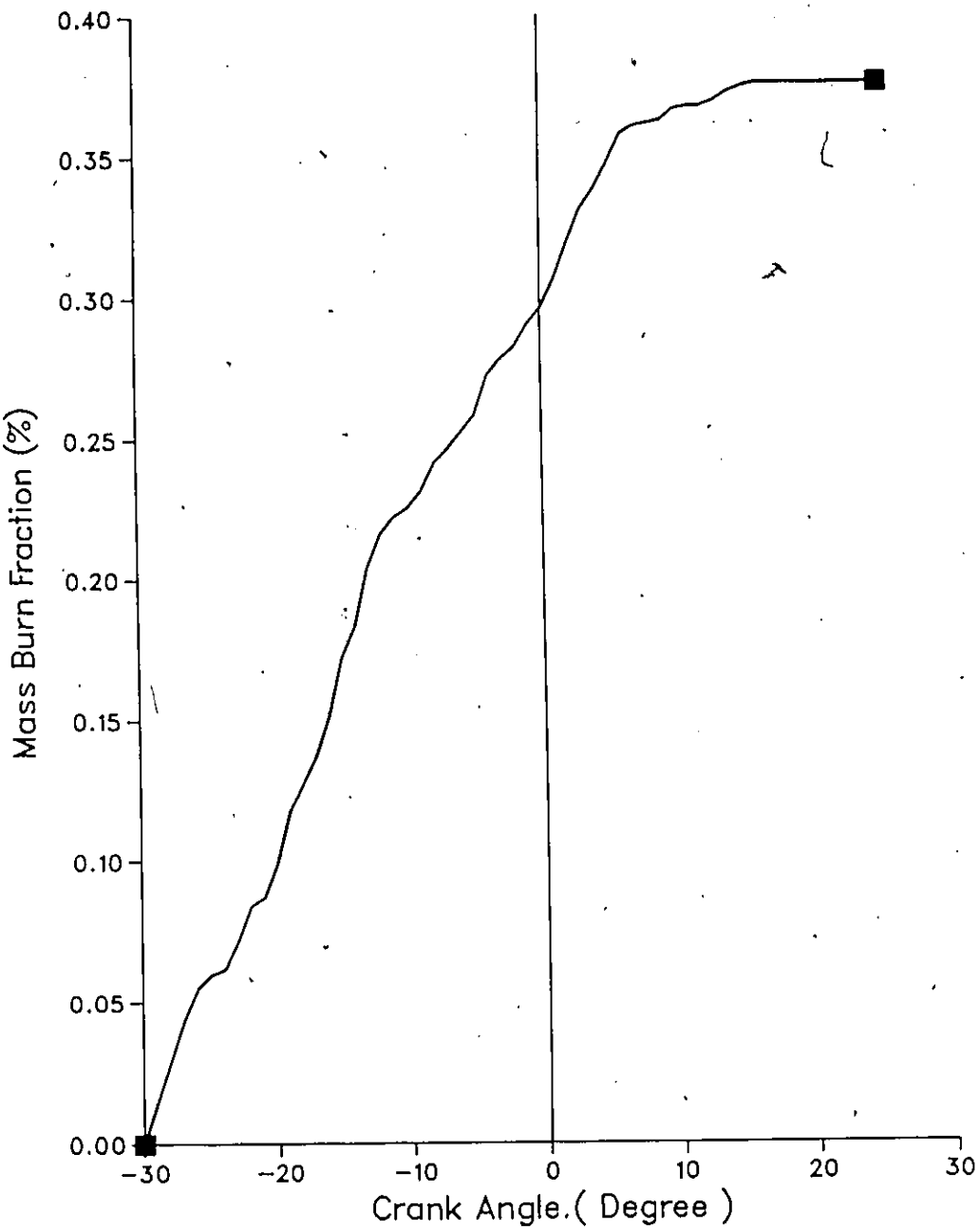


Figure 20. Mass Burn Fraction versus Crank Angle for the inclusion of Age Mixing

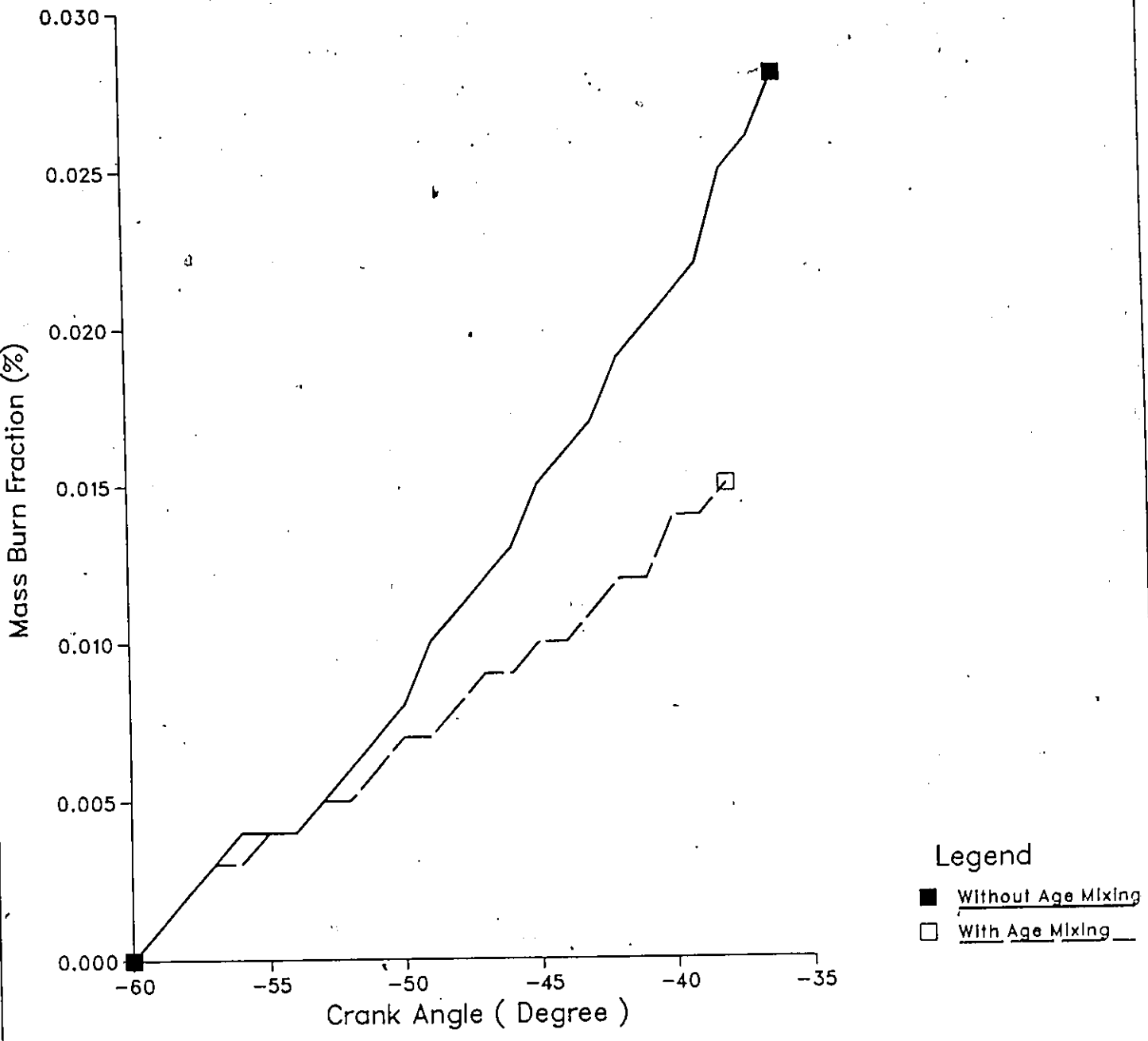


Figure 21. Mass Burn Fraction versus Crank Angle for the inclusion of Age Mixing at Partial Burn

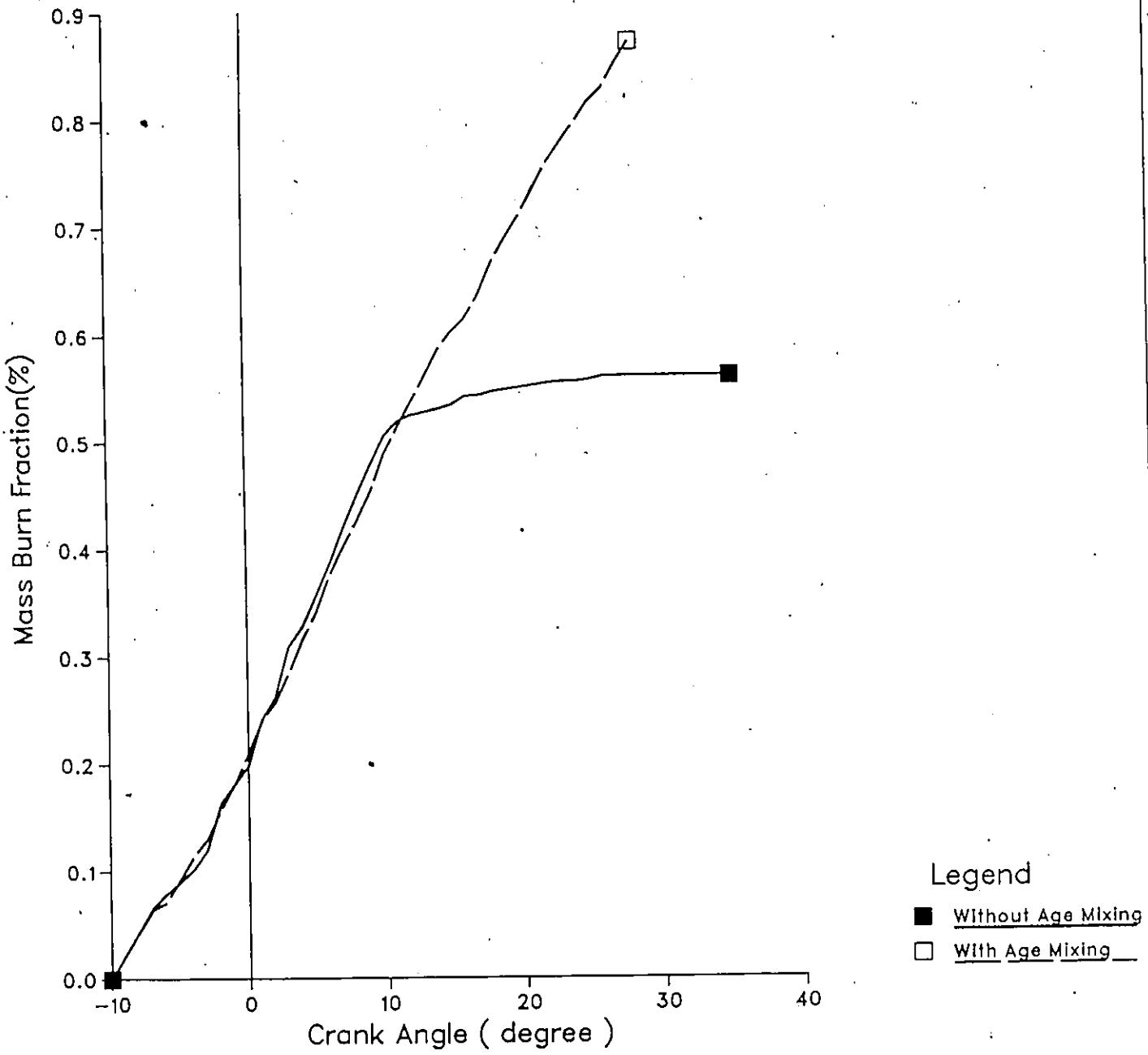
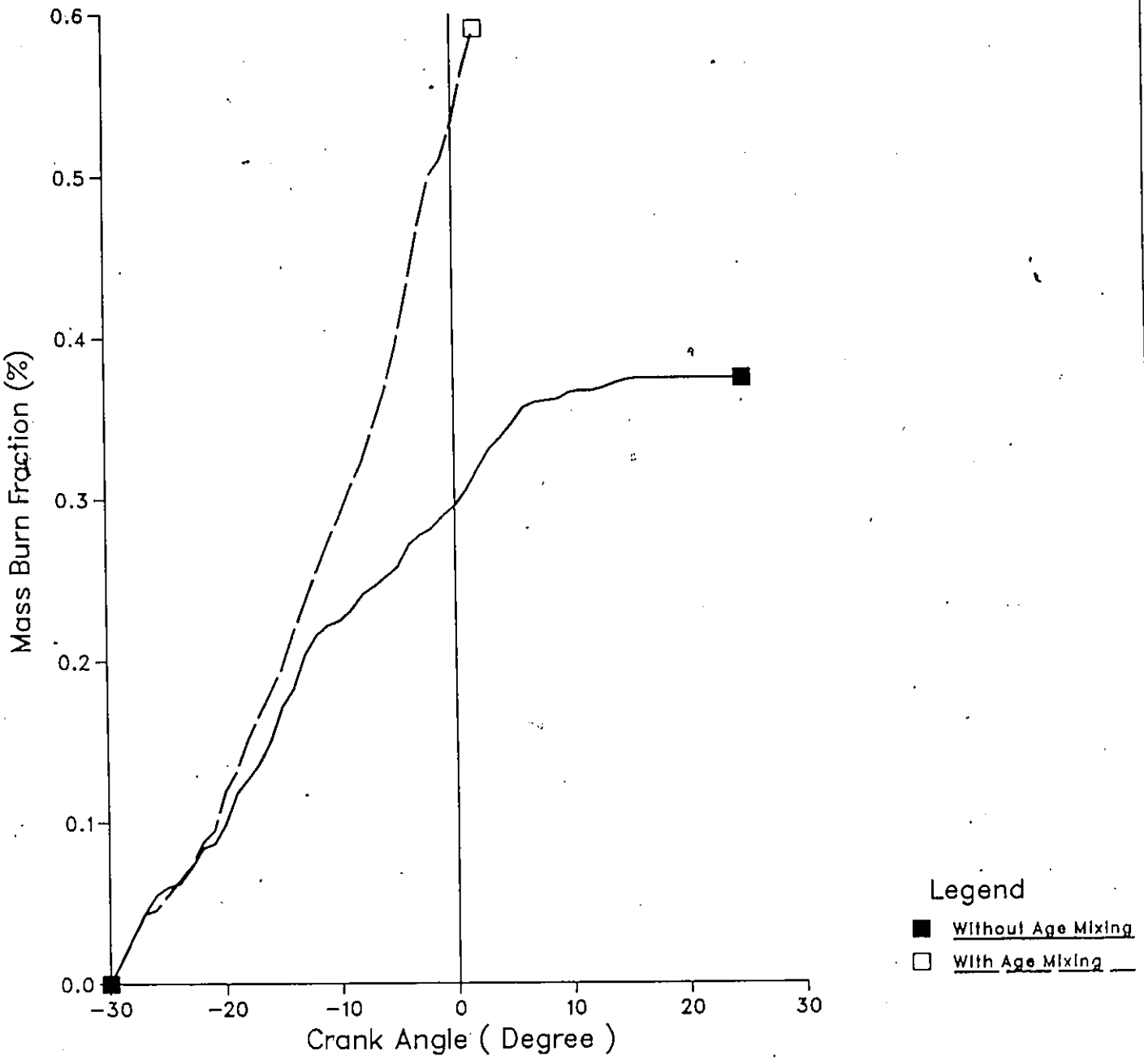


Figure 22. Mass Burn Fraction versus Crank Angle for the inclusion of Age Mixing at Partial Burn



APPENDIX A

```
      DIMENSION A(6,6,2)                                                APP00050
      EQUIVALENCE (A1(1),A(1,1,1))                                      APP00060
      EQUIVALENCE (A2(1),A(1,1,2))                                      APP00070
      COMMON/CNT/IUP,ICLD,IKIN                                          APP00080
      COMMON/CNTF/IF1,IF2,IF3                                           APP00090
      COMMON/JANAF/ A1(36),A2(36)                                       APP00100
       COMMON/UGASP/CCU(7),MBARU,RU,GAMU,CPU,HU,TU,RHOU                 APP00110
       COMMON/BGASP/CCB(7),MBARB,RB,GAMB,CPB,HB                         APP00120
       COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR                            APP00130
       COMMON/INPRS/PRESS                                               APP00140
       COMMON /FUEL/ ENW,CX,HY,OZ,AST                                   APP00150
       COMMON /OXDANT/XI                                                APP00160
       COMMON/CHARTH/RESFRK,RICH,LEAN                                   APP00170
       COMMON/CHARU/PHIFR,PHIEGR                                        APP00180
       COMMON/CHARB/PHI                                                 APP00190
       COMMON/MIX/MASS,F3,VOL3,TO3                                      APP00200
       COMMON/BURN/FFR(9999),IBURN(9999)                                APP00210
       COMMON/IDNUM/IDN(9999)                                           APP00220
       COMMON/AGE/NAGE,NP(500),FNM(500)                                 APP00230
       COMMON/PARNUM/N,NT,N1,N2,N3                                      APP00240
       COMMON/EQNUM/NQ                                                  APP00250
       COMMON/AFRN/V,TOTMX,P,M                                          APP00260
       COMMON/MOLWT/WM(7)                                               APP00270
       COMMON/TEMVOL/TEMP(9999),VOL(9999)                               APP00280
       COMMON/MOLES/TOTMXU,TOTMXB                                       APP00290
       COMMON/CRANGL/SA,CRG,CRGSTP                                      APP00300
       COMMON/STEP/TIMSTP                                               APP00310
       COMMON/CONST/PEC,B                                               APP00320
       REAL Y(1000),YPRIM(1000)                                         APP00330
       REAL X,XEND,INTER,M                                              APP00340
       REAL MU,MB,MBU,MSG,MBARU,MBARU1,MBARB1,MBARB,MBARAD              APP00350
       REAL MBARBU,MBARAV,MBARIS,MBARB2                                 APP00360
       REAL MASS,ME,NE,NB,RE,NM                                         APP00370
       DOUBLE PRECISION DSEED                                           APP00380
       DATA ERMAX,MAXITS/1.E-4,50/                                      APP00390
C-----------------------------------------------------------------------APP00400
C                                                                       APP00410
C   TO CALCULATE THE PRESSURE AND TEMPERATURE OF THE MIXTURE BEFORE     APP00420
C   IGNITION, THE INTAKE VALVE IS ASSUMED TO CLOSE AT 120 BTC, WHEN     APP00430
C   THE PRESSURE IS ASSUMED TO BE 0.6 ATM, AND TEMPERATURE TO BE 373 K. APP00440
C                                                                       APP00450
C   SAI = SPARK ADVANCE                                                 APP00460
C   SAIN = CRANK ANGLE AT CLOSE OF INTAKE VALVE (BTC)                   APP00470
C   GAMA = RATIO OF SPECIFIC HEAT                                       APP00480
C   PIN = PRESSURE AT CLOSE OF INTAKE VALVE                             APP00490
C   TIN = TEMPERATURE AT CLOSE OF INTAKE VALVE                          APP00500
C   PO = PRESSURE BEFORE IGNITION                                       APP00510
C   TO = TEMPERATURE BEFORE IGNITION                                    APP00520
C                                                                       APP00530
C-----------------------------------------------------------------------APP00540
       IUP=0                                                            APP00550
       ICLD=0                                                           APP00560
       IKIN=0                                                           APP00570
C                                                                       APP00580
C   INPUT PARAMETERS  ( EQUIVALENCE RATIO INPUT FROM BLOCK DATA )       APP00590
C                                                                       APP00600
       PEC = 4.3E+11                                                    APP00610
       B = 30000.                                                       APP00620
       C = 0.025                                                        APP00630
       PRINT*,' PEC =',PEC,' B =',B,' C =',C                            APP00640
       RPM = 3000.                                                      APP00650
       CRGSTP = 1./4.                                                   APP00660
       SAIN = -140.                                                     APP00670
       TIN = 270.                                                       APP00680
       PIN = 0.7                                                        APP00690
       U0 = 300.                                                        APP00700
       SAI = -10.                                                       APP00710
       SPDR = 2.                                                        APP00720
       EIGN = 6.E-03/4.184                                              APP00730
       GAP = 0.10                                                       APP00740
       NB = 5.                                                          APP00750
       SAF = 120.                                                       APP00760
```

```
      TIMSTP = 1./6./RPM * CRGSTP                                        APP00780
      SA1=SAIN                                                           APP00790
      CALL UPROP(PIN,TIN,ENTHU,CSUBP,RHO)                                APP00800
      RHO0=RHO                                                           APP00810
      PRINT*,'++++++++++++++++++ AT CLOSE OF INTAKE ++++++++++++++'      APP00820
      PRINT*,' RPM =',RPM,'  UPRIM =',U0,' CM/SEC'                       APP00830
      PRINT*,' SA1 =',SA1,'  VTO(SA1) =',VTO(SA1)                        APP00840
      PRINT*,' TIN =',TIN,'  PIN =',PIN                                  APP00850
      T1=TIN                                                             APP00860
      P1=PIN                                                             APP00870
     DO 100 SA= SA1,SAI,0.5                                              APP00880
      CALL UPROP(P1,T1,ENTHU,CSUBP,RHO)                                  APP00890
      PO=(VTO(SA)/VTO(SA1))**(-GAMU)*P1                                  APP00900
      TO=(PO/P1)**((GAMU-1)/GAMU)*T1                                     APP00910
      P1=PO                                                              APP00920
      T1=TO                                                              APP00930
      SA1=SA                                                             APP00940
 100  CONTINUE                                                           APP00950
      SA=SA1                                                             APP00960
      PRINT*,'++++++++++++++++++ AT IGNITION ++++++++++++++++++++'       APP00970
      PRINT*,' SA = ',SA,'  VTO(SA) = ',VTO(SA)                          APP00980
      PRINT*,' PO = ',PO,' TO = ',TO                                     APP00990
C-------------------------------------------------------------------     APP01000
C                                                                        APP01010
C    IGNITION IS MODELLED AS BURNING NB PARTICLES OF THE SIZE OF THE     APP01020
C            SPARK PLUG GAP IN THE ENSEMBLE OF N PARTICLES. IN THE       APP01030
C            FOLLOWING SECTION, EQUATIONS REPRESENTING THE VOLUME AND    APP01040
C            INTERNAL ENERGY ARE TO BE SOLVED FOR THE UNKNOWN            APP01050
C            BURNED PARTICLE PRESSURE AND TEMPERATURE.                   APP01060
C                                                                        APP01070
C                                                                        APP01080
C    EO = TOTAL INTERNAL ENERGY OF THE MIXTURE                           APP01090
C    EB1 = INTERNAL ENERGY OF THE BURNED PARTICLE                        APP01100
C    EU = INTTERNAL ENERGY OF THE UNBURNED PARTICLES                     APP01110
C    PO = CYLINDER PRESSURE BEFORE IGNITION                              APP01120
C    TO = TEMPERATURE BEFORE IGNITION                                    APP01130
C    VTO(SA) = CHAMBER VOLUME BEFORE IGNITION, AT SPARK ADVANCE (SA)     APP01140
C    PRESS = CYLINDER PRESSURE AFTER A PARTICLE IS BURNED                APP01150
C    TB1 = TEMPERATURE OF THE BURNED PARTICLE                            APP01160
C    TU = TEMPERATURE OF THE UNBURNED AFTER A PARTICLE IS BURNED         APP01170
C    V = VOLUME OF CHAMBER AFTER A PARTICLE IS BURNED                    APP01180
C    VB  = VOLUME OF THE BURNED PARTICLES                                APP01190
C    VU = VOLUME OF THE UNBURNED AFTER A PARTICLE IS BURNED              APP01200
C    N = TOTAL NUMBER OF PARTICLES IN CHAMBER                            APP01210
C    NB = NUMBER OF PARTICLES BURNED                                     APP01220
C    EIGN = IGNITION ENERGY, ASSUMED TO BE 30 MJ.( 1CAL=4.184J )         APP01230
C           ( 6. MJ IN 0.2 MSEC )                                        APP01240
C    SPDR = SPARK DURATION IN DEGREES OF CRANK ANGLE                     APP01250
C         = 2 DEGREES AT 1500 RPM FOR DURATION OF 0.2 MSEC.              APP01260
C                                                                        APP01270
C-------------------------------------------------------------------     APP01280
      PRINT*,' IGN ENERGY =',EIGN,' CAL, SPARK DURATION =',SPDR,'DEG'    APP01290
C..VOLUME OF SPARK IS CALCULATED AS THAT OF A CYLINDER WITH 0.25CM DIA.  APP01300
      VGAP=3.1416/4.*0.25**2.*GAP                                        APP01310
C..VOLUME OF SPARK IS CALCULATED AS THAT OF A SPHERE WITH DIA = GAP.     APP01320
C     VGAP=3.1416/6.*GAP**3.                                             APP01330
      N=VTO(SA)/VGAP*NB                                                  APP01340
      PRINT*,' N = ',N,' NB = ',NB                                       APP01350
      PRINT*,' GAP =',GAP,' IGN DIA =',(6./3.1415*VGAP)**(1./3.)         APP01360
      PRESS=PO                                                           APP01370
      V=VTO(SA+SPDR)                                                     APP01380
      CALL UPROP(PO,TO,ENTHU,CSUBP,RHO)                                  APP01390
      EO=ENTHU*1000.-RU*TO                                               APP01400
      MASS=RHO*VTO(SA)                                                   APP01410
      PRINT*,' MASS FLOW PER CYCLE =',MASS,' GRAM'                       APP01420
      EO=EO*MASS                                                         APP01430
      PRINT*,' PHI = ',PHI                                               APP01440
      EBI = (NB/N)*EO + EIGN                                             APP01450
      EUI = ((N-NB)/N)*EO                                                APP01460
      EOTI = EBI + EUI                                                   APP01470
C     PRINT*,' EBI,EUI :',EBI,EUI                                        APP01480
      X = 0.                                                             APP01490
      PPLUS = PO*0.00225*SPDR                                            APP01500
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      DO 25 I = 1,50                                                    APP01510
         TU = TO*(PRESS/PO)**((GAMU-1.)/GAMU)                           APP01520
         CALL UPROP(PRESS,TU,ENTHU,CSUBP,RHO)                           APP01530
         EU = ENTHU*1000.-RU*TU                                         APP01540
         EU = EU*MASS*(N-NB)/N                                          APP01550
         VU = ((N-NB)/N)*VTO(SA)*((PO/PRESS)**(1./GAMU))                APP01560
         WORKU = (PRESS+PO)*PSCALE*(VU-VTO(SA)*(N-NB)/N)/2.             APP01570
         VB = V-VU                                                      APP01580
         TB1 = 2000.                                                    APP01590
         CALL CLDPRD(PRESS,TB1,HB,CSUBP,RHOB,IER)                       APP01600
         TB1 = VB*PRESS/(RB/PSCALE)/(MASS*NB/N)                         APP01610
         DO 95 J =1,50                                                  APP01620
           CALL CLDPRD(PRESS,TB1,HB,CSUBP,RHOB,IER)                     APP01630
           TB2=TB1                                                      APP01640
           TB1 = VB*PRESS/(RB/PSCALE)/(MASS*NB/N)                       APP01650
           IF(ABS(TB2-TB1).LE.0.5) GO TO 96                             APP01660
 95      CONTINUE                                                       APP01670
 96      EB = HB*1000.-RB*TB1                                           APP01680
         EB = EB*MASS*NB/N                                              APP01690
         WORKB = (PRESS+PO)*PSCALE*(VB-VTO(SA)*NB/N)/2.                 APP01700
       EOT = EU+WORKU+EB+WORKB                                          APP01710
C     PRINT*,' PRESS,EB+WORKB,EU+WORKU :',PRESS,EB+WORKB,EU+WORKU       APP01720
       IF(ABS(EB+WORKB-EBI)/EBI.LE.0.010.AND.                           APP01730
     1   ABS(EU+WORKU-EUI)/EUI.LE.0.010) GO TO 15                       APP01740
      IF(I.GE.50)                                                       APP01750
     1  PRINT*,' NUMBER OF ITERATION EXCEEDS LIMIT AT IGNITION I'       APP01760
      IF(I.GE.50) STOP                                                  APP01770
      IF(X.EQ.0..AND.(EB+WORKB)/EBI.LT.1.) THEN                         APP01780
        PRESS = PRESS + PPLUS                                           APP01790
      ELSE                                                              APP01800
        X = X +1.                                                       APP01810
        IF((EB+WORKB)/EBI.LT.1.) THEN                                   APP01820
         PRESS = PRESS + (PPLUS/(2.**X))                                APP01830
        ELSE                                                            APP01840
         PRESS = PRESS - (PPLUS/(2.**X))                                APP01850
        ENDIF                                                           APP01860
      ENDIF                                                             APP01870
 25   CONTINUE                                                          APP01880
 15   SA=SA+SPDR                                                        APP01890
       PRINT*,'++++++++++++++++++++  AFTER IGNITION  +++++++++++++++++' APP01900
       PRINT *,' SA =',SA,' PRESS = ', PRESS,' ATM'                     APP01910
       PRINT *, ' TU = ', TU,' TB1 =',TB1                               APP01920
       PRINT*,' VU1 = ',VU/(N-NB),' VB1 =',VB/NB                        APP01930
       PRINT*,' BURNED DIA =',(6./3.1416*VB)**(1./3.)                   APP01940
       PRINT*,' RHO =',RHO,' RHO/RHOB =',RHO/RHOB                       APP01950
       PRINT*,' EU= ',EU,' EB = ',EB                                    APP01960
       PRINT*,' WORKU =',WORKU,'  WORKB =',WORKB                        APP01970
       PRINT*,' EOTI =',EOTI,'  EOT =',EOT                              APP01980
C                                                                       APP01990
C-----------------------------------------------------------------------APP02000
C                                                                       APP02010
C TEMP(I) = TEMP OF PARTICAL I                                          APP02020
C  VOL(I) = VOLUME OF PARTICAL I                                        APP02030
C  FFR(I) = FUEL FRACTION OF PARTICAL I                                 APP02040
C                                                                       APP02050
      DO 110 I = 1,NB                                                   APP02060
        TEMP(I) = TB1                                                   APP02070
        VOL(I)=VB/NB                                                    APP02080
        FFR(I)=0.                                                       APP02090
        IDN(I)=0                                                        APP02100
 110  CONTINUE                                                          APP02110
C                                                                       APP02120
C   FO = FUEL FRACTION OF AN UNBURNED PARTICLE                          APP02130
C                                                                       APP02140
      FO = 44./(44.+5*(32.+3.76*28.)/PHI)                               APP02150
      PRINT*,' UNBURNED FFR =',FO,' UBN FUEL CONC. =',FO/44.,' MOL/G'   APP02160
      DO 120 I = NB+1,MIN(N,9999)                                       APP02170
        TEMP(I) = TU                                                    APP02180
        VOL(I)=VU/(N-NB)                                                APP02190
        FFR(I)=FO                                                       APP02200
        IDN(I)=0                                                        APP02210
 120  CONTINUE                                                          APP02220
       NT=NB                                                            APP02230
      M = MASS/N                                                        APP02240
      ME=NT*M                                                           APP02250
      CALL COUNT(NT)                                                    APP02260
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      WM(1)=44.                                                          APP02290
      WM(2)=18.                                                          APP02300
      WM(3)=28.                                                          APP02310
      WM(4)=2.                                                           APP02320
      WM(5)=32.                                                          APP02330
      WM(6)=28.                                                          APP02340
      WM(7)=44.                                                          APP02350
C                                                                        APP02360
        FF1=FO                                                           APP02370
        X1=FF1/44.                                                       APP02380
        Y1=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                              APP02390
     1       -5.*(FO-FF1)*M*WM(5)/WM(7))/WM(5)/M                         APP02400
        V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                  APP02410
        TOTMXU=X1+Y1+V1                                                  APP02420
        FF1=0                                                            APP02430
        V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                  APP02440
        Z1=3.*(FO-FF1)*M*WM(1)/WM(7)/WM(7)/M                             APP02450
        W1=4.*(FO-FF1)*M*WM(2)/WM(7)/WM(2)/M                             APP02460
        TOTMXB=V1+W1+Z1                                                  APP02470
C                                                                        APP02480
      PRINT*,' CRGSTP =',CRGSTP,' TIMSTP =',TIMSTP                       APP02490
      WRITE(6,600)                                                       APP02500
 600  FORMAT(/4X,'SA',7X,'VTO',6X,'PCOM',5X,'PRESS',                     APP02510
     1       4X,'UPRIM',4X,'VER(%)',4X,'BMF(%)',6X,'NT',5X,'N1',5X,'N3', APP02520
     1  .       3X,'ETOTAL',3X,'T1AV',5X,'T3AV',6X,'TU')                APP02530
C                                                                        APP02540
       P1=PO                                                             APP02550
       T1=TO                                                             APP02560
       DP=0.                                                             APP02570
      WORK=0.                                                            APP02580
      HLAST=0.                                                           APP02590
      IUPT=0                                                             APP02600
      ICLDT=0                                                            APP02610
      IKINT=0                                                            APP02620
      FNT=0.                                                             APP02630
      DO 998 IAGE = 1,500                                                APP02640
       FNM(IAGE)=0.                                                      APP02650
 998  CONTINUE                                                           APP02660
      NAGE=0.                                                            APP02670
      DSEED=1234567.0D0                                                  APP02680
C                                                                        APP02690
      DO 999 CRNGL = SA,SAF,CRGSTP                                       APP02700
C                                                                        APP02710
C  TO CALCULATE PRESSURE AND TEMP FOR MOTORED CYCLE                      APP02720
C                                                                        APP02730
      DO 101 SS=SAI,SA+CRGSTP,CRGSTP                                     APP02740
       CALL UPROP(P1,T1,ENTHU,CSUBP,RHO)                                 APP02750
       PCOM=(VTO(SS)/VTO(SAI))**(-GAMU)*P1                               APP02760
       TCOM=(PCOM/P1)**((GAMU-1)/GAMU)*T1                                APP02770
       DPIS=(PCOM-P1)/TIMSTP                                             APP02780
       P1=PCOM                                                           APP02790
       T1=TCOM                                                           APP02800
       SAI=SS                                                            APP02810
 101  CONTINUE                                                           APP02820
C                                                                        APP02830
       PRESS1=PRESS                                                      APP02840
       DPDT=DP*PSCALE                                                    APP02850
       XEND=TIMSTP                                                       APP02860
C                                                                        APP02870
       IF(N1.EQ.0) THEN                                                  APP02880
         CALL ISCOMP(VTO(SA),VTO(SA+CRGSTP),PRESS,POUT)                  APP02890
         PRESS=POUT                                                      APP02900
       ENDIF                                                             APP02910
       IF(N1.EQ.0) GO TO 19                                              APP02920
C                                                                        APP02930
       IF1=0                                                             APP02940
       IF2=0                                                             APP02950
       IF3=0                                                             APP02960
       IUP=0                                                             APP02970
       ICLD=0                                                            APP02980
       IKIN=0                                                            APP02990
       CALL KINET(X,XEND,DPDT,Y,YPRIM,HLAST)                             APP03000
      IUPT=IUPT+IUP                                                      APP03010
      ICLDT=ICLDT+ICLD                                                   APP03020
      IKINT=IKINT+IKIN                                                   APP03030
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      CALL COUNT(NT)                                                    APP03090
      DO 131 I = 1,NT                                                   APP03100
        IF(IBURN(I).NE.1) IDN(I)=0                                      APP03110
  131 CONTINUE                                                          APP03120
C...  PRINT*,' N1 =',N1,' N3 =',N3                                      APP03130
   19 SA=SA+CRGSTP                                                      APP03140
      DP=(PRESS-PRESS1)/TIMSTP                                          APP03150
C     PRINT*,' DPDT OF COMPRESSION =',DPIS,' DPDT OF COMBUSTION =',DP   APP03160
      IF(N1+N3.EQ.0) PRINT*,' FLAME IS QUENCHED 1'                      APP03170
      IF(N1+N3.EQ.0) STOP                                               APP03180
C                                                                       APP03190
      T1AV=0.                                                           APP03200
      T3AV=0.                                                           APP03210
      DO 29 I = 1,NT                                                    APP03220
        IF(IBURN(I).EQ.1) T1AV=T1AV+TEMP(I)                             APP03230
        IF(IBURN(I).EQ.3) T3AV=T3AV+TEMP(I)                             APP03240
   29 CONTINUE                                                          APP03250
      IF(N1.NE.0)THEN                                                   APP03260
        T1AV=T1AV/N1                                                    APP03270
      ENDIF                                                             APP03280
      IF(N3.NE.0)THEN                                                   APP03290
        T3AV=T3AV/N3                                                    APP03300
      ENDIF                                                             APP03310
C                                                                       APP03320
C  TO CALCULATE TOTAL INTERNAL ENERGY OF THE SYSTEM                     APP03330
C    AND AVERAGE BURNING AND BURNED GAS DENSITY (RHOAVE)                APP03340
C                                                                       APP03350
      ETOTAL=0.                                                         APP03360
       IN=0                                                             APP03370
      VOLB = 0.                                                         APP03380
      DO 102 J=1,NT                                                     APP03390
       IF(IBURN(J).EQ.3) THEN                                           APP03400
         CALL CLDPRD(PRESS,TEMP(J),HB,CP,RHOB,IER)                      APP03410
         ETOTAL=ETOTAL+M*(HB*1000.-RB*TEMP(J))                          APP03420
         VOLB = VOLB+VOL(J)                                             APP03430
       ENDIF                                                            APP03440
       IF(IBURN(J).EQ.2) THEN                                           APP03450
         CALL UPROP(PRESS,TEMP(J),ENTHU,CSUBP,RHO)                      APP03460
         ETOTAL=ETOTAL+M*(ENTHU*1000.-RU*TEMP(J))                       APP03470
       ENDIF                                                            APP03480
       IF(IBURN(J).EQ.1.AND.IDN(J).EQ.0) THEN                           APP03490
         IN=IN+1                                                        APP03500
         JUMP=0                                                         APP03510
         CALL KINTER(Y,IN,WU,WCM,INTER)                                 APP03520
  302    ETOTAL=ETOTAL+INTER*M*TOTMX                                    APP03530
         VOLB = VOLB+VOL(J)                                             APP03540
         IF(JUMP.EQ.1) GO TO 102                                        APP03550
         DO 301 I = 1,NT                                                APP03560
          IF(IDN(I).EQ.J) JUMP=1                                        APP03570
          IF(IDN(I).EQ.J) GO TO 302                                     APP03580
  301    CONTINUE                                                       APP03590
       ENDIF                                                            APP03600
  102 CONTINUE                                                          APP03610
      RHOAVE=(N1+N3)*M/VOLB                                             APP03620
      CALL UPROP(PRESS,TEMP(NT+1),ENTHU,CSUBP,RHO)                      APP03630
      ETOTAL=ETOTAL+(N-NT)*M*(ENTHU*1000.-RU*TEMP(NT+1))                APP03640
      DWORK=(PRESS+PRESS1)*PSCALE*(VTO(SA)-VTO(SA-CRGSTP))/2.           APP03650
      WORK=WORK+DWORK                                                   APP03660
      ETOTAL=ETOTAL+WORK                                                APP03670
      IF(ABS((ETOTAL-EOT)/EOT).GT.0.10)                                 APP03680
     1   PRINT*,' EOT =',EOT,' ETOTAL =',ETOTAL,                        APP03690
     1          ' ... 1ST LAW IS VIOLATED 1'                            APP03700
      IF(ABS((ETOTAL-EOT)/EOT).GT.0.10) STOP                            APP03710
C                                                                       APP03720
C  VE = ENTRAINED VOLUME                                                APP03730
C                                                                       APP03740
      VE=0.                                                             APP03750
      VFL=0.                                                            APP03760
      DO 18 IE=1,NT+1                                                   APP03770
        IF(IE.LE.NT) VE=VE+VOL(IE)                                      APP03780
        IF(IE.GT.NT) VU=VOL(IE)*(N-NT)                                  APP03790
   18 CONTINUE                                                          APP03800
      VD=ABS(VE+VU-VTO(SA))/VTO(SA)                                     APP03810
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      IF(VD.GT.0.05)                                                    APP03820
     1  PRINT*,' VTO(SA) =',VTO(SA),' VE+VU =',VE+VU,                    APP03830
     1         ' ... PERFECT GAS LAW (VOLUME CONSTRAIN) IS VIOLATED !'   APP03840
      IF(VD.GT.0.05) STOP                                               APP03850
      VER=VE/(VE+VU)*100.                                               APP03860
C                                                                       APP03870
      CALL SHARE(SA,VE,H,RE,AE)                                         APP03880
C                                                                       APP03890
C  U0 = TURBULENT INTENSITY AT CLOSE OF INTAKE VALVE ( CM/SEC  )        APP03900
C  RHO0 = DENSITY (UNBURNED) AT CLOSE OF INTAKE VALVE                   APP03910
C  UPRIM = TURBULENT INTENSITY  ( CM/SEC)                               APP03920
C                                                                       APP03930
      TU=TEMP(NT+1)                                                     APP03940
      CALL SPEED(U0,RHO0,TU,PRESS,UPRIM,SL)                             APP03950
      UT=((2.*RHO)/(3.*RHOAVE))**.5*UPRIM+SL                            APP03960
      DT=TIMSTP                                                         APP03970
      RHO=(N-NT)*M/VU                                                   APP03980
      ME=ME+DT*AE*UT*RHO                                                APP03990
       NTP=NT                                                           APP04000
      NT=ME/M                                                           APP04010
      FNT=FNT+ME/M-NT                                                   APP04020
      IF(FNT.GE.1.) NT=NT+1                                             APP04030
      IF(FNT.GE.1.) FNT=FNT-1.                                          APP04040
      NAGE=NAGE+1                                                       APP04050
      IF(NAGE.GT.500) PRINT*,' NAGE > 500  !'                           APP04060
      IF(NAGE.GT.500) STOP                                              APP04070
      NP(NAGE)=NT-NTP                                                   APP04080
C...  PRINT*,' NAGE =',NAGE,' NP =',NP(NAGE)                            APP04090
      IF(NT.GT.9999) PRINT*,' PARTICLES ENTRAINED > 9999  !'            APP04100
      IF(NT.GT.9999) STOP                                               APP04110
      CALL COUNT(NT)                                                    APP04120
C                                                                       APP04130
C  BMF = BURNED MASS FRACTION OF THE SYSTEM                             APP04140
C                                                                       APP04150
      BMF=0.                                                            APP04160
      DO 31 I = 1,NT                                                    APP04170
        BMF = BMF+(1.-FFR(I))/FO)                                       APP04180
   31 CONTINUE                                                          APP04190
      BMF=BMF/N*100.                                                    APP04200
C                                                                       APP04210
C ...  CONSTANT C IS IN  SEC/CM**2                                      APP04220
      DELT=TIMSTP                                                       APP04230
      W=C*UPRIM**2.                                                     APP04240
C                                                                       APP04250
C   CALL RANMIX WITHOUT AGE MIXING, CALL AGEMIX WITH AGE MIXING         APP04260
C                                                                       APP04270
C...  CALL RANMIX(DELT,W,NM,FNM1,DSEED)                                APP04280
      CALL AGEMIX(DELT,W,NM,DSEED)                                      APP04290
C...  PRINT*,' W =',W,' NM =',NM                                        APP04300
      IF(ABS(SA-INT(SA)).EQ.0.) THEN                                    APP04310
      WRITE(6,601)SA,VTO(SA),PCOM,PRESS,UPRIM,VER,BMF,                  APP04320
     1   NT,N1,N3,ETOTAL,T1AV,T3AV,TEMP(NT+1)                           APP04330
 601  FORMAT(/3X,F6.2,3X,F6.2,3X,F6.3,3X,F6.3,3X,F6.1,                  APP04340
     1      3X,F7.3,3X,F7.3,3X,I4,3X,I4,3X,I4,3X,F6.2,                  APP04350
     1        3X,F6.1,3X,F6.1,3X,F5.1)                                  APP04360
      ENDIF                                                             APP04370
 999  CONTINUE                                                          APP04380
       STOP                                                             APP04390
       END                                                              APP04400
C------------ SUBROUTINE PRTY ------------------------------------------APP04410
C                                                                       APP04420
      SUBROUTINE PRTY(Y,NQ)                                             APP04430
      REAL Y(NQ)                                                        APP04440
      WRITE(6,601)                                                      APP04450
 601  FORMAT(/6X,'TEMP',16X,'C3H8')                                     APP04460
      WRITE(6,602)Y                                                     APP04470
 602  FORMAT(5X,F12.7,5X,F12.7)                                         APP04480
      RETURN                                                            APP04490
      END                                                               APP04500
C                                                                       APP04510
C------------ SUBROUTINE COUNT(IN)--------------------------------------APP04520
C                                                                       APP04530
C   IBURN(I)= 1 FOR BURNING PARTICLES                                   APP04540
C   IBURN(I)= 2 FOR UNBURNED PARTICLES                                  APP04550
C   IBURN(I)= 3 FOR FULLY BURNED PARTICLES                              APP04560
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      SUBROUTINE COUNT(IN)                                              APP04590
      COMMON/BURN/FFR(9999),IBURN(9999)                                 APP04600
      COMMON/PARNUM/N,NT,N1,N2,N3                                       APP04610
      COMMON/CHARB/PHI                                                  APP04620
      N1=0                                                              APP04630
      N2=0                                                              APP04640
      N3=0                                                              APP04650
      FO  =  44./(44.+5.*(32.+3.76*28.)/PHI)                            APP04660
C                                                                       APP04670
      DO 125 I=1,IN                                                     APP04680
      IBURN(I)=1                                                        APP04690
      IF(FFR(I).GE.FO*0.95 ) IBURN(I)=2                                 APP04700
      IF(FFR(I).EQ.0.) IBURN(I)=3                                       APP04710
        IF(IBURN(I).EQ.3)THEN                                           APP04720
          N3=N3+1                                                       APP04730
        ELSE                                                            APP04740
          IF(IBURN(I).EQ.2)THEN                                         APP04750
            N2=N2+1                                                     APP04760
          ELSE                                                          APP04770
            N1=N1+1                                                     APP04780
          ENDIF                                                         APP04790
        ENDIF                                                           APP04800
 125  CONTINUE                                                          APP04810
      IBURN(NT+1) = 2                                                   APP04820
      RETURN                                                            APP04830
      END                                                               APP04840
C                                                                       APP04850
C-----------------------------------------------------------------------APP04860
      BLOCK DATA                                                        APP04870
      DIMENSION A(6,6,2)                                                APP04880
      EQUIVALENCE (A1(1),A(1,1,1))                                      APP04890
      EQUIVALENCE (A2(1),A(1,1,2))                                      APP04900
      COMMON/JANAF/ A1(36),A2(36)                                       APP04910
      COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR                             APP04920
      COMMON /FUEL/ ENW,CX,HY,OZ,AST                                    APP04930
      COMMON /OXDANT/XI                                                 APP04940
       COMMON/CHARTH/RESFRK,RICH,LEAN                                   APP04950
       COMMON/CHARU/PHIFR,PHIEGR                                        APP04960
       COMMON/CHARB/PHI                                                 APP04970
C                                                                       APP04980
C                                                                       APP04990
C *** FUEL INFORMATION *****************                               APP05000
C                                                                       APP05010
      DATA ENW,CX,HY,OZ,AST/ 0., 3., 8., 0., 0.0/                       APP05020
      DATA A1/11.94033,2.088581,-0.47029,.037363,-.589447,-97.1418,     APP05030
     1 6.139094,4.60783,-.9356009,6.669498E-02,.0335801,-56.62588,      APP05040
     2  7.099556,1.275957,-.2877457,.022356,-.1598696,-27.73464,        APP05050
     3  5.555680,1.787191,-.2881342,1.951547E-02,.1611828, .76498,      APP05060
     4  7.865847,.6883719,-.031944,-2.68708E-03,-.2013873,-.893455,     APP05070
     5  6.807771,1.453404,-.328985,2.561035E-02,-.1189462,-.331835/     APP05080
      DATA A2/4.737305,16.65283,-11.23249,2.828001,6.76702E-03,-93.75793APP05090
     7 ,7.809672,-.2023519,3.418708,-1.179013,1.43629E-03,-57.08004,    APP05100
     8  6.97393,-.8238319,2.942042,-1.176239,4.132409E-04,-27.19597,    APP05110
     9  6.991878,.1617044,-.2182071,.2968197,-1.625234E-02,-.118189,    APP05120
     &  6.295715,2.388387,-.0314788,-.3267433,4.35925E-03,.103637,      APP05130
     \  7.0922,-1.2958,3.2069,-1.2022,-3.458E-04,-.013967/              APP05140
C *** CHEMICAL INFO  *****                                              APP05150
C                                                                       APP05160
       DATA RESFRK,PHI,PHIFR,PHIEGR/0.,0.5,0.5,0.5/                     APP05170
C                                                                       APP05180
C *** MOLAR N-O RATIO OF OXDANT ***                                     APP05190
C                                                                       APP05200
      DATA XI /3.76/                                                    APP05210
C                                                                       APP05220
      DATA R,RGSI,RO2,PSCALE,PSCOR                                      APP05230
     &      /1.9869,8.3143E7,.99345,2.42173E-2,1.2187E-2/               APP05240
      END                                                               APP05250
                                                                        APP05260
```

APPENDIX B

THERMODYNAMIC PROPERTIES OF PARTICLES

The thermodynamic properties of particles are functions of the temperatures and compositions. The overall reaction mechanism for the combustion of propane in air is assumed.

$$C_3H_8 + \frac{5}{\phi}O_2 + \frac{5\times3.76}{\phi}N_2 \rightarrow (\frac{5}{\phi} - 5)O_2 + 3CO_2 + 4H_2O + \frac{5\times3.76}{\phi}N_2$$

Equation (37)

where ϕ is the equivalence ratio defined as

$$\phi = \frac{actual\ air\ fuel\ ratio}{stoichiometric\ air\ fuel\ ratio}$$

The enthalpy, internal energy, specific heat at constant pressure and specific heat at constant volume are calculated using polynomial curve fitting of thermodynamic properties of the JANAF Table (1971). The polynomial function and coefficients are taken from Hire et al (1976). The specific enthalpy is calculated using the following function,

$$h = \sum_{i=1}^{6} X_i(\sum_{j=1}^{4}[a_{ij}T^j/j] - [a_{5j}/T] + a_{6j})$$

where h is the specific enthalpy in $Kcal/g$, X_i is the number of moles of species i (i is 1 for CO_2, 2 for H_2O, 3 for CO, 4 for H_2, 5 for O_2, and 6 for N_2), T is the temperature, and a_{ij} are the coefficients of the polynomial function. These coefficients are shown in Table 13. The internal energy in $cal/mole$ of fuel is calculated by the following expression,

$$u = R(0.233361 \times 10^{-10}T^5/5 - 0.545131 \times 10^{-7}T^4/4 + 0.351709 \times 10^{-4}T^3/3$$
$$+0.0157505T^2/2 + 1.31841T - 14091.3) + 201.1M_f$$

where R is the universal gas constant and M_f is the molecular weight of propane. The internal energy U in $Kcal$ is obtained by the relation,

$$U = H - RT$$

where H is the enthalpy in $Kcal$. The specific heat at constant pressure is calculated using the following polynomial function,

$$C_p = \sum_{i=1}^{6} X_i \sum_{j=1}^{4} (a_{ij} T^{j-1} + a_{5j}/T^2)$$

where C_p is the specific heat at constant pressure in $cal/g°K$. The specific heat at constant pressure of fuel is calculated by the following expression,

$$C_p = R/M_f(0.233361 \times 10^{-10}T^4 - 0.545131 \times 10^{-7}T^3$$
$$+0.351709 \times 10^{-4}T^2 + 0.0157505T + 1.31841) + R/M_f$$

The specific heat at constant volume C_v is obtained using the relation,

$$C_v = C_p - R$$

where R is the universal gas constant. The ratio of specifc heat can be calculated as,

$$\gamma = \frac{C_p}{C_v}$$

For an unburned particle, the above calculations are performed by subroutine UPROP, assuming the presence of the species on the left hand side of the reaction equation (37). For a burned particle, subroutine CLDPRD assumes that dissociation of products is neglegable and that the species on the right hand side of the reaction equation are present. For particles with frosen composition consist of all the species in the reaction equation, the above calculation is performed within the subroutine MIXFRO.

APPENDIX C

```
C----------  SUBROUTINE SPEED(UO,RHOO,TU,PRESS,UPRIM,SL)  ----------
C
C     GIVEN : UO = TURBULENT INTENSITY BEFORE IGNITION
C             RHOO = DENSITY (UNBURNED) BEFORE IGNITION
C             TU = UNBURNED TEMPERATURE
C             PRESS = PRESSURE IN ATM
C
C     RETURN : UPRIM = TURBULENT INTENSITY
C              SL = LAMINAR FLAME SPEED
C
C        NOTE : UO,UPRIM,CM,SL ARE IN CM/SEC
C
C-----------------------------------------------------------------------
C
      SUBROUTINE SPEED(UO,RHOO,TU,PRESS,UPRIM,SL)
      COMMON /UGASP/ X(7),MBAR,RU,GAMU,CPU,HU,TU1,RHOU
      COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR
      REAL MR,K
      DATA MR,ALPHA,A,B,E/31.,-0.06,-0.46,1.46,37.7/
      DATA ERMAX,MAXITS/0.01,25/
C
      CALL UPROP(PRESS,TU,ENTHLP,CSUBP,RHO)
      TGUESS=1900.
      CALL TEMPB(PRESS,TGUESS,ENTHLP,TB,ERMAX,MAXITS,IER)
      IF(IER.EQ.1)
     1  PRINT*,' ... NUMBER OF ITERATION EXCEEDS LIMIT IN "SPEED" !'
      IF(IER.EQ.1) STOP
      TM=TU+0.74*(TB-TU)
      CM=(8.*R*(4.184E7)*TM/(3.1416*MR))**(1./2.)
      K=(2.*TU/(3.07*TM))*((PRESS/1.)**ALPHA)
      YFOL=X(5)**B
      YFFL=X(7)**A
      SL=K*CM*(YFOL*YFFL*EXP(-E*1000./(R*TM)))**(1./2.)
      UPRIM=UO*(RHO/RHOO)**(1./3.)
C
      RETURN
      END
C
CTEMPB ************* VERSION 1.0 *** 5/29/74 **********************
C     SUBROUTINE TEMPB
C
C     PURPOSE
C        TO CALCULATE THE TEMPERATURE OF THE PRODUCTS OF HC-AIR
C        COMBUSTION, FOR GIVEN SPECIFIC ENTHALPY OF THE PRODUCT
C        FOR GIVEN ABSOLUTE PRESSURE
C
C     USAGE
C        CALL  TEMPB(P,TGUESS,ENTHLP,T,ERMAX,MAXITS,IER)
C
C     DESCRIPTION OF PARAMETERS
C      GIVEN
C        P      - ABSOLUTE PRESSURE OF THE PRODUCTS (ATM)
C        TGUESS- INITIAL GUESS FOR T (DEG K)
C        PHI    - EQUIVALENCE RATIO OF THE PRODUCTS
C        DEL    - MOLAR C H RATIO OF THE PRODUCTS
C        PSI    - MOLAR N O RATIO OF THE PRODUCTS
C        ENTHLP-  ENTHALPY OF THE PRODUCTS (KCAL/G)
C        ERMAX - MAXIMUM ALLOWABLE RELATIVE ERROR IN RESULTANT T
C        MAXITS- MAXIMUM NUMBER OF ALLOWABLE ITERATIONS WITHOUT
C                SUCCESS
C        IER    - FLAG, SET TO 1 IF NO SUCCESS WITHIN MAXITS ITERATIONS
C      RETURNS
C        T      - TEMPERATURE OF THE PRODUCTS  (DEG K)
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C        HPROD
C
C     METHOD
C        NEWTON-RAPHSON ITERATION
C
C*********************************************************************
```

APP05260 APP05270 APP05280 APP05290 APP05300 APP05310 APP05320 APP05330 APP05340 APP05350 APP05360 APP05370 APP05380 APP05390 APP05400 APP05410 APP05420 APP05430 APP05440 APP05450 APP05460 APP05470 APP05480 APP05490 APP05500 APP05510 APP05520 APP05530 APP05540 APP05550 APP05560 APP05570 APP05580 APP05590 APP05600 APP05610 APP05620 APP05630 APP05640 APP05650 APP05660 APP05670 APP05680 APP05690 APP05700 APP05710 APP05720 APP05730 APP05740 APP05750 APP05760 APP05770 APP05780 APP05790 APP05800 APP05810 APP05820 APP05830 APP05840 APP05850 APP05860 APP05870 APP05880 APP05890 APP05900 APP05910 APP05920 APP05930 APP05940 APP05950 APP05960 APP05970 APP05980 APP05990 APP06000 APP06010

```
      SUBROUTINE TEMPB(P,TGUESS,ENTHLP,T,ERMAX,MAXITS,IER)                APP06020
      T = TGUESS                                                          APP06030
      IER = 0                                                             APP06040
C                                                                         APP06050
      DO 10 I = 1,MAXITS                                                  APP06060
         CALL HPROD(P,T,AHG,CSUBP,CSUBT,RHO,DRHODT,DRHODP)                APP06070
         TOLD = T                                                         APP06080
         T = T + (ENTHLP - AHG)/(CSUBP * 1.0E-3)                          APP06090
         IF( ABS((T - TOLD)/ T)  .LE. ERMAX) GO TO 20                     APP06100
   10 CONTINUE                                                            APP06110
C                                                                         APP06120
      IER = 1                                                             APP06130
   20 RETURN                                                              APP06140
      END                                                                 APP06150
C                                                                         APP06160
CHPROD ************ VERSION 2.1 *** 1/05/78 ************************     APP06170
C                                                                         APP06180
C     SUBROUTINE HPROD                                                    APP06190
C                                                                         APP06200
C     PURPOSE                                                             APP06210
C        TO CALCULATE THE PROPERTIES OF THE PRODUCTS OF HYDROCA           APP06220
C        AIR COMBUSTION AS A FUNCTION OF TEMPERATURE AND PRESSURE,        APP06230
C        USING AN APPROXIMATE CORRECTION FOR DISSOCIATION.                APP06240
C        H AND RHO ARE CALCULATED AS FUNCTIONS OF P, T, AND PHI.          APP06250
C        THE PARTIAL DERIVATIVES OF H AND RHO WITH RESPECT TO             APP06260
C        P AND T ARE ALSO CALCULATED                                      APP06270
C                                                                         APP06280
C     USAGE                                                               APP06290
C        CALL HPROD (P, T,  H, CP, CT, RHO, DRHODT,DRHODP)                APP06300
C                                                                         APP06310
C     DESCRIPTION OF PARAMETERS                                           APP06320
C      GIVEN                                                              APP06330
C        P      - ABSOLUTE PRESSURE OF PRODUCTS (ATM)                     APP06340
C        T      - TEMPERATURE OF PRODUCTS (DEG K)                         APP06350
C      GIVEN IN COMMON AREA /CHARGE/                                      APP06360
C        PHI    - EQUIVALENCE RATIO (FUEL/AIR RATIO DIVIDED BY THE        APP06370
C                 CHEMICALLY CORRECT FUEL/AIR RATIO)                      APP06380
C      GIVEN IN COMMON AREA /PRODMR/                                      APP06390
C        DEL    - MOLAR C H RATIO OF THE PRODUCTS                         APP06400
C        PSI    - MOLAR N O RATIO OF THE PRODUCTS                         APP06410
C      GIVEN IN COMMON AREA /THERMS/                                      APP06420
C        PSCALE- CONST TO GIVE CAL FROM ATM-CC                            APP06430
C        R      - GAS CONSTANT                                            APP06440
C        ROVER2 - GAS CONSTANT DIVIDED BY TWO                             APP06450
C        PSCOR - PSCALE DIVIDED BY GAS CONSTANT                           APP06460
C      RETURNS                                                            APP06470
C        H      - SPECIFIC ENTHALPY OF THE PRODUCTS (KCAL/G)              APP06480
C        CP     - PARTIAL DERIVATIVE OF H WITH RESPECT TO T AT C          APP06490
C                 P AND PHI    (CAL/G-DEG K)                             APP06500
C        CT     - PARTIAL DERIVATIVE OF H WITH RESPECT TO P AT C          APP06510
C                 T AND PHI    (CC/G)                                    APP06520
C        RHO    - DENSITY OF THE PRODUCTS      (G/CC)                    APP06530
C        DRHODT- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO T AT           APP06540
C                 CONSTANT P AND PHI    (G/CC-DEG K)                      APP06550
C        DRHODP- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO P              APP06560
C                 CONSTANT T AND PHI    (G/CC-ATM)                        APP06570
C                                                                         APP06580
C      RETURNS IN COMMON AREA FROZEN                                      APP06590
C        CPFROZ- FROZEN SPECIFIC HEAT (CAL/G - DEG K)                     APP06600
C     REMARKS                                                             APP06610
C        1) ENTHALPY DATUM STATE IS AT T = 0 ABSOLUTE WITH                APP06620
C           O2, N2, H2 GASEOUS AND C SOLID GRAPHITE                       APP06630
C        2) MULTIPLY ATM-CC BY .0242173 TO CONVERT TO CAL                 APP06640
C                                                                         APP06650
C     SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                       APP06660
C        CLDPRD                                                           APP06670
C                                                                         APP06680
C     METHOD                                                              APP06690
C        SEE MARTIN & HEYWOOD 'APPROXIMATE RELATIONSHIPS FOR TH           APP06700
C        DYNAMIC PROPERTIES OF HYDROCARBON-AIR COMBUSTION PRODU           APP06710
C                                                                         APP06720
C                                                                         APP06730
C                                                                         APP06740
C*************************************************************************APP06750
```

```
      SUBROUTINE HPROD(P,T,H,CP,CT,RHO,CCT,CCP)                          APP06770
      LOGICAL RICH, LEAN, NOTHOT, NOTWRM, NOTCLD                         APP06780
      REAL MCP, MWT, K1, K2                                              APP06790
      COMMON/CHARB/PHI                                                   APP06800
       COMMON/CHARTH/RESFRK,RICH,LEAN                                    APP06810
      COMMON /PRODMR/DEL,CHI,DUM,DUMY,EPSO,EPS                           APP06820
      COMMON /BGASP/CCB(7),MWT,RB,GAMMAB,CPB,HB                          APP06830
      COMMON/THERMO/RGAS,RGSI,ROVER2,PSCALE,PSCOR                        APP06840
      COMMON/FUEL/ENN,CX,HY,OZ,AST                                       APP06850
      COMMON/OXDANT/PSI                                                  APP06860
      DATA I1/0/                                                         APP06870
C                                                                        APP06880
C     INITIALIZE PARAMETERS USED IN THE CALCULATION                      APP06890
C                                                                        APP06900
      DATA TCOLD, THOT /1000., 1100./                                    APP06910
C                                                                        APP06920
      NOTHOT = T .LT. THOT                                               APP06930
      NOTCLD = T .GT. TCOLD                                              APP06940
      NOTWRM = .NOT. (NOTCLD .AND. NOTHOT)                               APP06950
      IF(T.GE.2800.) T=2800.                                             APP06960
C                                                                        APP06970
C     USE SIMPLE ROUTINE FOR LOW TEMPERATURE MIXES                       APP06980
C                                                                        APP06990
      IF (NOTCLD) GO TO 1                                                APP07000
      CALL CLDPRD(P,T,H,CP,RHO,IER)                                      APP07010
      RETURN                                                             APP07020
    1 IF(I1) 3,2,3                                                       APP07030
C                                                                        APP07040
C *** DO THIS ONLY FIRST TIME                                            APP07050
C                                                                        APP07060
    2 I1=1                                                               APP07070
      DEL=CX/HY                                                          APP07080
      EPS=(4.*DEL)/(1. + 4.*DEL)                                         APP07090
      C5 = 2.- EPS + PSI                                                 APP07100
      C6 = EPS + 2.*C5                                                   APP07110
      C3 = (121.5 + 29.59*EPS)*1000.                                     APP07120
      C4 = 1.175E5                                                       APP07130
      T5 = 3.*C5                                                         APP07140
      TV = (3256.- 2400.*EPS + 300.*PSI)/(1.- .5*EPS + .09*PSI)          APP07150
    3 DEL=3./8.                                                          APP07160
      EPS=(4.*DEL)/(1. + 4.*DEL)                                         APP07170
      HFO=PHI*(20372.*EPS-114942.)                                       APP07180
      MCP    = (8.*EPS + 4.)*PHI + 32. + 28.*PSI                         APP07190
      RO2MCP=ROVER2/MCP                                                  APP07200
      LEAN=PHI.LE.1.                                                     APP07210
      IF (LEAN)  GO TO 4                                                 APP07220
C           RICH CASE                                                    APP07230
      HFO=HFO + 1000.*(134.39 - 6.5/EPS)*(PHI - 1.)                      APP07240
      C10= 2. + 2.*(7.- 4.*EPS)*PHI + 7.*PSI                             APP07250
      C20= 8. + 2.*(2.- 3.*EPS)*PHI + 2.*PSI                             APP07260
      DO=PHI*(2.-EPS)+PSI                                                APP07270
      GO TO 5                                                            APP07280
C             LEAN CASE                                                  APP07290
    4 C10= 7. +    (9.- 8.*EPS)*PHI + 7.*PSI                           APP07300
      C20= 2. + 2.*(5.- 3.*EPS)*PHI + 2.*PSI                             APP07310
      DO=1.+PHI*(1.-EPS)+PSI                                             APP07320
C                                                                        APP07330
C *** ENTRY AFTER FIRST CALL                                             APP07340
C                                                                        APP07350
C     CALCULATE EQUILIBRIUM CONSTANTS FOR DISSOCIATION                   APP07360
C     (NOTE THAT THESE HAVE UNITS ATM**(.5) )                            APP07370
C                                                                        APP07380
    5 K1 = 5.819E-6 * EXP(.9674*EPS + 35810./T)                          APP07390
      K2 = 2.961E-5 * EXP(2.593*EPS + 28980./T)                          APP07400
C                                                                        APP07410
C     CALCULATE A, X, Y, & U                                             APP07420
C                                                                        APP07430
C     IF((4.*P*K1*K1*EPS).EQ.0.)STOP                                     APP07440
      A  = ( C5/(4.*P*K1*K1*EPS) )**(.33333333)                          APP07450
      AA=T5*(1.+A+A)+2.*C6*A*A                                           APP07460
C                                                                        APP07470
      X  = A*EPS*(T5+C6*A)/AA                                            APP07480
C                                                                        APP07490
      Z = ABS((1.- PHI)/X)                                               APP07500
                                                                         APP07510
```

```
      U = C5*(EPS - 2.*X)/(4.*K1*K2*P*X)                                APP07520
      IF(LEAN) GOTO 10                                                  APP07530
      Y=X/(1.+.6666667*Z+.3333333*Z*Z-.6666667*(PHI-1.))                APP07540
      DYDX= (Y*Y)/(X*X)*(1.+ 4.*Z/3. + Z*Z - 2.*(PHI-1.)/3.)            APP07550
      GOTO 20                                                           APP07560
   10 ACH=1.+.6666667*Z+1.3333333*(1.-PHI)                              APP07570
      Y=X/(SQRT(ACH))                                                   APP07580
      DYDX=(Y/X)**3*(1.+Z+1.333333*(1.-PHI))                            APP07590
C                                                                       APP07600
C     CALCULATE THE ENTHALPY OF FORMATION FOR THIS APPROXIMATE          APP07610
C     COMPOSITION
C     ALSO GET THE COEFFICIENTS FOR T & TV TERMS
C                                                                       APP07640
   20 HF = HF0 +C3*Y +C4*U                                              APP07650
      C1 = C10 +5.*Y + 3.*U                                             APP07660
      C2 = C20 -6.*Y -2.*U                                              APP07670
      D = D0 + Y+ U                                                     APP07680
C                                                                       APP07690
C     ADD IN TRANSLATIONAL,VIBRATIONAL, AND ROTATIONAL TERMS TO GET     APP07700
C     TOTAL ENTHALPY
C                                                                       APP07720
      EXPTVT= EXP(TV/T)                                                 APP07730
      TVTIL = TV/( EXPTVT - 1.)                                         APP07740
C                                                                       APP07750
      H     = .001*RO2MCP*(C1*T + C2*TVTIL + HF)                        APP07760
C                                                                       APP07770
C     CALCULATE AVERAGE MOLECULAR WEIGHT, AND GET DENSITY BY            APP07780
C     USING THE PERFECT GAS LAW
C                                                                       APP07800
      MWT = MCP/D                                                       APP07810
      RHO = MWT*P*PSCOR/T                                               APP07820
      RHOB=RHO                                                          APP07830
      RB=RGAS/MWT                                                       APP07840
C                                                                       APP07850
C     GET PARTIAL DERIVATIVES IF DESIRED                                APP07860
C                                                                       APP07870
C                                                                       APP07900
C                                                                       APP07910
      DUDTPX = 64790.*U/(T*T)                                           APP07920
      DUDPTX = -U/P                                                     APP07930
      DUDXPT = -U*EPS/(X*(EPS - 2.*X))                                  APP07940
C                                                                       APP07950
      DADTP = 23873.*A/(T*T)                                            APP07960
      DADPT = -A/(3.*P)                                                 APP07970
C                                                                       APP07980
      DXDA=T5*EPS*(T5+2.*C6*A)/AA/AA                                    APP07990
C                                                                       APP08000
C                                                                       APP08030
      DYDTP = DYDX*DXDA*DADTP                                           APP08040
      DYDPT = DYDX*DXDA*DADPT                                           APP08050
      DUDTP = DUDXPT*DXDA*DADTP + DUDTPX                                APP08060
      DUDPT = DUDXPT*DXDA*DADPT + DUDPTX                                APP08070
C                                                                       APP08080
      DHFDPT = C3*DYDPT + C4*DUDPT                                      APP08090
      DC2DPT = -2.*(3.*DYDPT + DUDPT)                                   APP08100
      DC1DPT = 5.*DYDPT + 3.*DUDPT                                      APP08110
      DHFDTP = C3 * DYDTP + C4*DUDTP                                    APP08120
      DC2DTP = -2.*(3.*DYDTP + DUDTP)                                   APP08130
      DC1DTP = 5.*DYDTP + 3.*DUDTP                                      APP08140
C                                                                       APP08150
      DTVDTP = (TVTIL*TVTIL)/(T*T)*EXPTVT                               APP08160
C                                                                       APP08170
      CPFROZ = RO2MCP*(C1 + C2*DTVDTP)                                  APP08200
C                                                                       APP08210
      CP = RO2MCP*(T*DC1DTP+TVTIL*DC2DTP+DHFDTP)+CPFROZ                 APP08220
      CT = RO2MCP*(T*DC1DPT + TVTIL*DC2DPT + DHFDPT)/PSCALE             APP08230
      CPB=CP                                                            APP08240
      G     =MWT/D                                                      APP08280
      DMDTP = G*(DYDTP + DUDTP)                                         APP08290
      DMDPT = G*(DYDPT + DUDPT)                                         APP08300
C                                                                       APP08310
      CCT=1.-DMDTP*T/MWT                                                APP08320
      CCP=1.+DMDPT*P/MWT                                                APP08330
      GAMMAB=CP/(CP-RB)                                                 APP08340
```

```
C     IF CALCULATING FOR AN INTERMEDIATE TEMPERATURE, USE A WEIGHTED    APP08360
C     AVERAGE OF THE RESULTS FROM THIS ROUTINE AND THOSE FROM THE       APP08370
C     SIMPLE ROUTINE                                                    APP08380
C                                                                       APP08390
      IF (NOTWRM) RETURN                                                APP08400
C                                                                       APP08410
      CALL CLDPRD(P,T,TH,TCP,TRHO,IER)                                  APP08420
      W1 = (T - TCOLD)/(THOT - TCOLD)                                   APP08430
      W2 = 1.0 - W1                                                     APP08440
C                                                                       APP08450
      H    = W1*H    + W2*TH                                            APP08460
      RHOB = W1*RHO + W2*TRHO                                           APP08470
      CP   = W1*CP   + W2*TCP                                           APP08480
      CT   = W1*CT                                                      APP08490
      CCT=W1*CCT+W2                                                     APP08500
      CCP=W1*CCP+W2                                                     APP08510
      MWT=(RHO*T)/(PSCOR*P)                                             APP08520
      CPB=CP                                                            APP08530
C                                                                       APP08540
      IF(GAMMAB.LT.1..OR.GAMMAB.GT.2.)THEN                              APP08550
      PRINT*,' '                                                        APP08560
      PRINT*,'************** EXECUTION STOPPED AT HPROD **************'APP08570
      PRINT*,' '                                                        APP08580
      PRINT*,'T =',T,' P =',P                                           APP08590
      PRINT*,'CPB =',CPB,' RB =',RB                                     APP08600
      PRINT*,'GAMMAB =',GAMMAB                                          APP08610
      PRINT*,' '                                                        APP08620
      PRINT*,'************** EXECUTION STOPPED AT HPROD **************'APP08630
      PRINT*,' '                                                        APP08640
      ENDIF                                                             APP08650
      IF(GAMMAB.LT.1..OR.GAMMAB.GT.2.) STOP                             APP08660
C                                                                       APP08670
      RETURN                                                            APP08680
      END                                                               APP08690
```

APPENDIX D

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C  SUBROUTINE MIXFRO
C
C  USAGE : TO CALCULATE NEW COMPOSITION AND THERMODYNAMIC PROPERTIES
C          OF A PAIR OF IDENTICAL PARTICLES RESULTED FROM A BINARY
C          MIXING.IT IS ASSUMED THAT THE VOLUME AND PRESSURE HAVE NOT
C          CHANGED, AND THE PROPERTIES AND COMPOSITION ARE FROZEN
C          DURING THE MIXING PROCESS.
C
C  INPUT : COMPOSITION OF PARTICLE 1 AND 2
C              X1, X2 = MOLES OF FUEL/ G
C              Y1, Y2 = MOLES OF O2 / G
C              V1, V2 = MOLES OF N2 / G
C              Z1, Z2 = MOLES OF CO2 / G
C              W1, W2 = MOLES OF H2O / G
C          THERMODYNAMIC PROPERTIES OF PARTICLE 1 AND 2
C              VOL1, VOL2 = VOLUME OF EACH PARTICLE
C              T1, T2 = TEMPERATURE OF EACH PARTICLE
C
C  OUTPUT : NEW COMPOSITION OF EACH PARTICLE AFTER MIXING
C              XO, YO, VO, ZO, WO  ( MOLES / G )
C            TEMPERATURE OF EACH PARTICLE AFTER MIXING, TO (K)
C
C  SUBROUTINE NEEDED : NONE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE MIXFRO(F1,F2,VOL1,VOL2,T1,T2)
      LOGICAL RICH,LEAN
      DIMENSION TABLE(7),A(6,6,2),LEC(10),MX(7,3),X(10),WM(10)
      EQUIVALENCE (A1(1),A(1,1,1)),(A2(1),A(1,1,2))
      REAL  MBAR,MX,INTER
      REAL T,M,MASS
      REAL TEMP(3)
      COMMON/MIX/MASS,F3,VOL3,TO
      COMMON/PARNUM/N,NT,N1,N2,N3
      COMMON /FUEL/ ENW,CX,HY,OZ,AST
      COMMON/JANAF/ A1(36),A2(36)
      COMMON/CHARU/PHIFR,PHIEGR
      COMMON/CHARB/PHI
      COMMON/CHARTH/RESFRK,RICH,LEAN
      COMMON /OXDANT/XI
      COMMON/THERMO/RGAS,RGSI,RO2,PSCALE,PSCOR
      DATA TABLE /-1.,1.,1.,-1.,0.,0.,0./
      DATA ERMAX,MAXITS/5.E-04,50/
C
C     MOLECULAR WEIGHT OF SPECIES
C
      WM(1)=44.
      WM(2)=18.
      WM(3)=28.
      WM(4)=2.
      WM(5)=32.
      WM(6)=28.
      WM(7)=44.
C
      M = MASS/N
      FO=44./(44.+5.*(32.+3.76*28)/PHI)
C
      X1=M*F1/WM(7)/M
      Y1=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))
     1    -5.*(FO-F1)*M*WM(5)/WM(7))/WM(5)/M
      V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M
      Z1=3.*(FO-F1)*M*WM(1)/WM(7)/WM(7)/M
      W1=4.*(FO-F1)*M*WM(2)/WM(7)/WM(2)/M
      X2=M*F2/WM(7)/M
      Y2=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))
     1    -5.*(FO-F2)*M*WM(5)/WM(7))/WM(5)/M
      V2=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M
```

```
      Z2=3.*(FO-F2)*M*WM(1)/WM(7)/WM(7)/M                                APP09450
      W2=4.*(FO-F2)*M*WM(2)/WM(7)/WM(2)/M                                APP09460
C                                                                        APP09470
      TOTMX1=X1+Y1+V1+W1+Z1                                              APP09480
      TOTMX2=X2+Y2+V2+W2+Z2                                              APP09490
C                                                                        APP09500
C---------- TOTAL INTERNAL ENERGY OF THE TWO MIXING PARTICLES ----------APP09510
C                                                                        APP09520
C     NUMBER OF MOLES PER UNIT MASS.                                     APP09530
      MX(1,1)=Z1                                                         APP09540
      MX(2,1)=W1                                                         APP09550
      MX(3,1)=0                                                          APP09560
      MX(4,1)=0                                                          APP09570
      MX(5,1)=Y1                                                         APP09580
      MX(6,1)=V1                                                         APP09590
      MX(7,1)=X1                                                         APP09600
      MX(1,2)=Z2                                                         APP09610
      MX(2,2)=W2                                                         APP09620
      MX(3,2)=0                                                          APP09630
      MX(4,2)=0                                                          APP09640
      MX(5,2)=Y2                                                         APP09650
      MX(6,2)=V2                                                         APP09660
      MX(7,2)=X2                                                         APP09670
C     TEMPERATURE AND VOLUME                                             APP09680
      TEMP(1)=T1                                                         APP09690
      TEMP(2)=T2                                                         APP09700
C                                                                        APP09710
C***  ENTRY FOR CALCULATION OF ENTHALPY                                  APP09720
C                                                                        APP09730
C                                                                        APP09740
C        CALCULATE H, CP, AND CT AS IN WRITEUP, USING FITTED             APP09750
C        COEFFICIENTS FROM JANAF TABLES                                  APP09760
C                                                                        APP09770
      INTER=0.                                                           APP09780
C.....TU IS IN CAL/MOLE OF SPECIES                                       APP09790
C.....TCVS,TCVF IN CAL/MOLE/K                                            APP09800
      DO 10 K=1,2                                                        APP09810
        IR = 1                                                           APP09820
        T=TEMP(K)                                                        APP09830
        IF( T .LT.500.) IR = 2                                           APP09840
        ST=T/1000.                                                       APP09850
      DO 40 J = 1,6                                                      APP09860
        TU = ((((  A(4,J,IR)/4.*ST + A(3,J,IR)/3. )*ST                  APP09870
     1     +   A(2,J,IR)/2.)*ST + A(1,J,IR)  )*ST                       APP09880
     1     - A(5,J,IR)/ST  +  A(6,J,IR))*1000. -1.98726*T                APP09890
        INTER=INTER+TU*MX(J,K)*M                                         APP09900
   40 CONTINUE                                                           APP09910
C     THIS PART IS FOR FUEL PROPANE                                      APP09920
        FM=44.09                                                         APP09930
        RFV=RGAS/FM                                                      APP09940
        TU= RGAS*(((((0.233361E-10/5.*T - 0.545131E-7/4.)*T              APP09950
     1              +0.351709E-4/3.)*T                                   APP09960
     1             +0.157505E-1/2.)*T                                    APP09970
     1            +1.31841)*T                                           APP09980
     1           -14091.3) + 201.1*FM                                    APP09990
        INTER=INTER+TU*MX(7,K)*M                                         APP10000
   10 CONTINUE                                                           APP10010
      U=INTER                                                            APP10020
C                                                                        APP10030
C---- NEW COMPOSITION AFTER MIXING ---------------------------------------APP10040
C                                                                        APP10050
      F3=(F1+F2)/2.                                                      APP10060
      VOL3=(VOL1+VOL2)/2.                                                APP10070
      XO=M*F3/WM(7)/M                                                    APP10080
      YO=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                                APP10090
     1    -5.*(FO-F3)*M*WM(5)/WM(7))/WM(5)/M                             APP10100
      VO=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                    APP10110
      ZO=3.*(FO-F3)*M*WM(1)/WM(7)/WM(7)/M                                APP10120
      WO=4.*(FO-F3)*M*WM(2)/WM(7)/WM(2)/M                                APP10130
C                                                                        APP10140
C---------- NEW VALUE OF TEMPERATURE AFTER MIXING ----------------------APP10150
C                                                                        APP10160
      MX(1,3)=ZO                                                         APP10170
      MX(2,3)=WO                                                         APP10180
      MX(3,3)=0                                                          APP10190
```

```
      MX(4,3)=0                                                                  APP10200
      MX(5,3)=YO                                                                 APP10210
      MX(6,3)=VO                                                                 APP10220
      MX(7,3)=XO                                                                 APP10230
      TEMP(3)=(TOTMX1*T1+TOTMX2*T2)/(TOTMX1+TOTMX2)                              APP10240
C                                                                                APP10250
C                                                                                APP10260
      DO 20 I=1,MAXITS                                                           APP10270
      INTER=0.                                                                   APP10280
      TCV=0.                                                                     APP10290
        T=TEMP(3)                                                                APP10300
        ST=T /1000.                                                              APP10310
        IR = 1                                                                   APP10320
        IF(T.LT.500.) IR = 2                                                     APP10330
      DO 50 J = 1,6                                                              APP10340
        TU = (((( A(4,J,IR)/4.*ST + A(3,J,IR)/3. )*ST                           APP10350
     1     +   A(2,J,IR)/2.)*ST + A(1,J,IR)   )*ST                              APP10360
     1     - A(5,J,IR)/ST  +  A(6,J,IR))*1000. -1.98726*T                      APP10370
        INTER=INTER+TU*MX(J,3)*M*2.                                              APP10380
        TCVS=(( A(4,J,IR)*ST+A(3,J,IR) )*ST + A(2,J,IR))*ST                      APP10390
     1      + A(1,J,IR)+A(5,J,IR)/ST**2 -1.98726                                APP10400
        TCV=TCV+TCVS*MX(J,3)*M*2.                                                APP10410
   50 CONTINUE                                                                   APP10420
C     THIS PART IS FOR FUEL PROPANE                                              APP10430
        FM=44.09                                                                 APP10440
        RFV=RGAS/FM                                                              APP10450
        TU= RGAS*(((((0.233361E-10/5.*T - 0.545131E-7/4.)*T                      APP10460
     1              +0.351709E-4/3.)*T                                           APP10470
     1             +0.157505E-1/2.)*T                                            APP10480
     1            +1.31841)*T                                                   APP10490
     1           -14091.3) + 201.1*FM                                           APP10500
        INTER=INTER+TU*MX(7,3)*M*2.                                              APP10510
        TCVF=RFV*((((0.233361E-10*T -0.545131E-7)*T                              APP10520
     1       +0.351709E-4)*T +0.157505E-1)*T +1.31841)                           APP10530
        TCV=TCV+FM*TCVF*MX(7,3)*M*2.                                             APP10540
      TO=TEMP(3)                                                                 APP10550
      TEMP(3)=TEMP(3)+(U-INTER)/TCV                                              APP10560
      IF(ABS(U-INTER)/U.LE.ERMAX) GO TO 30                                       APP10570
      IF(I.GE.MAXITS) PRINT*,' (U-INTER)/U =',(U-INTER)/U                        APP10580
      IF(I.GE.MAXITS)                                                            APP10590
     1  PRINT*,' ... NUMBER OF ITERATION EXCEEDS LIMIT IN "MIXFRO" !'            APP10600
      IF(I.GE.MAXITS) STOP                                                       APP10610
   20 CONTINUE                                                                   APP10620
   30 TO=TEMP(3)                                                                 APP10630
      RETURN                                                                     APP10640
      END                                                                        APP10650
```

APPENDIX E

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE RANMIX(DELT,W,NM,FNM1,DSEED)
C
      COMMON/MIX/MASS,F3,VOL3,TO3
      COMMON/PARNUM/N,NT,N1,N2,N3
      COMMON/BURN/FFR(9999),IBURN(9999)
      COMMON/TEMVOL/TEMP(9999),VOL(9999)
      COMMON/IDNUM/IDN(9999)
      REAL NM,CHOSEN(9999)
      INTEGER IR(2),K,NR
      DOUBLE PRECISION DSEED
C
C    NM = NUMBER OF PAIRS TO BE MIXED AT A FREQUENCY OF 'W'.
C
      DO 100 I = 1,NT
        CHOSEN(I)=0.
 100  CONTINUE
C
      XNM = DELT*W*NT
      NM = INT(XNM)
      FNM1=FNM1+XNM-NM
      IF(FNM1.GE.1.) NM=NM+1
      IF(FNM1.GE.1.) FNM1=FNM1-1.
C...  PRINT*,' NUMBER OF PAIRS TO BE MIXED =',NM
C
C  RANDOM GENERATOR "GGUD" GENERATES NR INTEGERS FROM 1 TO K
C   ( INITIAL SEED DSEED RANGES FROM 1.0D0 TO 2147483647.0D0 )
C
      K = NT
      NR = 2
C
      DO 130 I = 1,NM
 22     CALL GGUD(DSEED,K,NR,IR)
        I1=IR(1)
        I2=IR(2)
        IF(CHOSEN(I1).EQ.1..OR.CHOSEN(I2).EQ.1.)GO TO 22
         CHOSEN(I1)=1.
         CHOSEN(I2)=1.
       IF(IBURN(I1).NE.IBURN(I2).OR.
     1    (IBURN(I1).EQ.1.AND.IBURN(I2).EQ.1)) THEN
C...   PRINT*,I,' MIXING :',I1,I2
        CALL MIXFRO(FFR(I1),FFR(I2),VOL(I1),VOL(I2),TEMP(I1),TEMP(I2))
        FFR(I1)=F3
        FFR(I2)=F3
        VOL(I1)=VOL3
        VOL(I2)=VOL3
        TEMP(I1)=TO3
        TEMP(I2)=TO3
        DO 8 J = 1,NT
         IF(IDN(J).EQ.I1.OR.IDN(J).EQ.I2) IDN(J)=0
 8      CONTINUE
        IDN(I1)=0
        IDN(I2)=I1
       ENDIF
 130  CONTINUE
      CALL COUNT(NT)
C
      RETURN
      END
```

APPENDIX F

```
CKINETCCCCCCCCCCCCCCCCC10/04/87CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C   SUBROUTINE KINET
C
C   PURPOSE
C   TO CALCULATE THE EVOLUTION OF SPECIES CONCENTRATION AND TEMPERATURE
C   IN A TIME STEP DT. THE EVOLUTION OF SPECIES IS CALCULATED USING
C   A SINGLE STEP REACTION MECHANISM DESCRIBED IN WESTBROOK AND DRYER.
C   THE 1ST LAW IS USED IN DIFFERENTIAL FORM.
C
C   GIVEN:
C
C         X (SECOND) TIME AT WHICH INITIAL VALUES ARE GIVEN
C         XEND (SECOND) TIME AT WHICH VALUES ARE DESIRED
C         P (ATM) PRESSURE AT TIME XEND
C
C   GIVEN INITIAL VALUES AT TIME X FOR
C
C         Y(1)  (K) TEMPERATURE
C         Y(2)  (MOLES/G) CONCENTRATION OF PROPANE FUEL
C
C   RETURN VALUES AT XEND FOR
C
C         Y(1)  (K) TEMPERATURE
C         Y(2)  (MOLES/G) CONCENTRATION OF PROPANE FUEL
C
C  SUBROUTINES AND FUNCTION PROGRAM NEEDED
C    -SUBROUTINE FCN
C    -FUNCTION F2 CALCULATE THE DERIVATIVE OF TEMPERATURE WITH
C     RESPECT TO TIME
C    -FUNCTION F1 CALCULATE THE RATE OF DEPLETION OF PROPANE FUEL
C    -BLOCK DATA CONTAINS COEFFICIENTS USED TO CALCULATE INTERNAL
C     ENERGY AND SPECIFIC HEAT (SEE SAE PAPER BY HIRES ET AL )
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE KINET(X,XEND,DPDT,Y,YPRIM,HLAST)
C
      COMMON/CHARU/PHIFR,PHIEGR
      COMMON/AFRN/V,TOTMX,P,M
      COMMON/TEMVOL/TEMP(9999),VOL(9999)
      COMMON/BURN/FFR(9999),IBURN(9999)
      COMMON/IDNUM/IDN(9999)
      COMMON/PARNUM/N,NT,N1,N2,N3
      COMMON/EQNUM/NQ
      COMMON/CHARB/PHI
      COMMON/CHARTH/RESFRK,RICH,LEAN
      COMMON/UGASP/UX(7),MBAR,RU,GAMU,CPU,HU,TU,RHOU
      COMMON /BGASP/CCB(7),MWT,RB,GAMB,CPB,HB
      COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR
      COMMON/MOLES/TOTMXU,TOTMXB
      COMMON/INPRS/PRESS
      COMMON/MOLWT/WM(7)
      COMMON/CRANGL/SA,CRG,CRGSTP
      COMMON/STEP/TIMSTP
      COMMON/CONST/PEC,B
      REAL Y(NQ),YPRIM(NQ),X,XEND
      REAL MBAR,INEREA,INER,INTER,M
C
C INITIAL VALUES
C
      ITS=0
    8 X=0.
      IN=0
      DO 10 J=1,NT
      IF(IBURN(J).EQ.1.AND.IDN(J).EQ.0) THEN
       IN=IN+1
       K=(IN-1)*2
       Y(1+K)= TEMP(J)
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      Y(2+K)= FFR(J)/44.                                                APP12080
      ENDIF                                                             APP12090
   10 CONTINUE                                                          APP12100
      NQ=2*IN                                                           APP12110
C...  PRINT*,' NQ =',NQ                                                 APP12120
C     CALL PRTY(Y,NQ)                                                   APP12130
C                                                                       APP12140
C   EPS1 = ERROR TOLERANCE FOR FIRST STEP SIZE IN "CODE".               APP12150
C   EPS2 = ERROR TOLERANCE FOR CONVERGENCE OF EACH STEP IN "CODE".      APP12160
C   EPS3 = ERROR TOLERANCE FOR CONVERGENCE OF PRESSURE IN "KINET".      APP12170
C                                                                       APP12180
      EPS1=1.E-02                                                       APP12190
      EPS2=1.E-02                                                       APP12200
      EPS3=1.E-02                                                       APP12210
C                                                                       APP12220
      CALL CODE(X,XEND,Y,YPRIM,DPDT,NQ,EPS1,EPS2,HLAST)                 APP12230
C                                                                       APP12240
      ITS=ITS+1                                                         APP12250
      FO=44./(44.+5.*(32.+3.76*28)/PHI)                                 APP12260
      P=PRESS*PSCALE+X*DPDT                                             APP12270
      PM=(PRESS+P/PSCALE)/2.                                            APP12280
      IN=0                                                              APP12290
      TOVOL=0.                                                          APP12300
      UNB=0.                                                            APP12310
      DO 4 I = 1,NT                                                     APP12320
       IF(IBURN(I).EQ.1.AND.IDN(I).EQ.0) THEN                           APP12330
        IN=IN+1                                                         APP12340
        FF1=Y(2+(IN-1)*2)*44.                                           APP12350
        T1=Y(1+(IN-1)*2)                                                APP12360
        X1=FF1/44.                                                      APP12370
        Y1=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                             APP12380
     1        -5.*(FO-FF1)*M*WM(5)/WM(7))/WM(5)/M                       APP12390
        V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                 APP12400
        Z1=3.*(FO-FF1)*M*WM(1)/WM(7)/WM(7)/M                            APP12410
        W1=4.*(FO-FF1)*M*WM(2)/WM(7)/WM(2)/M                            APP12420
        TOTMX=X1+Y1+V1+W1+Z1                                            APP12430
        TOVOL=TOVOL+M*TOTMX*1.987*T1/P                                  APP12440
        DO 32 J = 1,NT                                                  APP12450
         IF(IDN(J).EQ.I) TOVOL=TOVOL+M*TOTMX*1.987*T1/P                 APP12460
   32   CONTINUE                                                        APP12470
       ENDIF                                                            APP12480
       IF(IBURN(I).EQ.2) THEN                                           APP12490
        IF(UNB.EQ.0.) THEN                                              APP12500
        UNB=1.                                                          APP12510
        ENDIF                                                           APP12520
        TOVOL=TOVOL+VU                                                  APP12530
       ENDIF                                                            APP12540
       IF(IBURN(I).EQ.3) THEN                                           APP12550
        CALL CLDPRD(PM,TEMP(I),ENTHLP,CSUBP,RHOB,IER)                   APP12560
        T1=TEMP(I)*(P/PSCALE/PRESS)**((GAMB-1)/GAMB)                    APP12570
        TOVOL=TOVOL+M*TOTMXB*1.987*T1/P                                 APP12580
       ENDIF                                                            APP12590
    4  CONTINUE                                                         APP12600
       CALL UPROP(PM,TEMP(NT+1),ENTHLP,CSUBP,RHO)                       APP12610
       TU=TEMP(NT+1)*(P/PSCALE/PRESS)**((GAMU-1)/GAMU)                  APP12620
       VU=M*TOTMXU*1.987*TU/P                                           APP12630
       TOVOL=TOVOL+(N-NT)*VU                                            APP12640
C      PRINT*,' VTO =',VTO(SA+1),' TOVOL =',TOVOL                       APP12650
C                                                                       APP12660
       IF(ABS(TOVOL-VTO(SA+1))/VTO(SA+1).LE.EPS3) GO TO 9               APP12670
       IF(ITS.GE.3)                                                     APP12680
     1 PRINT*,' 4TH ITERATION ON PRESSURE RISE ...'                     APP12690
       IF(ITS.GE.4)                                                     APP12700
     1 PRINT*,' PRESSURE DOES NOT CONVERGE AFTER 4 ITERATIONS !'        APP12710
       IF(ITS.GE.4) STOP                                                APP12720
       PNEXT=P*(TOVOL/VTO(SA+1))                                        APP12730
       DPDT=(PNEXT-PRESS*PSCALE)/TIMSTP                                 APP12740
       IF(ITS.LT.4) GO TO 8                                             APP12750
C                                                                       APP12760
C  TO UPDATE FFR(I), TEMP(I) AND VOL(I) FOR ALL PARTICLES               APP12770
C                                                                       APP12780
    9  IN=0.                                                            APP12790
       UNB=0.                                                           APP12800
       DO 2 I=1,NT                                                      APP12810
         IF(IBURN(I).EQ.1.AND.IDN(I).EQ.0) THEN                         APP12820
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```
          IN=IN+1                                                          APP12830
          FFR(I)=Y(2+(IN-1)*2)*44.                                         APP12840
          TEMP(I)=Y(1+(IN-1)*2)                                            APP12850
          IF(TEMP(I).LT.TEMIN) TEMIN=TEMP(I)                               APP12860
          IF(FFR(I).GT.FUMAX) FUMAX=FFR(I)                                 APP12870
           FF1=FFR(I)                                                      APP12880
           X1=FF1/44.                                                      APP12890
           Y1=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                             APP12900
     1        -5.*(FO-FF1)*M*WM(5)/WM(7))/WM(5)/M                          APP12910
           V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                 APP12920
           Z1=3.*(FO-FF1)*M*WM(1)/WM(7)/WM(7)/M                            APP12930
           W1=4.*(FO-FF1)*M*WM(2)/WM(7)/WM(2)/M                            APP12940
           TOTMX=X1+Y1+V1+W1+Z1                                            APP12950
          VOL(I)=M*TOTMX*1.987*TEMP(I)/P                                   APP12960
          DO 31 J = 1,NT                                                   APP12970
           IF(IDN(J).EQ.I) THEN                                            APP12980
            TEMP(J)=TEMP(I)                                                APP12990
            FFR(J)=FFR(I)                                                  APP13000
            VOL(J)=VOL(I)                                                  APP13010
           ENDIF                                                           APP13020
  31      CONTINUE                                                         APP13030
         ENDIF                                                             APP13040
         IF(IBURN(I).EQ.2) THEN                                            APP13050
          IF(UNB.EQ.0.) THEN                                               APP13060
          CALL UPROP(PM,TEMP(I),ENTHLP,CSUBP,RHO)                          APP13070
          UNB=1.                                                           APP13080
          ENDIF                                                            APP13090
          TEMP(I)=TEMP(I)*(P/PSCALE/PRESS)**((GAMU-1)/GAMU)                APP13100
          VOL(I)=M*TOTMXU*1.987*TEMP(I)/P                                  APP13110
         ENDIF                                                             APP13120
         IF(IBURN(I).EQ.3) THEN                                            APP13130
          CALL CLDPRD(PM,TEMP(I),ENTHLP,CSUBP,RHOB,IER)                    APP13140
          TEMP(I)=TEMP(I)*(P/PSCALE/PRESS)**((GAMB-1)/GAMB)                APP13150
          VOL(I)=M*TOTMXB*1.987*TEMP(I)/P                                  APP13160
         ENDIF                                                             APP13170
  2    CONTINUE                                                           APP13180
       DO 3 I = NT+1,MIN(N,9999)                                          APP13190
         TEMP(I)=TU                                                       APP13200
         VOL(I)=VU                                                        APP13210
  3    CONTINUE                                                           APP13220
       PRESS=P/PSCALE                                                     APP13230
C                                                                         APP13240
       RETURN                                                             APP13250
       END                                                                APP13260
C                                                                         APP13270
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCAPP13280
C                                                                         APP13290
C    SUBROUTINE  FCN SPECIFIES THE DERIVATIVES WITH RESPECT TO            APP13300
C    TIME                                                                 APP13310
C                                                                         APP13320
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCAPP13330
       SUBROUTINE FCN(NQ,X,Y,YPRIM,DPDT)                                  APP13340
       INTEGER NQ                                                         APP13350
       COMMON/TEMVOL/TEMP(9999),VOL(9999)                                 APP13360
       COMMON/BURN/FFR(9999),IBURN(9999)                                  APP13370
       COMMON/IDNUM/IDN(9999)                                             APP13380
       COMMON/PARNUM/N,NT,N1,N2,N3                                        APP13390
       COMMON/CRANGL/SA,CRG,CRGSTP                                        APP13400
       COMMON/STEP/TIMSTP                                                 APP13410
       COMMON/CONST/PEC,B                                                 APP13420
       REAL Y(NQ),YPRIM(NQ),X                                             APP13430
C                                                                         APP13440
       CRG=SA+X/TIMSTP*CRGSTP                                             APP13450
C                                                                         APP13460
        IN=0                                                              APP13470
       DO 10 J=1,NT                                                       APP13480
       IF(IBURN(J).EQ.1.AND.IDN(J).EQ.0)THEN                              APP13490
        IN=IN+1                                                           APP13500
       FU2=F2(Y,IN,DPDT)                                                  APP13510
       FU1=F1(Y,IN)                                                       APP13520
        K=(IN-1)*2                                                        APP13530
       YPRIM(1+K)=+FU2                                                    APP13540
       YPRIM(2+K)=+FU1                                                    APP13550
       ENDIF                                                              APP13560
  10   CONTINUE                                                           APP13570
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      RETURN                                                                    APP13590
       END                                                                      APP13600
CF1CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC APP13610
C                                                                              APP13620
C      FUNCTION F1(Y,J)                                                        APP13630
C                                                                              APP13640
C      CALCULATE THE RATE OF DEPLETION OF FUEL PROPANE USING A SINGLE          APP13650
C      REACTION MECHANISM FROM WESTBROOK AND DRYER.                            APP13660
C                                                                              APP13670
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCAPP13680
C                                                                              APP13690
      FUNCTION F1(Y,J)                                                         APP13700
      COMMON/CNTF/IF1,IF2,IF3                                                  APP13710
      COMMON/AFRN/V,TOTMX,P,M                                                  APP13720
      COMMON/CHARB/PHI                                                         APP13730
      COMMON/TEMVOL/TEMP(9999),VOL(9999)                                       APP13740
      COMMON/BURN/FFR(9999),IBURN(9999)                                        APP13750
      COMMON/IDNUM/IDN(9999)                                                   APP13760
      COMMON/MOLWT/WM(7)                                                       APP13770
      COMMON/PARNUM/N,NT,N1,N2,N3                                              APP13780
      COMMON/EQNUM/NQ                                                          APP13790
      COMMON/CRANGL/SA,CRG,CRGSTP                                              APP13800
      COMMON/INPRS/PRESS                                                       APP13810
      COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR                                    APP13820
      COMMON/CONST/PEC,B                                                       APP13830
      REAL Y(NQ),M                                                             APP13840
       IF1=IF1+1                                                               APP13850
C                                                                              APP13860
      PO=PRESS*PSCALE                                                          APP13870
      P=PO+TIMSTP*(CRG-SA)/CRGSTP*DPDT                                         APP13880
      FO=44./(44.+5.*(32.+3.76*28)/PHI)                                        APP13890
       IN=0                                                                    APP13900
      DO 1 I=1,NT                                                              APP13910
      IF(IBURN(I).EQ.1.AND.IDN(I).EQ.0) THEN                                   APP13920
      IN=IN+1                                                                  APP13930
      IF(IN.EQ.J) THEN                                                         APP13940
         FF1=FFR(I)                                                            APP13950
         X01=M*FF1/WM(7)/M                                                     APP13960
         Y01=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                                  APP13970
     1        -5.*(FO-FF1)*M*WM(5)/WM(7))/WM(5)/M                              APP13980
      ENDIF                                                                    APP13990
      ENDIF                                                                    APP14000
    1 CONTINUE                                                                 APP14010
C                                                                              APP14020
       K=(J-1)*2                                                               APP14030
       IF(Y(2+K).LE.FO/44.*0.050) Y(2+K)=0.                                    APP14040
      FF1=Y(2+K)*WM(7)                                                         APP14050
      Y1=Y01+5.*(Y(2+K)-X01)                                                   APP14060
      V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                          APP14070
      Z1=3.*(FO-FF1)*M*WM(1)/WM(7)/WM(7)/M                                     APP14080
      W1=4.*(FO-FF1)*M*WM(2)/WM(7)/WM(2)/M                                     APP14090
       IF(Y1.LE.Y01*0.050) Y1=0.                                               APP14100
      TOTMXJ=Y(2+K)+Y1+V1+W1+Z1                                                APP14110
      V=TOTMXJ*1.987*Y(1+K)/P                                                  APP14120
C                                                                              APP14130
      IF(Y(2+K).LT.0..OR.Y1.LT.0..OR.V.LE.0.)                                  APP14140
     1  PRINT*,' Y(2+K) =',Y(2+K),' Y1 =',Y1,' V =',V,' ... IN "F1" !'         APP14150
      IF(Y(2+K).LT.0..OR.Y1.LT.0..OR.V.LE.0.) STOP                             APP14160
C                                                                              APP14170
      F1=-PEC*V*EXP(-B/Y(1+K)/1.987)*((Y(2+K)/V)**.1)*((Y1/V)**1.65)           APP14180
C                                                                              APP14190
       RETURN                                                                  APP14200
       END                                                                     APP14210
C                                                                              APP14220
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC APP14230
C                                                                              APP14240
C      FUNCTION F2(Y,J) = DTDTI FOR EACH BURNING PARTICALS                     APP14250
C                                                                              APP14260
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC APP14270
      FUNCTION F2(Y,J,DPDT)                                                    APP14280
      COMMON/CNTF/IF1,IF2,IF3                                                  APP14290
      COMMON/AFRN/V,TOTMX,P,M                                                  APP14300
      COMMON/UGASP/CCU(7),MBARU,RU,GAMU,CPU,HU,TU,RHOU                         APP14310
      COMMON/BGASP/CCB(7),MBARB,RB,GAMB,CPB,HB                                 APP14320
      COMMON/THERMO/R,RGSI,RO2,PSCALE,PSCOR                                    APP14330
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      COMMON/PARNUM/N,NT,N1,N2,N3                                          APP14340
      COMMON/EQNUM/NQ                                                      APP14350
      COMMON/INPRS/PRESS                                                   APP14360
      COMMON/STEP/TIMSTP                                                   APP14370
      COMMON/CRANGL/SA,CRG,CRGSTP                                          APP14380
      REAL Y(NQ),M,INTER                                                   APP14390
      IF2=IF2+1                                                            APP14400
C                                                                          APP14410
      FU1=F1(Y,J)                                                          APP14420
      CALL KINTER(Y,J,WU,WCM,INTER)                                        APP14430
C                                                                          APP14440
C.....P IN DTDTI IS IN CAL/CC                                              APP14450
      PO=PRESS*PSCALE                                                      APP14460
      P=PO+TIMSTP*(CRG-SA)/CRGSTP*DPDT                                     APP14470
       K=(J-1)*2                                                           APP14480
      T = Y(1+K)                                                           APP14490
C                                                                          APP14500
      DTDTI=(FU1*(1.987*T-WU)+TOTMX*1.987*T/P*DPDT)/                       APP14510
     1       (WCM+TOTMX*1.987)                                             APP14520
C                                                                          APP14530
      F2=DTDTI                                                             APP14540
C                                                                          APP14550
      RETURN                                                               APP14560
      END                                                                  APP14570
C                                                                          APP14580
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC APP14590
C                                                                          APP14600
C     SUBROUTINE KINTER                                                    APP14610
C                                                                          APP14620
C     PURPOSE                                                              APP14630
C        TO CALCULATE THE DERATIVE OF TEMPERATURE WITH RESPECT TO          APP14640
C        TIME AND THE INTERNAL ENERGY OF MIXTURE.                          APP14650
C                                                                          APP14660
C     USAGE                                                                APP14670
C        CALL INTER(Y)                                                     APP14680
C                                                                          APP14690
C     DESCRIPTION OF PARAMETERS                                            APP14700
C                                                                          APP14710
C   GIVEN:                                                                 APP14720
C                                                                          APP14730
C         P (ATM) PRESSURE                                                 APP14740
C                                                                          APP14750
C  GIVEN                                                                   APP14760
C                                                                          APP14770
C         Y(1)  (K) TEMPERATURE                                            APP14780
C         Y(2)  (MOLES/G) CONCENTRATION OF PROPANE FUEL                    APP14790
C         Y(3)  (MOLES/G) CONCENTRATION OF OXYGEN                          APP14800
C         Y(4)  (MOLES/G) CONCENTRATION OF NITROGEN                        APP14810
C         Y(5)  (MOLES/G) CONCENTRATION OF CARBON DIOXIDE                  APP14820
C         Y(6)  (MOLES/G) CONCENTRATION OF WATER VAPOR                     APP14830
C                                                                          APP14840
C      GIVEN IN COMMON AREA /FUEL/                                         APP14850
C        AF(I) - 6 DIMENSIONAL VECTOR OF ENTHALPY COEFFICIENTS SUCH        APP14860
C                THAT THE ENTHALPY OF FUEL VAPOR AS A FUNCTION             APP14870
C                OF TEMPERATURE ( T DEG K ) IS GIVEN BY                    APP14880
C                  H(T) = AF(1)*ST + (AF(2)*ST**2)/2 + (AF(3)*ST**3)/3     APP14890
C                       + (AF(4)*ST**4)/4 - AF(5)/ST + AF(6)               APP14900
C                  WHERE ST = T/1000 AND H(T) = <KCAL/MOLE>                APP14910
C                FOR MOST APPLICATIONS THE ENTHALPY FUNCTION H(            APP14920
C                BE VALID OVER AT LEAST THE FOLLOWING TEMPERATURE RAN      APP14930
C                                   300 < T < 1000                         APP14940
C                ENTHALPY DATUM STATE IS AT T = 0 ABSOLUTE WITH O2,N2      APP14950
C                AND H2 GASEOUS AND C SOLID GRAPHITE.                      APP14960
C                HYDROCARBON-OXIDANT COMBUSTION                            APP14970
C      RETURNS                                                             APP14980
C        DTDTI - DERIVATIVE OF TEMPERATURE WITH RESPECT TO TIME            APP14990
C                (DEG K /SECOND )                                          APP15000
C        INTER - INTERNAL ENERGY OF MIXTURE (CAL/MOLE OF MIXTURE)          APP15010
C                                                                          APP15020
C     REMARKS                                                              APP15030
C        1)  ENTHALPY DATUM STATE IS AT T = 0 ABSOLUTE WITH                APP15040
C            O2,N2,H2 GASEOUS AND C SOLID GRAPHITE                         APP15050
C        2) THE VARIABLES HAVE DIFFERENT INDICES IN THERMO                 APP15060
C           SUBROUTINES AND DGEAR .THEY ARE AS FOLLOWS:                    APP15070
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C          THERMO. PROP.        DGEAR          SPECIES                  APP15080
C                                                                        APP15090
C               1                  5              CO2                    APP15100
C               2                  6              H2O                    APP15110
C               5                  3              O2                     APP15120
C               6                  4              N2                     APP15130
C               7                  2              C3H8                   APP15140
C                                                                        APP15150
C     SUBROUTINES AND FUNCTION SUBPROGRAMS NEEDED                        APP15160
C          F1                                                            APP15170
C                                                                        APP15180
C                                                                        APP15190
C*************************************************************************APP15200
      SUBROUTINE KINTER(Y,J,WU,WCM,INTER)                                APP15210
      LOGICAL RICH,LEAN                                                  APP15220
      DIMENSION TABLE(7),A(6,6,2),LEC(10),MX(10),X(10),WM(10)            APP15230
      EQUIVALENCE (A1(1),A(1,1,1)),(A2(1),A(1,1,2))                      APP15240
      REAL*4  MBAR,MX,INTER                                              APP15250
      COMMON/CNT/IUP,ICLD,IKIN                                           APP15260
      COMMON /FUEL/ ENN,CX,HY,OZ,AST                                     APP15270
      COMMON/JANAF/ A1(36),A2(36)                                        APP15280
      COMMON/CHARU/PHIFR,PHIEGR                                          APP15290
      COMMON/CHARB/PHI                                                   APP15300
      COMMON/AFRN/V,TOTMX,P,M                                            APP15310
      COMMON/BURN/FFR(9999),IBURN(9999)                                  APP15320
      COMMON/PARNUM/N,NT,N1,N2,N3                                        APP15330
      COMMON/EQNUM/NQ                                                    APP15340
      COMMON/CHARTH/RESFRK,RICH,LEAN                                     APP15350
      COMMON /OXDANT/XI                                                  APP15360
      COMMON/THERMO/RGAS,RGSI,RO2,PSCALE,PSCOR                           APP15370
      REAL Y(NQ),M                                                       APP15380
      DATA TABLE /-1.,1.,1.,-1.,0.,0.,0./                                APP15390
      IKIN=IKIN+1                                                        APP15400
C                                                                        APP15410
C     COEFFICIENTS IN 1ST LAW EXPRESSION                                 APP15420
      LEC(1)=-3                                                          APP15430
      LEC(2)=-4                                                          APP15440
      LEC(3)=0                                                           APP15450
      LEC(4)=0                                                           APP15460
      LEC(5)=5                                                           APP15470
      LEC(6)=0                                                           APP15480
      LEC(7)=1                                                           APP15490
C     MOLECULAR WEIGHT                                                   APP15500
      WM(1)=44                                                           APP15510
      WM(2)=18                                                           APP15520
      WM(3)=0                                                            APP15530
      WM(4)=0                                                            APP15540
      WM(5)=32                                                           APP15550
      WM(6)=28                                                           APP15560
      WM(7)=44                                                           APP15570
C     NUMBER OF MOLES PER UNIT VOLUME                                    APP15580
      FO=44./(44.+5.*(32.+3.76*28)/PHI)                                  APP15590
       K=(J-1)*2                                                         APP15600
      FF1=Y(2+K)*44.                                                     APP15610
      Y1=(M*(1.-FO)/(1.+3.76*WM(6)/WM(5))                                APP15620
     1    -5.*(FO-FF1)*M*WM(5)/WM(7))/WM(5)/M                            APP15630
      V1=3.76*M*(1.-FO)/WM(5)/(1.+3.76*WM(6)/WM(5))/M                    APP15640
      Z1=3.*(FO-FF1)*M*WM(1)/WM(7)/WM(7)/M                               APP15650
      W1=4.*(FO-FF1)*M*WM(2)/WM(7)/WM(2)/M                               APP15660
      MX(1)=Z1                                                           APP15670
      MX(2)=W1                                                           APP15680
      MX(3)=0                                                            APP15690
      MX(4)=0                                                            APP15700
      MX(5)=Y1                                                           APP15710
      MX(6)=V1                                                           APP15720
      MX(7)=Y(2+K)                                                       APP15730
      TOTMX=MX(1)+MX(2)+MX(3)+MX(4)+MX(5)+MX(6)+MX(7)                    APP15740
C     TEMPERATURE                                                        APP15750
      T=Y(1+K)                                                           APP15760
C                                                                        APP15770
C***  ENTRY FOR CALCULATION OF ENTHALPY                                  APP15780
C                                                                        APP15790
      IR = 1                                                             APP15800
      IF (T .LT. 500.) IR = 2                                            APP15810
```

```
C        CALCULATE H, CP, AND CT AS IN WRITEUP, USING FITTED
C        COEFFICIENTS FROM JANAF TABLES
C
      WU=0.
      WCM=0.
      INTER=0.
      ST = T/1000.
C.....TU IS IN CAL/MOLE OF SPECIES
C.....TCV IN CAL/MOLE/K
      DO 40 K = 1,6
         TU = (((( A(4,K,IR)/4.*ST + A(3,K,IR)/3. )*ST
     1     +   A(2,K,IR)/2.)*ST + A(1,K,IR)  )*ST
     1     - A(5,K,IR)/ST  +  A(6,K,IR))*1000. -1.98726*T
         INTER=INTER+TU*MX(K)/TOTMX
         TCV = (( A(4,K,IR)*ST + A(3,K,IR) )*ST
     1     + A(2,K,IR))*ST + A(1,K,IR)+A(5,K,IR)/ST**2 -1.98726
         WU=WU + TU*LEC(K)
         WCM=WCM+MX(K)*TCV
   40 CONTINUE
C     THIS PART IS FOR FUEL PROPANE
         FM=44.09
         RFV=RGAS/FM
         TU= RGAS*(((((0.233361E-10/5.*T - 0.545131E-7/4.)*T
     1              +0.351709E-4/3.)*T
     1             +0.157505E-1/2.)*T
     1            +1.31841)*T
     1           -14091.3) + 201.1*FM
         INTER=INTER+TU*MX(7)/TOTMX
         TCV=RFV*((((0.233361E-10*T - 0.545131E-7)*T
     1              +0.351709E-4)*T
     1             +0.157505E-1)*T
     1            +1.31841)
         TCV=FM*TCV
         WU=WU + TU*LEC(7)
         WCM=WCM+MX(7)*TCV
C
      RETURN
      END
```

APP15830
APP15840
APP15850
APP15860
APP15870
APP15880
APP15890
APP15900
APP15910
APP15920
APP15930
APP15940
APP15950
APP15960
APP15970
APP15980
APP15990
APP16000
APP16010
APP16020
APP16030
APP16040
APP16050
APP16060
APP16070
APP16080
APP16090
APP16100
APP16110
APP16120
APP16130
APP16140
APP16150
APP16160
APP16170
APP16180
APP16190
APP16200

APPENDIX G

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C     VTO(CRKINT) IS THE VOLUME OF THE CHAMBER AS A FUNCTION OF
C                 THE CRANK ANGLE.
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      FUNCTION VTO(CRKINT)
      COMMON/BBORE/BORE
C
        BORE=4.0
        STROKE=4.0
        CONLEN=7.5
        CR=8.0
        DATA RADIAN/57.29578/
        B1=0.39269908*BORE*BORE*STROKE
        B2=(CONLEN*2./STROKE)**2.-1.
        B3=1.0+2.*CONLEN/STROKE
        THBEG=CRKINT
        AREA=3.14*BORE*BORE/4
        VTDC=AREA*STROKE/(CR-1.)
        CAS=COS(THBEG/RADIAN)
        VTO=VTDC+B1*(B3-CAS-SQRT(CAS**2+B2))
        RETURN
        END
```

APP16220
APP16230
APP16240
APP16250
APP16260
APP16270
APP16280
APP16290
APP16300
APP16310
APP16320
APP16330
APP16340
APP16350
APP16360
APP16370
APP16380
APP16390
APP16400
APP16410
APP16420
APP16430
APP16440
APP16450
APP16460
APP16470
APP16480
APP16490
APP16500
APP16510

APPENDIX H

```
CCLDPRD************ VERSION 2.1 *** 1/10 76 ************************
C
C     SUBROUTINE CLDPRD
C
C     PURPOSE
C        TO CALCULATE THE SPECIFIC ENTHALPY OF THE PRODUCTS OF
C        COMBUSTION AT TEMPERATURES AND PRESSURES WHERE DISSOCIATI
C        OF THE PRODUCT GASES MAY BE IGNORED.  THE DENSITY OF THE
C        PRODUCT GAS IS ALSO CALCULATED, AS ARE THE PARTIAL
C        DERIVATIVES OF BOTH OF THESE QUANTITIES WITH RESPECT TO
C        PRESSURE AND TEMPERATURE.
C
C     USAGE
C        CALL CLDPRD(P,T,ENTHLP,CSUBP,CSUBT,RHO,DRHODT,DRHOD
C
C     DESCRIPTION OF PARAMETERS
C      GIVEN
C        P      - ABSOLUTE PRESSURE OF PRODUCTS (ATM)
C        T      - TEMPERATURE OF PRODUCTS (DEG K)
C      GIVEN IN COMMON AREA /CHARGE/
C        PHI    - EQUIVALENCE RATIO (FUEL/AIR RATIO DIVIDED BY THE
C                 CHEMICALLY CORRECT FUEL/AIR RATIO)
C      GIVEN IN COMMON AREA /PRODMR/
C        DEL    - MOLAR C H RATIO OF THE PRODUCTS
C        PSI    - MOLAR N O RATIO OF THE PRODUCTS
C      RETURNS
C        ENTHLP- SPECIFIC ENTHALPY OF THE GAS (KCAL/G)
C        CSUBP - PARTIAL DERIVATIVE OF ENTHLP WITH RESPECT T
C                AT CONSTANT P    (CAL/G-DEG K)
C        CSUBT - PARTIAL DERIVATIVE OF ENTHLP WITH RESPECT TO P
C                AT CONSTANT T    (CC/G)
C        RHO    - DENSITY OF THE MIXTURE (G/CC)
C        DRHODT- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO T AT
C                CONSTANT P (G/CC-DEG K)
C        DRHODP- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO P
C                CONSTANT T (G/CC-ATM)
C        IER    - FLAG, SET TO 1 FOR T<100 DEG K
C                               2 FOR T> 6000 DEG K
C                               0 OTHERWISE
C      RETURNS IN COMMON AREA FROZEN
C        CPFROZ- FROZEN SPECIFIC HEAT (CAL/G - DEG K)
C
C     REMARKS
C        1)  ENTHALPY DATUM STATE IS AT T  =  0 ABSOLUTE WITH
C            O2,N2,H2 GASEOUS AND C SOLID GRAPHITE
C
C     SUBROUTINES AND FUNCTION SUBPROGRAMS NEEDED    NONE
C
C     METHOD
C        DESCRIBED IN APPENDIX A OF HIRES ET AL, SAE PAPER #
C
C*********************************************************************
      SUBROUTINE CLDPRD(P,T,ENTHLP,CSUBP,RHOB,IER)
C
      LOGICAL RICH,LEAN
      DIMENSION TABLE(7),A(6,6,2)
      EQUIVALENCE (A1(1),A(1,1,1))
      EQUIVALENCE (A2(1),A(1,1,2))
      REAL*4  MBAR,K
      COMMON/CNT/IUP,ICLD,IKIN
      COMMON/CHARB/PHI
       COMMON/CHARU/PHIFR,PHIEGR
      COMMON/CHARTH/RESFRK,RICH,LEAN
      COMMON/THERMO/RGAS,RGSI,RO2,PSCALE,PSCOR
      COMMON /PRODMR/DEL,CHI,DUMM,DUMY,EPS0,EPS
      COMMON /FUEL/ ENW,CX,HY,OZ,AST
      COMMON /BGASP/X(7),MBAR,RB,GAMB ,CPB,HB
      COMMON/JANAF/ A1(36),A2(36)
      COMMON/OXDANT/PSI
      DATA TABLE /-1.,1.,1.,-1.,0.,0.,0./
```

APP16530 APP16540 APP16550 APP16560 APP16570 APP16580 APP16590 APP16600 APP16610 APP16620 APP16630 APP16640 APP16650 APP16660 APP16670 APP16680 APP16690 APP16700 APP16710 APP16720 APP16730 APP16740 APP16750 APP16760 APP16770 APP16780 APP16790 APP16800 APP16810 APP16820 APP16830 APP16840 APP16850 APP16860 APP16870 APP16880 APP16890 APP16900 APP16910 APP16920 APP16930 APP16940 APP16950 APP16960 APP16970 APP16980 APP16990 APP17000 APP17010 APP17020 APP17030 APP17040 APP17050 APP17060 APP17070 APP17080 APP17090 APP17100 APP17110 APP17120 APP17130 APP17140 APP17150 APP17160 APP17170 APP17180 APP17190 APP17200 APP17210 APP17220 APP17230 APP17240 APP17250 APP17260 APP17270

```
      ICLD=ICLD+1                                                       APP17280
C                                                                       APP17290
   1  I1 = 2                                                           APP17300
      RICH = PHIFR.GT.1.0                                               APP17310
      LEAN = .NOT.RICH                                                  APP17320
      DEL = CX/HY                                                       APP17330
      EPS=4.*DEL/(1.+4.*DEL)                                            APP17340
      MBAR =  (8.*EPS + 4.)*PHI + 32. + 28.*PSI                         APP17350
C                                                                       APP17360
C        GET THE COMPOSITION IN MOLES/MOLE OXYGEN                       APP17370
C                                                                       APP17380
      IF (RICH)  GO TO 13                                               APP17390
C                                                                       APP17400
C *** LEAN CASE  SHIFT JUMP TO 35 AFTER THIS                            APP17410
C                                                                       APP17420
      I1 = 3                                                            APP17430
      TMOLES = 1.+PSI+PHI*(1.-EPS)                                      APP17440
      X(1) = EPS*PHI/TMOLES                                             APP17450
      X(2) = 2.*(1.- EPS)*PHI/TMOLES                                    APP17460
      X(3) = 0.                                                         APP17470
      X(4) = 0.                                                         APP17480
      X(5) = (1.-PHI)/TMOLES                                            APP17490
      X(6) = PSI/TMOLES                                                 APP17500
      X(7) = 0.                                                         APP17510
      MBAR = MBAR/TMOLES                                                APP17520
      DCDT = 0.                                                         APP17530
      GO TO 35                                                          APP17540
C                                                                       APP17550
C *** RICH CASE INITIALIZATION                                          APP17560
C                                                                       APP17570
  13  TMOLES = PSI+ PHI*(2.-EPS)                                        APP17580
      X(5) = 0.                                                         APP17590
      X(6) = PSI/TMOLES                                                 APP17600
      X(7) = 0.                                                         APP17610
      MBAR = MBAR/TMOLES                                                APP17620
      BETA0 = 2.*(1.-EPS*PHI)                                           APP17630
      CB1 = 2.*(PHI-1.) + EPS*PHI                                       APP17640
      GA1 = 2.*EPS*PHI*(PHI-1.)                                         APP17650
C                                                                       APP17660
C *** RICH CASE ENTRY AFTER FIRST TIME                                  APP17670
C                                                                       APP17680
  20  Z = 1000./T                                                       APP17690
      K = EXP(2.743 + Z*(-1.761 + Z*(-1.611 + Z*.2803)))                APP17700
      DKDT = -K*Z*(-1.761 + Z*(-3.222 + Z*.9409))/T                     APP17710
      ALPHA = 1. - K                                                    APP17720
      BETA = BETA0 + CB1*K                                              APP17730
      GAMMA = GA1*K                                                     APP17740
      C = ( - BETA + SQRT(BETA*BETA + 4.*ALPHA*GAMMA))/(2.*ALPHA)       APP17750
      DCDT=-DKDT*(C*(CB1+C)-GA1)                                        APP17760
      DCDT = DCDT/(2.*ALPHA*C + BETA)/TMOLES                            APP17770
      X(1) =(EPS*PHI - C)/TMOLES                                        APP17780
      X(2) = (BETA0 + C)/TMOLES                                         APP17790
      X(3) = C/TMOLES                                                   APP17800
      X(4) = (2.*(PHI-1.)-C)/TMOLES                                     APP17810
C                                                                       APP17820
C        CONVERT COMPOSITION TO MOLE FRACTIONS AND CALCULATE AVERAGE     APP17830
C        MOLECULAR WEIGHT                                               APP17840
C                                                                       APP17850
  35  IER = 0                                                           APP17860
      IF (T .LT. 100.) IER = 1                                          APP17870
      IF (T .GT. 6000.) IER  =  2                                       APP17880
      IR = 1                                                            APP17890
      IF (T .LT. 500.) IR = 2                                           APP17900
C                                                                       APP17910
C        CALCULATE H, CP, AND CT AS IN WRITEUP  USING FITTED            APP17920
C        COEFFICIENTS FROM JANAF TABLES                                 APP17930
C                                                                       APP17940
      ENTHLP = 0.                                                       APP17950
      CSUBP = 0.                                                        APP17960
      CPFROZ = 0.                                                       APP17970
      ST = T/1000.                                                      APP17980
      DO 40 J = 1,6                                                     APP17990
      TH = ((( A(4,J,IR)/4.*ST + A(3,J,IR)/3. )*ST                      APP18000
     1       + A(2,J,IR)/2. )*ST + A(1,J,IR) )*ST                       APP18010
      TCP = (( A(4,J,IR)*ST + A(3,J,IR) )*ST                            APP18020
     1       +A(2,J,IR))*ST+A(1,J,IR)+A(5,J,IR)/ST**2                   APP18030
```

```
      TH  = TH - A(5,J,IR)/ST  +  A(6,J,IR)                              APP18040
      ENTHLP  =  ENTHLP  +  TH*X(J)                                      APP18050
      CPFROZ = CPFROZ + TCP*X(J)                                         APP18060
   40 CSUBP  =  CSUBP  + 1000.*TH*DCDT*TABLE(J)                          APP18070
      ENTHLP = ENTHLP/MBAR                                               APP18080
      CPFROZ=CPFROZ/MBAR                                                 APP18090
      CSUBP=CPFROZ+CSUBP/MBAR                                            APP18100
      CPB=CSUBP                                                          APP18110
C                                                                        APP18120
C        NOW CALCULATE RHO AND ITS PARTIAL DERIVATIVES                   APP18130
C        USING PERFECT GAS LAW                                           APP18140
C                                                                        APP18150
      RHOB= PSCOR*MBAR*P/T                                               APP18160
      RB=RGAS/MBAR                                                       APP18170
      GAMB=CPB/(CPB-RB)                                                  APP18180
C                                                                        APP18190
      IF(GAMB.LT.1..OR.GAMB.GT.2.)THEN                                   APP18200
      PRINT*,' '                                                         APP18210
      PRINT*,'*********** EXECUTION STOPPED AT CLDPRD ************'     APP18220
      PRINT*,' '                                                         APP18230
      PRINT*,'T =',T,' P =',P                                            APP18240
      PRINT*,'X(1)=',X(1),' X(2)=',X(2)                                  APP18250
      PRINT*,'X(3)=',X(3),' X(4)=',X(4)                                  APP18260
      PRINT*,'X(5)=',X(5),' X(6)=',X(6)                                  APP18270
      PRINT*,'X(7)=',X(7),' RB=',RB                                      APP18280
      PRINT*,'CPB=',CPB,' GAMB =',GAMB                                   APP18290
      PRINT*,' '                                                         APP18300
      PRINT*,'*********** EXECUTION STOPPED AT CLDPRD ************'     APP18310
      PRINT*,' '                                                         APP18320
      ENDIF                                                              APP18330
      IF(GAMB.LT.1..OR.GAMB.GT.2.) STOP                                  APP18340
C                                                                        APP18350
C     * ALL DONE                                                        APP18360
      RETURN                                                             APP18370
      END                                                                APP18380
CUPROP ****************** VERSION 2.0  1/10/76  ***************         APP18390
C                                                                        APP18400
C     SUBROUTINE UPROP                                                   APP18410
C                                                                        APP18420
C     PURPOSE                                                            APP18430
C        TO CALCULATE THE ENTHALPY AND DENSITY OF A HOMOGENOUS MIXTUR    APP18440
C        OF AIR, RESIDUAL GAS, AND FUEL AS A FUNCTION OF                 APP18450
C        EQUIVALENCE RATIO, TEMPERATURE, AND PRESSURE                    APP18460
C                                                                        APP18470
C     USAGE                                                              APP18480
C        CALL UPROP(P,T,ENTHLP,CSUBP,RHO)                                APP18490
C                                                                        APP18500
C     DESCRIPTION OF PARAMETERS                                          APP18510
C      GIVEN                                                             APP18520
C        P      - ABSOLUTE PRESSURE OF PRODUCTS (ATM)                    APP18530
C        T      - TEMPERATURE OF PRODUCTS (DEG K)                        APP18540
C      GIVEN IN COMMON AREA /CHARGE/                                     APP18550
C        RESFRK- RESIDUAL GAS FRACTION                                   APP18560
C        PHI    - EQUIVALENCE RATIO (FUEL/AIR RATIO DIVIDED BY THE       APP18570
C                 CHEMICALLY CORRECT FUEL/AIR RATIO)                     APP18580
C      GIVEN IN COMMON AREA /FUEL/                                       APP18590
C        AF(I) - 6 DIMENSIONAL VECTOR OF ENTHALPY COEFFICIENTS SUCH      APP18600
C                THAT THE ENTHALPY OF FUEL VAPOR AS A FUNCTION           APP18610
C                OF TEMPERATURE ( T DEG K ) IS GIVEN BY                  APP18620
C                  H(T) = AF(1)*ST + (AF(2)*ST**2)/2 + (AF(3)*ST**3)/3   APP18630
C                       + (AF(4)*ST**4)/4 - AF(5)/ST + AF(6)             APP18640
C                  WHERE ST = T/1000 AND H(T) = <KCAL/MOLE>              APP18650
C                FOR MOST APPLICATIONS THE ENTHALPY FUNCTION H(          APP18660
C                BE VALID OVER AT LEAST THE FOLLOWING TEMPERATURE RAN    APP18670
C                                  300 < T < 1000                        APP18680
C                ENTHALPY DATUM STATE IS AT T = 0 ABSOLUTE WITH O2,N2    APP18690
C                AND H2 GASEOUS AND C SOLID GRAPHITE.                    APP18700
C        ENW    - AVERAGE NUMBER OF NITROGEN ATOMS PER FUEL MOLECULE     APP18710
C        CX     - AVERAGE NUMBER OF CARBON ATOMS PER FUEL MOLECULE       APP18720
C        HY     - AVERAGE NUMBER OF HYDROGEN ATOMS PER FUEL MOLECULE     APP18730
C        OZ     - AVERAGE NUMBER OF OXYGEN ATOMS PER FUEL MOLECULE       APP18740
C        QLOWER- LOWER HEATING VALUE (KCAL/G)                            APP18750
C      GIVEN IN COMMON AREA/OXDANT/                                      APP18760
C        XI     - MOLAR N O RATIO OF THE OXIDANT (FOR AIR XI = 3.76)     APP18770
C                                                                        APP18780
```

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C      RETURNS IN COMMON AREA /PRODMR/                                          APP18790
C        DEL   - MOLAR C H RATIO OF THE PRODUCTS                                APP18800
C        PSI   - MOLAR N O RATIO OF THE PRODUCTS                                APP18810
C        CHI   - EQUIVALENCE RATIO OF THE PRODUCTS FOR AN EQUIVALENT            APP18820
C                HYDROCARBON-OXIDANT COMBUSTION                                 APP18830
C      RETURNS                                                                  APP18840
C        ENTHLP- SPECIFIC ENTHALPY OF THE PRODUCTS (KCAL/G)                     APP18850
C        CSUBP - PARTIAL DERIVATIVE OF ENTHLP WITH RESPECT T                    APP18860
C                AT CONSTANT P    (CAL/G-DEG K)                                 APP18870
C        CSUBT - PARTIAL DERIVATIVE OF ENTHLP WITH RESPECT TO P                 APP18880
C                AT CONSTANT T    (CC/G)                                        APP18890
C        RHO   - DENSITY OF THE PRODUCTS      (G/CC)                            APP18900
C        DRHODT- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO T AT                 APP18910
C                CONSTANT P    (G/CC-DEG K)                                     APP18920
C        DRHODP- PARTIAL DERIVATIVE OF RHO WITH RESPECT TO P                    APP18930
C                CONSTANT T    (G/CC-ATM)                                       APP18940
C      RETURNS IN COMMON AREA CMPSTN                                            APP18950
C        X(1)  - CARBON DIOXIDE MOLE FRACTION                                   APP18960
C        X(2)  - WATER VAPOR MOLE FRACTION                                      APP18970
C        X(3)  - CARBON MONOXIDE MOLE FRACTION                                  APP18980
C        X(4)  - HYDROGEN MOLE FRACTION                                         APP18990
C        X(5)  - OXYGEN MOLE FRACTION                                           APP19000
C        X(6)  - NITROGEN MOLE FRACTION                                         APP19010
C        X(7)  - FUEL MOLE FRACTION                                             APP19020
C        MBAR  - MOLECULAR WEIGHT OF UNBURNED MIXTURE                           APP19030
C                                                                               APP19040
C      REMARKS                                                                  APP19050
C         1)  ENTHALPY DATUM STATE IS AT T = 0 ABSOLUTE WITH                    APP19060
C             O2,N2,H2 GASEOUS AND C SOLID GRAPHITE                             APP19070
C                                                                               APP19080
C      SUBROUTINES AND FUNCTION SUBPROGRAMS NEEDED   NONE                       APP19090
C                                                                               APP19100
C                                                                               APP19110
C     METHOD                                                                    APP19120
C         DESCRIBED IN APPENDIX A OF HIRES ET AL, SAE PAPER #                   APP19130
C                                                                               APP19140
C*****************************************************************************APP19150
      SUBROUTINE UPROP(P,T,ENTHLP,CSUBP,RHO)                                    APP19160
      LOGICAL RICH,LEAN                                                         APP19170
      DIMENSION TABLE(7),A(6,6,2)                                               APP19180
      EQUIVALENCE (A1(1),A(1,1,1))                                              APP19190
      EQUIVALENCE (A2(1),A(1,1,2))                                              APP19200
      REAL*4  MBAR,K                                                            APP19210
      COMMON/CNT/IUP,ICLD,IKIN                                                  APP19220
      COMMON /FUEL/ ENW,CX,HY,OZ,AST                                            APP19230
      COMMON/JANAF/ A1(36),A2(36)                                               APP19240
      COMMON/CHARU/PHIFR,PHIEGR                                                 APP19250
       COMMON/CHARB/PHI                                                         APP19260
      COMMON/CHARTH/RESFRK,RICH,LEAN                                            APP19270
      COMMON /OXDANT/XI                                                         APP19280
      COMMON /UGASP/ X(7),MBAR,RU,GAMU,CPU,HU,TU,RHOU                           APP19290
      COMMON /PRODMR/DEL,CHI,W,Z,EPS1,EPS                                       APP19300
      COMMON/THERMO/RGAS,RGS1,RO2,PSCALE,PSCOR                                  APP19310
      DATA TABLE /-1.,1.,1.,-1.,0.,0.,0./                                       APP19320
      IUP=IUP+1                                                                 APP19330
C                                                                               APP19340
C        ENTER INTO ARRAYS A1 AND A2 THE FUEL PARAMETERS                        APP19350
C                                                                               APP19360
    1 I1 = 2                                                                    APP19370
      RICH = PHIFR  .GT. 1.0                                                    APP19380
      LEAN =  .NOT. RICH                                                        APP19390
      CX=3.                                                                     APP19400
      HY=8.                                                                     APP19410
      W = ENW/CX                                                                APP19420
      Z = OZ/CX                                                                 APP19430
      DEL = CX/HY                                                               APP19440
      EPS = 4.*DEL/(1. + 4.*DEL - 2.*DEL*Z)                                     APP19450
C                                                                               APP19460
C        CALCULATE PSI AND CHI FOR BURNED GASES                                 APP19470
C                                                                               APP19480
C                                                                               APP19490
C *** THESE VALUES ARE RETURNED IN COMMON /CHARGE/ /PRODMR / /CMPS              APP19500
C     IER = 0                                                                   APP19510
C     IF (T .LT. 100.) IER = 1                                                  APP19520
C     IF (T .GT. 6000.) IER  =  2                                               APP19530
C
```

```
C       GET THE COMPOSITION IN MOLES/MOLE OXYGEN OF OXIDANT                  APP19540
C                                                                            APP19550
      PCTRES = RESFRK                                                        APP19560
      PCTNEW = 1.0 - RESFRK                                                  APP19570
      MBAR=(12.+1./DEL)*(PHIFR*PCTNEW+PHIEGR*PCTRES)*EPS+32.+28.*XI          APP19580
      IF (RICH) GO TO 13                                                     APP19590
C                                                                            APP19600
C *** THE LEAN VALUES NOT DEPENDENT ON TEMP. (CONSTANT)                      APP19610
C                                                                            APP19620
      I1 = 3                                                                 APP19630
      TMOLES=XI+(1.+EPS*PHIFR/CX)*PCTNEW                                     APP19640
     &    +(1.+(1.-EPS)*PHIEGR+EPS*PHIEGR*(Z+W/2.))*PCTRES                   APP19650
      X(1) = EPS*PHIEGR*PCTRES/TMOLES                                        APP19660
      X(2) = (2.*(1. - EPS) + EPS*Z)*PHIEGR*PCTRES/TMOLES                    APP19670
      X(3) = 0.                                                              APP19680
      X(4) = 0.                                                              APP19690
      X(5) = ((1.-PHIEGR)*PCTRES+PCTNEW)/TMOLES                              APP19700
      X(6) = (XI + EPS*PHIEGR*W/2.*PCTRES)/TMOLES                            APP19710
      X(7) = PCTNEW*EPS*PHIFR/CX/TMOLES                                      APP19720
C                                                                            APP19730
      MBAR = MBAR/TMOLES                                                     APP19740
      DCDT = 0.                                                              APP19750
      GO TO 35                                                               APP19760
C                                                                            APP19770
C *** THE RICH CASE                                                          APP19780
C                                                                            APP19790
   13 TMOLES= XI+(1.+EPS*PHIFR/CX)*PCTNEW                                    APP19800
     1  +((2.-EPS)*PHIEGR+EPS*PHIEGR*(Z+W/2.))*PCTRES                       APP19810
      X(5) = PCTNEW/TMOLES                                                   APP19820
      X(6) = (XI+EPS*PHIEGR*W/2.*PCTRES)/TMOLES                              APP19830
      X(7) = PCTNEW*EPS*PHIFR/CX/TMOLES                                      APP19840
      MBAR = MBAR/TMOLES                                                     APP19850
C                                                                            APP19860
C *** THE CALCULATIONS THAT MUST BE PERFORMED EACH TIME                      APP19870
      CB1 = 2.*(PHIEGR-1.) + EPS*PHIEGR                                      APP19880
      GA1 = 2.*EPS*PHIEGR*(PHIEGR-1.)                                        APP19890
      BETA0 = EPS*PHIEGR*Z + 2.*(1.-EPS*PHIEGR)                              APP19900
C                                                                            APP19910
C *** THE RICH CASE ENTRY                                                    APP19920
   20 ZT = 1000./T                                                           APP19930
      K = EXP(2.743 + ZT*(-1.761 + ZT*(-1.611 + ZT*.2803)))                  APP19940
      DKDT = -K*ZT*(-1.761 + ZT*(-3.222 + ZT*.9409))/T                       APP19950
      ALPHA = 1.0 - K                                                        APP19960
      BETA = BETA0 + CB1*K                                                   APP19970
      GAMMA = GA1*K                                                          APP19980
      XX= BETA*BETA +4.*ALPHA*GAMMA                                          APP19990
C     PRINT*,XX                                                              APP20000
      C = (-BETA + SQRT(BETA*BETA + 4.*ALPHA*GAMMA))/(2.*ALPHA)              APP20010
      DCDT=-DKDT*(C*(CB1+C)-GA1)                                             APP20020
      DCDT = DCDT/(2.*ALPHA*C + BETA)/TMOLES                                 APP20030
      X(1) = (EPS*PHIEGR - C)*PCTRES/TMOLES                                  APP20040
      X(2) = (BETA0 + C)*PCTRES/TMOLES                                       APP20050
      X(3) = C*PCTRES/TMOLES                                                 APP20060
      X(4) = (2.0*(PHIEGR - 1.) - C)*PCTRES/TMOLES                           APP20070
C                                                                            APP20080
C***  ENTRY FOR CALCULATION OF ENTHALPY                                      APP20090
C                                                                            APP20100
   35 IR = 1                                                                 APP20110
      IF (T .LT. 500.) IR = 2                                                APP20120
C                                                                            APP20130
C        CALCULATE H, CP, AND CT AS IN WRITEUP, USING FITTED                 APP20140
C        COEFFICIENTS FROM JANAF TABLES                                      APP20150
C                                                                            APP20160
      ENTHLP = 0.                                                            APP20170
      CSUBP = 0.                                                             APP20180
      CSUBT = 0.                                                             APP20190
      ST = T/1000.                                                           APP20200
      DO 40 J = 1,6                                                          APP20210
      TH = ((( A(4,J,IR)/4.*ST + A(3,J,IR)/3. )*ST                          APP20220
     1       +  A(2,J,IR)/2.)*ST + A(1,J,IR)  )*ST                          APP20230
      TCP = (( A(4,J,IR)*ST + A(3,J,IR) )*ST                                 APP20240
     1        + A(2,J,IR))*ST + A(1,J,IR)+A(5,J,IR)/ST**2                    APP20250
      TH  =  TH - A(5,J,IR)/ST  +  A(6,J,IR)                                 APP20260
      ENTHLP  =  ENTHLP  +  TH*X(J)                                          APP20270
   40 CSUBP  =  CSUBP  +  TCP*X(J)+ 1000.*TH*DCDT*PCTRES*TABLE(J)            APP20280
```

```
C     THIS PART IS FOR FUEL PROPANE                                          APP20290
      FM=44.09                                                               APP20300
      RFV=RGAS/FM                                                            APP20310
      TH= RFV*(((((0.233361E-10/5.*T - 0.545131E-7/4.)*T                     APP20320
     1             +0.351709E-4/3.)*T                                        APP20330
     1            +0.157505E-1/2.)*T                                         APP20340
     1           +1.31841)*T                                                 APP20350
     1          -14091.3) + 201.1 +RFV*T                                    APP20360
      TH=TH*1.0E-3*FM                                                        APP20370
      TCP=RFV*((((0.233361E-10*T - 0.545131E-7)*T                            APP20380
     1             +0.351709E-4)*T                                           APP20390
     1            +0.157505E-1)*T                                            APP20400
     1           +1.31841) + RFV                                             APP20410
      TCP=FM*TCP                                                             APP20420
      ENTHLP= ENTHLP + TH*X(7)                                               APP20430
      CSUBP= CSUBP + TCP*X(7) + 1000.*TH*DCDT*PCTRES*TABLE(7)                APP20440
     ENTHLP = ENTHLP/MBAR                                                    APP20450
     CSUBP = CSUBP/MBAR                                                      APP20460
     CPU=CSUBP                                                               APP20470
C                                                                            APP20480
C        NOW CALCULATE RHO AND ITS PARTIAL DERIVATIVES                       APP20490
C        USING PERFECT GAS LAW                                               APP20500
C                                                                            APP20510
     RHO=PSCOR*MBAR*P/T                                                      APP20520
     RHOU=RHO                                                                APP20530
     RU=RGAS/MBAR                                                            APP20540
     GAMU=CSUBP/(CSUBP-RU)                                                   APP20550
C                                                                            APP20560
     IF(GAMU.LT.1..OR.GAMU.GT.2.)THEN                                        APP20570
     PRINT*,' '                                                              APP20580
     PRINT*,'************ EXECUTION STOPPED AT UPROP *************'         APP20590
     PRINT*,' '                                                              APP20600
     PRINT*,'T =',T,' P =',P                                                 APP20610
     PRINT*,'X(1)=',X(1),' X(2)=',X(2)                                       APP20620
     PRINT*,'X(3)=',X(3),' X(4)=',X(4)                                       APP20630
     PRINT*,'X(5)=',X(5),' X(6)=',X(6)                                       APP20640
     PRINT*,'X(7)=',X(7),' RU=',RU                                           APP20650
     PRINT*,'CPU=',CPU,' GAMU =',GAMU                                        APP20660
     PRINT*,' '                                                              APP20670
     PRINT*,'************ EXECUTION STOPPED AT UPROP *************'         APP20680
     PRINT*,' '                                                              APP20690
     ENDIF                                                                   APP20700
     IF(GAMU.LT.1..OR.GAMU.GT.2.) STOP                                       APP20710
C                                                                            APP20720
C        ALL DONE                                                            APP20730
     RETURN                                                                  APP20740
```

APPENDIX I

```
C------------ SUBROUTINE SHAPE ------------------------------------------
C
C     GIVEN : CRG = CRANK ANGLE
C             VE = ENTRAINED VOLUME
C
C     GIVEN AS CONSTANTS : RR = RADIUS OF CYLINDER ( HALF BORE )
C                          RS = SPARK LOCATION FROM CENTER
C
C     RETURN : H = CHAMBER HEIGHT
C              RE = ENTRAINMENT RADIUS
C              AE = ENTRAINMENT SURFACE AREA
C
C-----------------------------------------------------------------------
C
      SUBROUTINE SHAPE(CRG,VE,H,RE,AE)
      COMMON/BBORE/BORE
C
      RR=BORE/2.
      RS=0.75
      H=VTO(CRG)/3.1416/RR**2.
C
      RE=(3./2.*VE/3.1416)**(1./3.)
      IF(RE.LE.H.AND.RE.LE.RR-RS) AE = 2.*3.1416*RE**2.
      IF(RE.LE.H.AND.RE.LE.RR-RS) GO TO 4
C
      DO 2 I =1,50
         FRE=0.
         AE=0.
         ZO=0.
         RO=(RE**2.-ZO**2.)**0.5
         ALFO=3.1416
         BETO=0.
         IF(RO.GE.RR-RS)THEN
          IF(RO.GE.RR+RS)THEN
            AFLO=0.
            BETO=3.1416
          ELSE
            ALFO=ACOS(((RS**2.)+(RO**2.)-(RR**2.))/(2.*RS*RO))
            BETO=ACOS(((RS**2.)+(RR**2.)-(RO**2.))/(2.*RS*RR))
          ENDIF
         ENDIF
C
         DO 1 Z = H/50.,H,H/50.
             R=0.
             IF(RE.GT.Z) R=(RE**2.-Z**2.)**0.5
             ALF=3.1416
             BET=0.
             IF(R.GE.RR-RS)THEN
              IF(R.GE.RR+RS)THEN
                ALF=0.
                BET=3.1416
              ELSE
                ALF=ACOS((RS**2.+R**2.-RR**2.)/(2.*RS*R))
                BET=ACOS((RS**2.+RR**2.-R**2.)/(2.*RS*RR))
              ENDIF
             ENDIF
           FRE=FRE+(ALF*R**2.+BET*RR**2.+RS*RR*SIN(BET)+
     1           ALFO*RO**2.+BETO*RR**2.+RS*RR*SIN(BETO))*(Z-ZO)/2.
           AE=AE+(ALF+ALFO)*(Z-ZO)/2.
             RO=R
             ALFO=ALF
             BETO=BET
             ZO=Z
    1    CONTINUE
C
         FRE=FRE-VE
         AE=2.*RE*AE
         RE=RE-FRE/AE/2.
         IF(I.GE.50)
     1     PRINT*,' ... NUMBER OF ITERATION EXCEEDS LIMIT IN "SHAPE" !'
```

APP20750 APP20760 APP20770 APP20780 APP20790 APP20800 APP20810 APP20820 APP20830 APP20840 APP20850 APP20860 APP20870 APP20880 APP20890 APP20900 APP20910 APP20920 APP20930 APP20940 APP20950 APP20960 APP20970 APP20980 APP20990 APP21000 APP21010 APP21020 APP21030 APP21040 APP21050 APP21060 APP21070 APP21080 APP21090 APP21100 APP21110 APP21120 APP21130 APP21140 APP21150 APP21160 APP21170 APP21180 APP21190 APP21200 APP21210 APP21220 APP21230 APP21240 APP21250 APP21260 APP21270 APP21280 APP21290 APP21300 APP21310 APP21320 APP21330 APP21340 APP21350 APP21360 APP21370 APP21380 APP21390 APP21400 APP21410 APP21420 APP21430 APP21440 APP21450 APP21460 APP21470 APP21480 APP21490

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      IF(I.GE.50) STOP                                                  APP21500
      IF(ABS(FRE)/VE.LE.1.E-03) GO TO 3                                 APP21510
    2 CONTINUE                                                          APP21520
    3 IF(RE.GE.((RR+RS)**2.+H**2.)**.5)THEN                             APP21530
       RE = ((RR+RS)**2.+H**2.)**.5                                     APP21540
       AE = 0.                                                          APP21550
      ENDIF                                                             APP21560
C                                                                       APP21570
    4 RETURN                                                            APP21580
      END                                                               APP21590
```

APPENDIX J

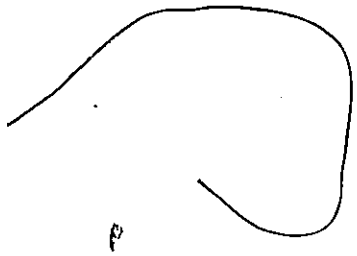
```
C------------------  SUBROUTINE ISCOMP  ------------------------------------
C
C    GIVEN : VOLI = TOTAL VOLUME BEFORE COMPRESSION
C            VOLF = TOTAL VOLUME AFTER COMPRESSION
C            PIN = PRESSURE BEFORE COMPRESSION
C    GIVEN IN COMMON BLOCK :
C            TEMP(I) = TEMPERATURE OF EACH PARTICLE BEFORE COMPRESSION
C            VOL(I) = VOLUME OF EACH PARTICLE BEFORE COMPRESSION
C            FFR(I) = FUEL FRACTION OF EACH PARTICLE
C
C    RETURN : POUT = PRESSURE AFTER COMPRESSION
C    RETURN IN COMMON BLOCK :
C             TEMP(I) = TEMPERATURE OF EACH PARTICLE AFTER COMPRESSION
C             VOL(I) = VOLUME OF EACH PARTICLE AFTER COMPRESSION
C
C    SUBROUTINE NEEDED : UPROP, CLDPRD
C
C-------------------------------------------------------------------------
C
      SUBROUTINE ISCOMP(VOLI,VOLF,PIN,POUT)
      COMMON/BURN/FFR(9999),IBURN(9999)
      COMMON/TEMVOL/TEMP(9999),VOL(9999)
      COMMON/PARNUM/N,NT,N1,N2,N3
      COMMON/UGASP/CCU(7),MBARU,RU,GAMU,CPU,HU,TU,RHOU
      COMMON/BGASP/CCB(7),MBARB,RB,GAMB,CPB,HB
      COMMON/CHARB/PHI
      REAL VNEW(9999)
C
      FO=44./(44.+5.*(32.+3.76*28)/PHI)
C
      CALL UPROP(PIN,TEMP(NT+1),ENTHLP,CSUBP,RHO)
      POUT = PIN*(VOLI/VOLF)**GAMU
      DO 2 ITS = 1,50
      TOVOL=0.
      UNB=0.
      DO 1 I =1,NT+1
        IF(IBURN(I).EQ.2) THEN
          IF(UNB.EQ.0.) THEN
          CALL UPROP(PIN,TEMP(I),ENTHLP,CSUBP,RHO)
          UBN=1.
          ENDIF
          VNEW(I) = VOL(I)*(POUT/PIN)**(-1./GAMU)
          TOVOL=TOVOL+VNEW(I)
        ELSE
          CALL CLDPRD(PIN,TEMP(I),H,CP,RHO,IER)
          VNEW(I) = VOL(I)*(POUT/PIN)**(-1./GAMB)
          TOVOL=TOVOL+VNEW(I)
        ENDIF
    1 CONTINUE
      TOVOL = TOVOL + (N-NT-1.)*VNEW(NT+1)
C
      POUT=POUT*(TOVOL/VOLF)**GAMB
      IF(ABS(TOVOL-VOLF)/VOLF.LE.1.E-05) GO TO 9
      IF(ITS.GE.50) PRINT*,
     1 ' ... NUMBER OF ITERATION EXCEEDS LIMIT IN "ISCOMP" !'
      IF(ITS.GE.50) STOP
    2 CONTINUE
C
    9 UNB=0.
      DO 3 I =1,MIN(N,9999)
       IF(I.LE.NT+1) THEN
        IF(IBURN(I).EQ.2) THEN
          IF(UBN.EQ.0.) THEN
          CALL UPROP(PIN,TEMP(I),ENTHLP,CSUBP,RHO)
          UNB=1.
          ENDIF
          VOL(I)=VNEW(I)
          TEMP(I)=TEMP(I)*(POUT/PIN)**((GAMU-1.)/GAMU)
        ELSE
          CALL CLDPRD(PIN,TEMP(I),H,CP,RHO,IER)
```

```
          VOL(I)=VNEW(I)                                                    APP22360
          TEMP(I)=TEMP(I)*(POUT/PIN)**((GAMB-1.)/GAMB)                      APP22370
         ENDIF                                                              APP22380
        ELSE                                                                APP22390
         VOL(I) = VOL(NT+1)                                                 APP22400
         TEMP(I) = TEMP(NT+1)                                               APP22410
        ENDIF                                                               APP22420
    3  CONTINUE                                                            APP22430
C                                                                           APP22440
      RETURN                                                                APP22450
      END                                                                   APP22460
```

APPENDIX K

```
C-----------------------------------------------------------------------APP22480
C                                                                       APP22490
      SUBROUTINE CODE(X,XEND,Y,YPRIM,DPDT,NQ,EPS1,EPS2,HLAST)           APP22500
      COMMON/BURN/FFR(9999),IBURN(9999)                                 APP22510
      COMMON/TEMVOL/TEMP(9999),VOL(9999)                                APP22520
      COMMON/CRANGL/SA,CRG,CRGSTP                                       APP22530
      REAL YY(1000),YP(1000),YYPRIM(1000)                               APP22540
      REAL Y(NQ),YPRIM(NQ)                                              APP22550
C                                                                       APP22560
      IF(NQ.GT.1000) PRINT*,' NUM OF EQUATIONS > 1000 !'                APP22570
      IF(NQ.GT.1000) STOP                                               APP22580
C                                                                       APP22590
        CALL FCN(NQ,X,Y,YPRIM,DPDT)                                     APP22600
        TERMIN=ABS(Y(1)/YPRIM(1))                                       APP22610
        DO 7 I = 2,NQ                                                   APP22620
          IF(Y(I).EQ.0..OR.YPRIM(I).EQ.0.) GO TO 7                      APP22630
          IF(ABS(Y(I)/YPRIM(I)).LT.TERMIN) TERMIN=ABS(Y(I)/YPRIM(I))    APP22640
    7   CONTINUE                                                        APP22650
        H=AMAX1(EPS1*TERMIN,HLAST,XEND/10)                              APP22660
C       PRINT*,' FIRST H =',H                                           APP22670
        NITS=0                                                          APP22680
        NRH=0                                                           APP22690
        NIH=0                                                           APP22700
      DO 10 ISTEP = 1,100                                               APP22710
        IF(ISTEP.EQ.51) PRINT*,' WRN : NUM OF STEP > 50  AT CRG =',CRG  APP22720
        IF(ISTEP.GT.99) PRINT*,' NUM OF STEP > 99  AT CRG =',CRG        APP22730
        IF(ISTEP.GT.99) STOP                                            APP22740
        IFLAG = 0                                                       APP22750
        IF(X+H.GT.XEND) HLAST=H                                         APP22760
        IF(X+H.GT.XEND) H=XEND-X                                        APP22770
    8   ITS = 0                                                         APP22780
        CALL FCN(NQ,X,Y,YPRIM,DPDT)                                     APP22790
        DO 11 I = 1,NQ                                                  APP22800
          YY(I)=Y(I)                                                    APP22810
          YYPRIM(I)=YPRIM(I)                                            APP22820
          Y(I)=Y(I)+H*YPRIM(I)                                          APP22830
   11   CONTINUE                                                        APP22840
    9   DO 12 I = 1,NQ                                                  APP22850
          YP(I)=Y(I)                                                    APP22860
   12   CONTINUE                                                        APP22870
        CALL FCN(NQ,X+H,Y,YPRIM,DPDT)                                   APP22880
        DO 13 I = 1,NQ                                                  APP22890
          Y(I)=YY(I)+H/2.*(YPRIM(I)+YYPRIM(I))                          APP22900
   13   CONTINUE                                                        APP22910
        ITS=ITS+1                                                       APP22920
        NITS=NITS+1                                                     APP22930
        DO 14 I = 1,NQ                                                  APP22940
          IF(Y(I).EQ.0..OR.YP(I).EQ.0.) GO TO 14                        APP22950
          DIF=ABS(Y(I)-YP(I))/AMIN1(Y(I),YP(I))                         APP22960
          IF(DIF.GE.EPS2.AND.ITS.LT.5 ) GO TO 9                         APP22970
          IF(DIF.GE.EPS2.AND.ITS.GE.5 ) THEN                            APP22980
          IF(IFLAG.EQ.2)                                                APP22990
     1      PRINT*,' WRN : H IS REDUCED THE 3RD TIME AT STEP',ISTEP     APP23000
          IF(IFLAG.GE.3)                                                APP23010
     1      PRINT*,' STEP CONVERGENCE FAILED. DIF/EPS2 =',DIF/EPS2      APP23020
          IF(IFLAG.GE.3) STOP                                           APP23030
          H=AMAX1(AMIN1(H/2.,H/DIF*EPS2),H/5.)                          APP23040
          IFLAG=IFLAG+1                                                 APP23050
          NRH=NRH+1                                                     APP23060
          DO 15 J = 1,NQ                                                APP23070
            Y(J)=YY(J)                                                  APP23080
   15     CONTINUE                                                      APP23090
          IF(IFLAG.LE.3) GO TO 8                                        APP23100
          ENDIF                                                         APP23110
          IF(ISTEP.EQ.1) THEN                                           APP23120
          ENDIF                                                         APP23130
   14   CONTINUE                                                       APP23140
        X=X+H                                                           APP23150
        IF(X.EQ.XEND) GO TO 20                                          APP23160
        IF(ITS.LE.2) H=H*1.5                                            APP23170
                                                                        APP23180
                                                                        APP23190
                                                                        APP23200
                                                                        APP23210
                                                                        APP23220
```

```
      IF(ITS.LE.2) NIH=NIH+1                                          APP23230
   10 CONTINUE                                                        APP23240
C                                                                     APP23250
C  20 PRINT*,' STEPS TAKEN =',ISTEP,' CORRECTOR ITERATION =',NITS     APP23260
C     PRINT*,' STEPSIZE REDUCTION =',NRH,' STEPSIZE INCREASE =',NIH   APP23270
C     PRINT*,' LAST H =',HLAST                                        APP23280
   20 RETURN                                                          APP23290
      END                                                             APP23300
```



APPENDIX L

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE AGEMIX(DELT,W,NM,DSEED)
C
      COMMON/MIX/MASS,F3,VOL3,TO3
      COMMON/PARNUM/N,NT,N1,N2,N3
      COMMON/BURN/FFR(9999),IBURN(9999)
      COMMON/TEMVOL/TEMP(9999),VOL(9999)
      COMMON/IDNUM/IDN(9999)
      COMMON/AGE/NAGE,NP(500),FNM(500)
      REAL NM,CHOSEN(9999)
      INTEGER IR(2),K,NR
      DOUBLE PRECISION DSEED
C
C   NM = NUMBER OF PAIRS TO BE MIXED AT A FREQUENCY OF 'W'.
C
      IF(W*DELT.GT.0.5) PRINT*,' W*DELT =',W*DELT,'> 0.5 !'
      IF(W*DELT.GT.0.5) STOP
      DO 100 I = 1,NT
        CHOSEN(I)=0.
 100  CONTINUE
C
      NP2=0.
      DO 99 IAGE = 2, NAGE
      IF(IAGE.NE.2) NP2 = NP2 + NP(IAGE-2)
      XNM = DELT*W*(NP(IAGE)+NP(IAGE-1))
      NM = INT(XNM)
      FNM(IAGE)=FNM(IAGE)+XNM-NM
      IF(FNM(IAGE).GE.1.) NM=NM+1
      IF(FNM(IAGE).GE.1.) FNM(IAGE)=FNM(IAGE)-1.
C
C  RANDOM GENERATOR "GGUD" GENERATES NR INTEGERS FROM 1 TO K
C   ( INITIAL SEED DSEED RANGES FROM 1.0D0 TO 2147483647.0D0 )
C
      K = NP(IAGE)+NP(IAGE-1)
      NR = 2
C
      DO 130 I = 1,NM
         CHOUNT=0.
 22     CALL GGUD(DSEED,K,NR,IR)
        I1=IR(1)+NP2
        I2=IR(2)+NP2
        IF(CHOSEN(I1).EQ.1..OR.CHOSEN(I2).EQ.1.) CHOUNT=CHOUNT+1.
         IF(CHOUNT.GT.K**2) PRINT*,' K =',K,' NM =',NM
         IF(CHOUNT.GT.K**2) PRINT*,' I =',I,' CHOUNT >',CHOUNT
         IF(CHOUNT.GT.K**2) STOP
        IF(CHOSEN(I1).EQ.1..OR.CHOSEN(I2).EQ.1.)GO TO 22
         CHOSEN(I1)=1.
         CHOSEN(I2)=1.
       IF(IBURN(I1).NE.IBURN(I2).OR.
     1   (IBURN(I1).EQ.1.AND.IBURN(I2).EQ.1)) THEN
        IF(IAGE.EQ.2) GO TO 97
 97     CALL MIXFRO(FFR(I1),FFR(I2),VOL(I1),VOL(I2),TEMP(I1),TEMP(I2))
        FFR(I1)=F3
        FFR(I2)=F3
        VOL(I1)=VOL3
        VOL(I2)=VOL3
        TEMP(I1)=TO3
        TEMP(I2)=TO3
        DO 8 J = 1,NP(IAGE)
         IF(IDN(J).EQ.I1.OR.IDN(J).EQ.I2) IDN(J)=0
   8    CONTINUE
        IDN(I1)=0
        IDN(I2)=I1
       ENDIF
 130  CONTINUE
 99   CONTINUE
      CALL COUNT(NT)
C
      RETURN
      END
C
```