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APPLICATION OF ALTERNATIVE FUELS FOR INTERNAL  
COMBUSTION ENGINES, IIP, DEHRA DUN

DP/IND/82/001/11-52 and 11-54

INDIA

Technical report: Mathematical modeling of the thermofluid process  
of a two-stroke engine using methanol\*

Prepared for the government of India  
by the United Nations Industrial Development Organization,  
acting as executing agency for the United Nations Development Programme

Based on the work of Messrs L. H. Browning and R. K. Refley,  
UNIDO consultants

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United Nations Industrial Development Organization  
Vienna

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**APPLICATION OF ALTERNATIVE FUELS FOR  
INTERNAL COMBUSTION ENGINES**

DP/IND/82/001

**ABSTRACT**

The fuel delivery system for the Indian 2-cycle, spark ignited engine is in need of redesign. This is based on its expected growth in use (production exceeding 5 million per year in the 1990's) and its accompanying excessive pollution (a 150 cc, 2-cycle vehicle produces hydrocarbon and carbon monoxide pollution levels approximating 10 American cars on a per mile basis).

The alternative fuels program at IIP includes evaluating 2-cycle engines on methanol. The experimental tests have shown some combustion instabilities in the engine. Mathematical modeling of the fuel delivery and combustion processes of the 2-cycle engine can be an invaluable aid in the design evolution of this engine as its emissions are reduced and its fuel changed from gasoline to alcohol.

Thermofluid and chemical kinetics models of the two-stroke engine were developed during this consulting contract which simulate the engine processes from the point of air induction to the exhaust. It includes air-fuel charging by carburetion and throttle control, intake and exhaust product mixing, compression, combustion, and cylinder scavenging. Flame speed and heat transfer considerations are structured to allow for matching to specific engine configurations. Combustion kinetics reveals the mechanisms of instability and allows the prediction of the unstable combustion domain and the influence of operating parameters on that domain.

A key modeling factor is shown in this study to be the ratio of mixing of the exhaust residual and the fresh charge during the exhaust/intake process.

The model has been tuned to a specific engine and a set of operating conditions and the model's results are compared with the experimental evidence. A culmination of this comparison is the model's chemical kinetics prediction of hot gas ignition which represents an experimentally observed combustion instability.

The duration of this activity is from May 1, 1987 through October 31, 1987.

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## INTRODUCTION

Historically, the two-stroke, spark ignited engine has been used extensively for personal transportation because of its high horsepower to weight ratio and easy maintenance. Today it remains popular in many countries that do not have emission controls. However in its historic form with the lubricating oil mixed in the fuel and the fuel mixed in the engine's scavenging air, it suffers from poor fuel economy and excessive hydrocarbons (HC) and carbon monoxide (CO) emissions. The fuel delivery system for the Indian two-cycle, spark ignited engine is in need of redesign. This is based on its expected growth in use (production exceeding 5 million per year in the 1990's) and its accompanying excessive pollution (a 150 cc, two-cycle vehicle produces hydrocarbon and carbon monoxide pollution levels approximating 10 American cars on a per mile basis).

There are several possible ways of enhancing the performance and suppressing the emissions from two-cycle engines. Switching fuels from gasoline to methanol is one possibility since methanol is relatively unreactive photochemically in comparison to gasoline. This change alone would reduce photochemical smog. However, if the conversion is combined with modern technology in terms of electronically controlled fuel injection the improvement could make the two-cycle spark-ignited engine competitive with the four-cycle engine in terms of performance and emissions [1]\*.

Early dynamometer studies with two-cycle engines converted to run on methanol have shown some combustion instabilities at high speeds and light loads which can result in poor performance and high emissions [2]. This is believed to be caused by premature ignition by hot residual gases in the cylinder. Such phenomena must be understood and eliminated.

In order to study improvements in fuel delivery systems and the related fuel-air exhaust mixing and underlying processes occurring within a two-stroke engine, a computer simulation of the basic thermofluid processes has been developed. This model can be matched to specific engine performance and then used for design studies associated with improved gasoline performance as well as those associated with converting the engine to methanol. Subsequent inclusion of chemical kinetics in the model allows study of the premature or hot gas ignition problem [3].

The opportunity to develop a mathematical model of the two-stroke cycle engine arose through the authors' participation in an NSF project at Santa Clara University and the UNIDO project at the Indian Institute of Petroleum at Dehra Dun. One aspect of this project is to develop and establish suitable technologies for the utilization of alcohol as an alternative fuel in two-stroke spark-ignited engines. The development of a

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\*References at the end of this report.

mathematical simulation of two-stroke engine working processes to optimize two-stroke engines for methanol usage is a part of the project. The first phase of the simulation study was begun by L. Browning in early August 1986 with funding from the National Science Foundation. The work funded by UNIDO began in the United States on September 17, 1986 and continued in India until October 29, 1986 [4].

The second phase of the study began in the U.S. on May 1, 1987. During the three weeks home-base assignment, a chemical kinetics model was developed that would examine both normal and abnormal combustion. This model required data to be generated from the thermofluids engine model developed in the first phase of the project. The model was debugged and three initial runs were made. In addition several modifications were made to the first model to facilitate the marriage of the two models and to better simulate the two-stroke engines used in India.

It was expected that during the 7 1/2 month period between the first and second phases of the study that the Indian Institute of Petroleum (IIP) engineers would modify the engine model to simulate their test engine as they had all the coding to do this. They could have tuned the model's empirical equations to their test engine data as well. This was not done due to the fact that the execution time for the model on the IBM 370 at the Institute of Petroleum Exploration (IPE) was approximately 1 hour even though runs on a personal computer required only two hours. Attempts by IIP engineers to increase step-size resulted in instabilities. Furthermore, attempts to modify the model, as they were directed, to include the rotary valve intake port found in their test engines resulted in failure. They had, however, reproduced the initial test run that was left with them.

In returning to India, Browning brought a revised thermofluids model and the new chemical kinetics model, as well as input data, on magnetic tape. The Indian portion of the second phase of the project began June 10, 1987. After a short briefing in New Delhi, Browning traveled to Dehra Dun and began work with the IIP engineers.

The first endeavor was to remove the programs from tape and install them on the IPE computer. This required much time as Browning was not allowed access to IPE due to a new policy and had to work through Mr. Semvol of IIP. This allowed for only one run per day resulting in slow progress.

During this period Browning worked with Mr. Abraham of IIP, describing to him how the kinetics model was developed and how it was used. In addition the thermofluids model was reviewed. Mr. Abraham suggested that heat transfer be added to the crankcase node of the thermofluids model, as this was a significant variable. Also in working with the initial run output of the model, Pefley, who had arrived at Dehra Dun on June 23, discovered that a more accurate mass accounting of the liquid fuel was required since there was no temperature drop for vaporization in the intake

node as there should be. In addition, a request was made to reduce run time for the thermofluids model. These modifications were made to the models as described in Section III.

During this time, Mr. Abraham of IIP was also trained on modeling techniques and how to tune the computer models to the existing engine data taken in the laboratory. In addition, experimental data was chosen for this purpose. Initial runs for both thermofluid and kinetic models in both the normal and abnormal combustion modes were set up for execution and initiated. At the time of Browning's departure from India, the kinetics model was running correctly, but the thermofluids model required some additional changes as Pefley's analysis of the thermofluid model had revealed some additional mass-energy discrepancies that needed attention. These modifications were done upon returning to the U.S.. In addition, the models were also transferred to 8" floppy disks so that they can be adapted for use on IIP's small computer system. Both the 8" diskettes and magnetic tape are being forwarded with this final report, albeit separately.

## RECOMMENDATIONS

1. In order to improve the predictive accuracy of the model, it is recommended that its tuning relative to the actual engine be extended to cover a full range of normal combustion and knocking conditions. Such a model would include improved matching of scavenging ratio, evaporated fuel fraction and the pressure-crank angle relationship.
2. In order to fully realize the purpose of this project, a detailed study of knock in the two-stroke engine is strongly suggested. By studying the reasons and conditions responsible for causing knock, the engines can be redesigned to eliminate knocking.
3. Ways of reducing exhaust emissions of two-stroke engines which use gasoline and/or methanol fuel should be examined.
  - (a) A study of scavenging with a view to improving the process is recommended. Wave mechanics should be added to the thermofluids model to enable such a study. The model can then also be used to optimize engine port sizes and locations to reduce fuel short-circuiting.
  - (b) Fuel short-circuiting can also be reduced by the use of port fuel injection or in-cylinder fuel injection. These options should be investigated.



## I. THE COMPUTER MODELS

The two models developed to simulate the 2-stroke engine working processes are the thermofluids and chemical kinetics models. They are companion models as the chemical kinetics model utilizes the data from the thermofluids model as part of its input program.

### A. The Thermofluids Model

This model simulates the fluid dynamic and thermodynamic processes occurring within a typical two-stroke engine. The model assumes that the liquid fuel occupies negligible volume and vaporizes as it is swept, at air velocity, along the intake runner. The model also assumes that it continues to vaporize during crankcase compression and the partially vaporized fuel mixture is then swept into the cylinder at air velocity. It is also assumed that fuel vapor is saturated at gas temperature and that vaporization and droplet heat transfer occur instantaneously to reach this condition at each time step. Furthermore, it is assumed that the mixture is homogeneous within a given node. Heat transfer occurs between the mixture and the engine surfaces.

The model is broken into seven distinct nodes as shown in Fig. 1. These nodes are (1) the intake manifold after the throttle, (2) the crankcase, (3) the transfer duct, (4) the cylinder, (5) the exhaust port area, (6) the exhaust pipe, and (7) the tailpipe. Conservation equations for each node have been derived using basic thermodynamic and fluid dynamic principles.

### Modifications to the Thermofluids Model

The thermofluids model required several modifications as a result of the first and second visits to India. The modifications carried out prior to the second visit involved adding the equations and coding to simulate a rotary valve intake ported engine and a piston ported intake engine as well as the reed valve simulation that was originally in the model. In addition, special output statements were written to provide the data needed by the chemical kinetics model.

Upon Browning's arrival in India in June of 1987, several requests were made to extend the heat transfer analysis to include the crankcase node and to reduce computation time for the model. Heat transfer equations were derived and coded into the model at the crankcase node. Run time was reduced by reducing the number of species used in calculations in the equilibrium combustion and expansion phases of the model and by increasing the time step used for cylinder computations during combustion and expansion. This reduced computation time by a factor of 2, with little or no reduction in accuracy.

Subsequently Pefley discovered that the liquid fuel mass was not totally accounted for in the model. Improved liquid fuel modeling was added. In addition, the prior logic of allowing vaporization up to the saturation point or condensation down to the saturation point led to instabilities in the calculations. Initially the model would vaporize sufficient liquid fuel to bring the gaseous fuel partial pressure to the saturation pressure at the node temperature. This caused a large reduction in temperature, thereby lowering the saturation pressure at the node temperature and requiring condensation of liquid fuel on the next time step. This condensation raised the node temperature, consequently requiring vaporization on the next time step. This oscillation caused the model to become unstable. This was corrected by allowing vaporization to the saturation point. If gaseous fuel pressure is larger than saturation pressure, no vaporization or condensation is allowed. By this technique the instability was eliminated yet the saturation pressure-temperature relationship was preserved. With this model stability the large temperature reduction in the intake node appeared as expected. Due to these corrections in the model, mass and energy balances at each node now account for all the mass and energy entering or leaving the system as shown in Table I. It should be noted that these corrections caused the saturated vapor pressure computed to be lower than the actual vapor pressure in the crankcase during induction of fresh mixture into the crankcase. This difference was up to .07 atmospheres or 50% of the actual vapor pressure for the case of a fully open throttle position. However, when viewed as a temperature difference this translates to only a 7 K difference and should not affect the overall modeling significantly.

Before tuning the model to experimental data, it was first brought into dimensional compatibility with the engine used in the experiment (see Table II for test engine dimensions and model tuning conditions). Upon initial tuning of the model to the experimental data, it was found that with the spark plug modeled in the center of the combustion zone, it did not correctly simulate the calculated burning pattern from the measured pressure trace. By modifying the burning pattern to a side spark plug model, which agrees with the actual engine configuration, the pressure versus crank angle evidence was brought into more reasonable alignment.

#### Tuning the Model to Experimental Data

Using all of the data obtained from the Bajaj Chetak engine connected to a dynamometer and instrumented to record temperatures and pressures during the engine cycle, the model's flame propagation equations were totally tuned. First the model's flame propagation equations were adjusted until the model's predicted mass fraction burned curve matched that of the actual engine. As mentioned previously, the model had to be modified from the center spark plug burning pattern to a side spark plug burning pattern in order to get good agreement between model and experiment. As shown in Fig. 2, the match between the actual and predicted mass fraction burned curves for the experimental test point are satisfactory.

The model's heat transfer equations were then adjusted to predict the overall horsepower measured from the engine. The horsepower comparison is directly related to the pressure crank angle evidence and an acceptable comparison of pressures after adjusting the model for burning rate and heat transfer is shown in Fig. 3. The match during most of the cycle is very good; however, the model produces a higher peak pressure than the actual engine. Table III shows a general comparison between the experimental data and the results from the model run. As can be seen from this table, the model's predictions are fairly close. The model was then considered to be tuned at least to one point of experimental data. Further matching to other conditions would improve the accuracy of the predictions, but lack of time has allowed tuning to only one engine condition.

### B. Chemical Kinetics Model

The chemical kinetics model\* was developed for study of both normal and abnormal combustion processes. It simulates a well-stirred reactor which allows mass addition or removal, volume changes and heat transfer. The temperature of the incoming charge can also be varied. By applying this model in different modes, it can simulate either the burned or unburned segment during the combustion process, or the burned charge during the expansion process. Two methanol reaction sets are supplied to model both low and high temperature oxidation of methanol. They are shown in Tables IV and V. The high temperature reaction set, Table IV, is used in both the burned segment during combustion and the expansion processes. The low temperature reaction set, Table V, is used in the unburned segment combustion process.

Study of normal combustion is examined by applying the model in the burned segment combustion mode. In this mode, the burned segment is modeled as a growing well-stirred volume with unburned mass surroundings. Segment volume, mass consumption rate, heat transfer rate and temperature of the unburned charge versus time equations are integrated over time until the flame has consumed all the unburned mass. The high temperature reaction set is used for kinetic calculations. This mode can be used to study kinetic reactions occurring in normal combustion, pollutant formation and lean burn flameout.

The expansion process is studied next by applying the model in the burned charge expansion mode. This mode is modeled as a well-stirred reactor of increasing volume with heat transfer. This starts at the end of the combustion process and continues until the exhaust valve opens. The time variation of volume and heat transfer rate are obtained from the thermofluids model. The high temperature reaction set is also used for this mode. This mode can be used to study pollutant reaction freezing and reduction of radicals as the charge expands.

\*A description of the organization of the chemical kinetic model program is given in Appendix A.

Finally abnormal combustion can be studied during the combustion process by applying the model to the unburned segment during the combustion mode. This is modeled as a well-stirred reactor with decreasing volume and mass, but no heat transfer. This process begins with flame initiation and ends at the end of the combustion process. If combustion of the unburned charge is shown during this run, knock is predicted. Again volume and mass consumption rate versus time curves are obtained from the thermofluids model run. The low temperature reaction set is used for this mode. Knock can be shown to occur with this model if unburned temperatures reach high enough levels.

After coupling the kinetics model to the thermofluids model, it and the thermofluids model were used to:

- a. predict performance variation with throttle opening;
- b. predict emissions for the model tuning test point;
- c. predict spontaneous ignition by hot gas containing radicals found in the exhaust gases.

## II. DISCUSSION OF RESULTS

The predicted performance of the engine with variation in throttle setting is shown in Fig. 4. The full throttle ( $2.27 \text{ cm}^2$ ) values in the graph correspond with the predicted values of Table III. This condition will be discussed next.

First note that the engine speed and equivalence ratio are identical. The difference of +2% in indicated horsepower is to be expected because of the cylinder pressure-crank angle matching as previously discussed.

The predicted fuel economy of the model (10% lower isfc) is significantly better than the actual engine. This 10% difference in isfc translates to approximately a 20% difference in thermal efficiency because of the difference in heating values of the M-90 and M-100. These differences between the engine and its model are primarily related to the values of the scavenging ratio. The 10% higher scavenging ratio for the engine means that more fuel is lost by the engine in the scavenging process. This agrees with the relative unburned fuel evidence.

The total comparison of exhaust products agrees well between the engine and its model but the scavenging ratio difference should be more closely aligned before conducting parametric comparisons.

The model's parametric excursion over the part load range as shown in Fig. 4 appears reasonable. A meaningful near term experimental program would be to overlay experimental evidence on this family of curves.

A major argument for the creation of the mathematical model is the need to understand "hot gas" ignition as it relates to methanol usage in two-cycle engines. As previously mentioned, the loss of combustion control associated with a flame front moving smoothly from spark ignition has been experimentally observed. If such a phenomenon could be observed at a match point in the mathematical model it could prove invaluable as a cost reduction tool for parametrically studying the mechanisms and precursors.

Figures 5 and 6 reveal the first model evidence of hot gas ignition. A fully closed throttle position with throttle area of  $0.25 \text{ cm}^2$  was used in the run shown in these figures. The pictorializations are from a well stirred pool of unreacted gas that is experiencing the effects of an approaching flame front. In Fig. 5 the variation of the mole fractions of some key species, methanol ( $\text{CH}_3\text{O}$ ), formaldehyde ( $\text{CH}_2\text{O}$ ), CO, and  $\text{H}_2$ , and temperature with crank angle clearly show the onset of "hot gas" ignition. In Fig. 6 the contrast between the temperature predicted by equilibrium thermodynamics ( $T_{\text{Equilibrium}}$ ) and that produced by the chemical kinetics program ( $T_{\text{Kinetic}}$ ) stand in clear contrast. Clearly the model is predicting ignition within the unburned gas pool.

This early evidence of "hot gas" ignition from the computer model is exciting and deserves extensive study. One very important observation is made here.

In early discussions it was not certain whether "hot gas" ignition was primarily a consequence of the presence of radicals in the gas pool or the temperature or a combination of both. The computer indicates very low concentrations of radicals hence, it is clear that ignition in this case is a consequence of temperature. This evidence corroborates experimental findings that also show that hot gas and not radicals are the cause of ignition [5].

### III. CONCLUSIONS

In summary, a mathematical model of the thermofluid processes of a Bajaj Chetak two-cycle engine has been successfully generated and tuned to match a specific engine operating point. It has been coupled to two different chemical kinetic reaction sets: one for high temperature gas regions and the other for low temperature gas regions. The former is useful for studying normal combustion and the latter for studying low temperature phenomena such as "hot gas" ignition.

The model has been used to show the effect of throttle variation on engine performance parameters and has been shown to predict the phenomenon of "hot gas" ignition.

Further utility of the model awaits transfer of the logic to the computer facilities available to the Indian Institute of Petroleum.

## APPENDIX A

## CHEMICAL KINETICS PROGRAM ORGANIZATION

The chemical kinetics program is organized into the following four sections: (1) control, (2) input/output, (3) chemical kinetics, and (4) numerical integration. The following sections describe the function of each program section and of each subroutine in each section. The names of non-standard entry points into a subroutine are given in parentheses following the subroutine name.

Control Section

The main program of TWOKIN is the control section. It provides the problem set up through a series of subroutine calls. It also monitors the numerical integration and provides an output call whenever a print station is reached.

Input/Output Section

This section provides for the reading, converting and writing of all input data and kinetic results. It also performs all the necessary bookkeeping functions such as building tables, setting switches and storing data for later use.

KINP (RINP) - Provides for the processing of all input data. It initializes, sets all standard options, reads input data, calculates reference conditions, builds tables and curve-fits them for later interpolation.

BLOCK DATA - Contains, in block data format, the master species list and molecular weight of each species in that list. It also contains alphanumeric data for testing and output.

INIT - Reads the initial conditions for the kinetics run.

OUTP (OUT1, OUT2, OUT3) - Provides all output. It calculates parameters which are required only as output such as total entropy and net energy exchange rates.

Chemical Kinetics Section

The calculation of all chemical and state parameters is performed in this section. In particular, thermodynamic functions are evaluated, reaction and species production rates are computed and required partial and total derivatives are calculated.

PRED (PRED1) - Performs all necessary pre-derivative calculations. This routine calls for or computes directly the thermodynamic properties, reaction rates, equilibrium constants, pressure and specific heat ratio as



well as other parameters required for the calculation of derivatives.

DERV - Calculates all partial and total derivatives with respect to time.

PARD - Calculates all partial derivatives with respect to all chemical and state variables.

THRM - Computes the (dimensionless) thermodynamic properties  $h_i/RT$ ,  $G_i/RT$ ,  $S_i/R$ ,  $Cp_i/R$  and  $(dCp/dT)_i/R$  from polynomial curve fits.

CUBS (CINP) - Provides for the calculation of the assigned variable and its derivatives. If the assigned variable is specified by a table, then the variable and its derivatives are computed by a cubic spline interpolation.

### Numerical Integration Section

This section sets up and solves the implicit equations, computes the relative error, and performs the step-size optimization at each step. It contains the automatic species elimination calculations for omitting from error considerations these species with non-representative errors.

INTE (INTI, INTC, INTG) - Provides control of the numerical integration procedure during each step. It calls for the implicit equations to be set up and solved, checks for restart conditions, and calls for the step-size optimization.

CASM (CASI, CASG) - Sets up the implicit equations as an augmented matrix, calls for the solution, and updates all dependent variables after the increments have been calculated.

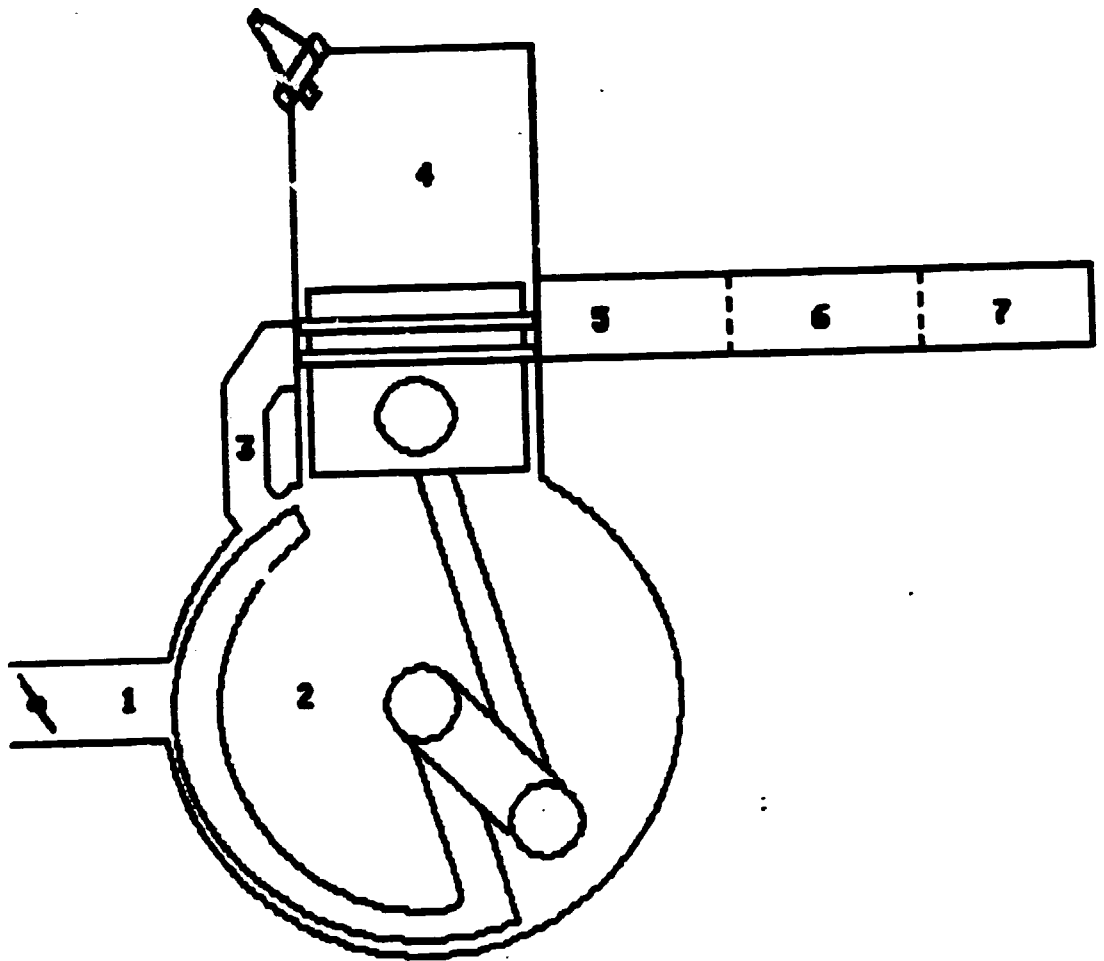
LESV - Solves the implicit equations for increments  $K_{i, n+1}$  using the matrix provided by CASM.

ERROR - Computes the relative error and determines the controlling variable at each step.

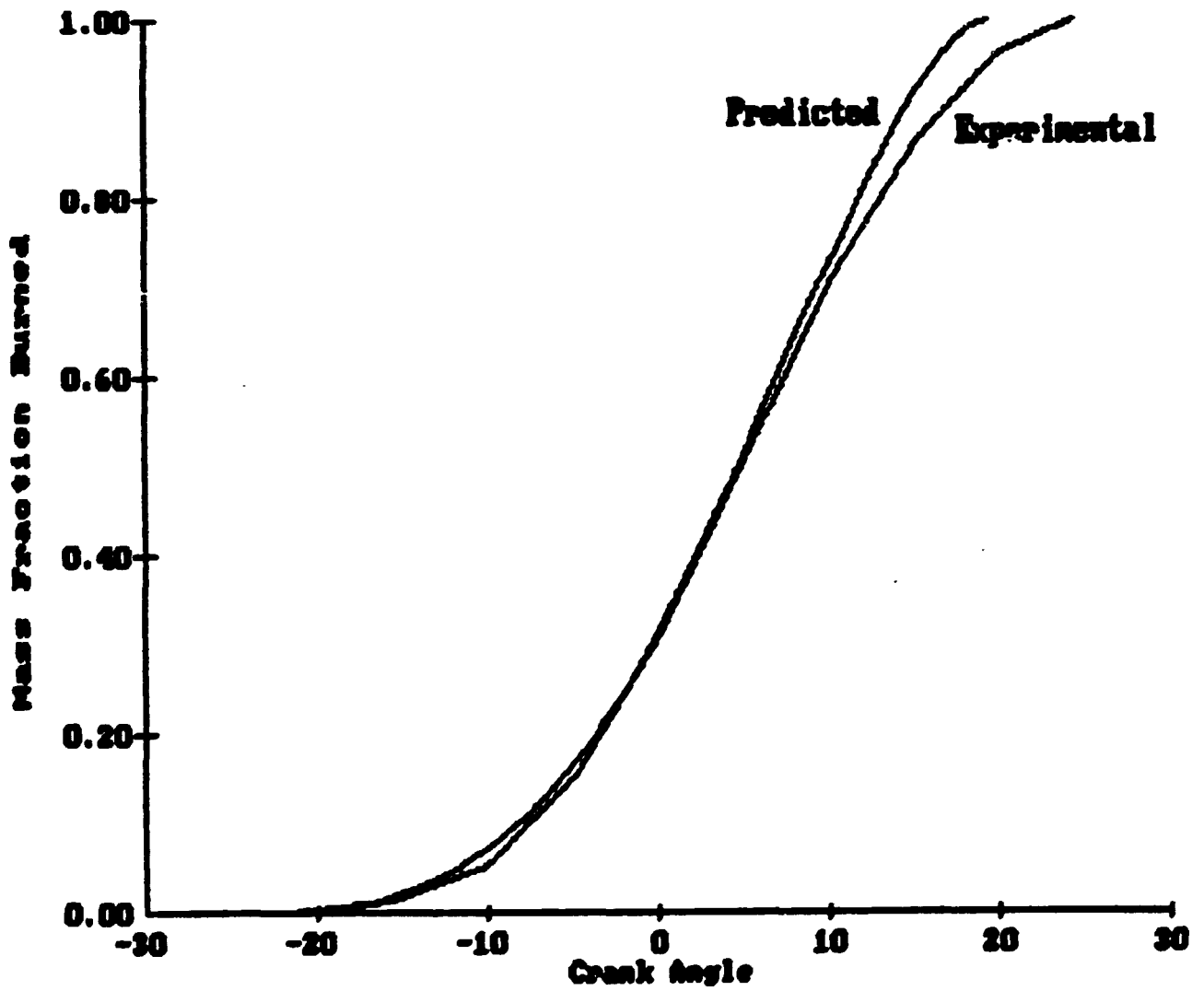
PERR - Provides an approximate error for any assigned step size by optimizing an approximate solution of the implicit equations. This routine is used in the step-size optimization procedure to predict the error which can be expected from any given step size.

AUTO - Provides for automatic elimination from error considerations of species with non-representative errors. A species error  $E_i$  is considered to be non-representative if  $E_i > 15 * E_m$  where  $E_m$  is the median of the errors associated with those species which have not been permanently neglected from all error considerations.

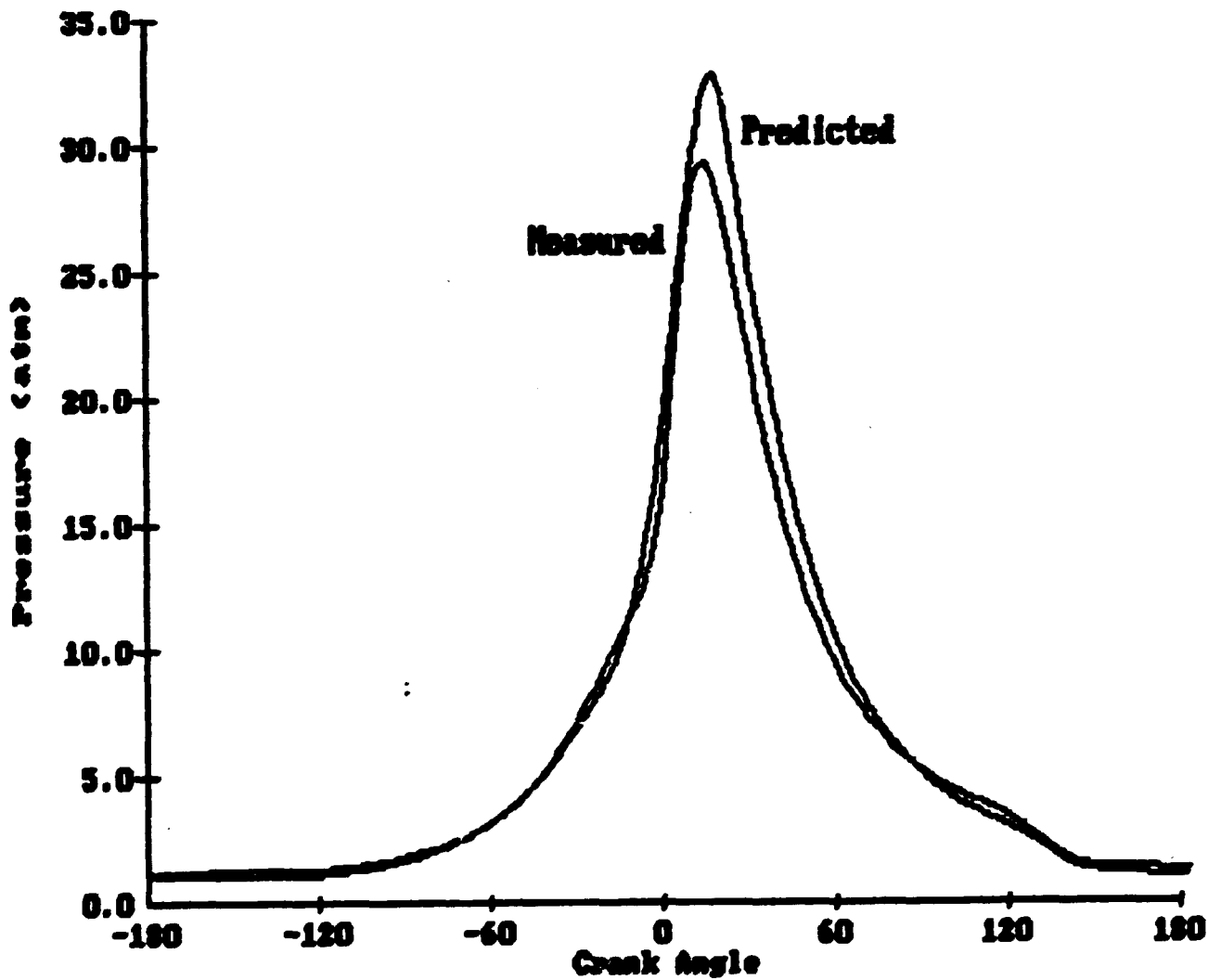
SEARCH - A sequential direct search routine which is used in the step-size optimization procedure.



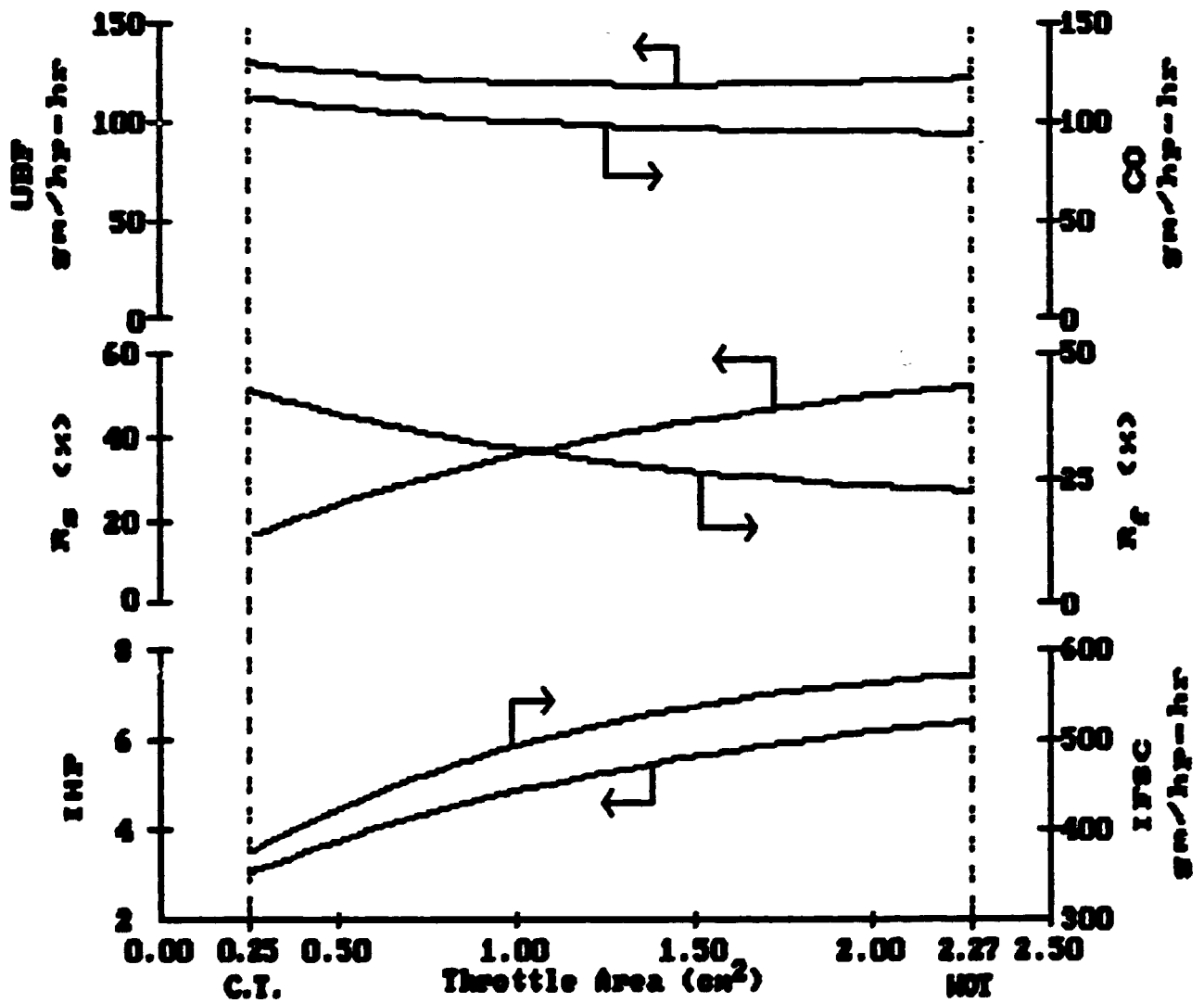
**Figure 1: Node Schematic of Engine Model**



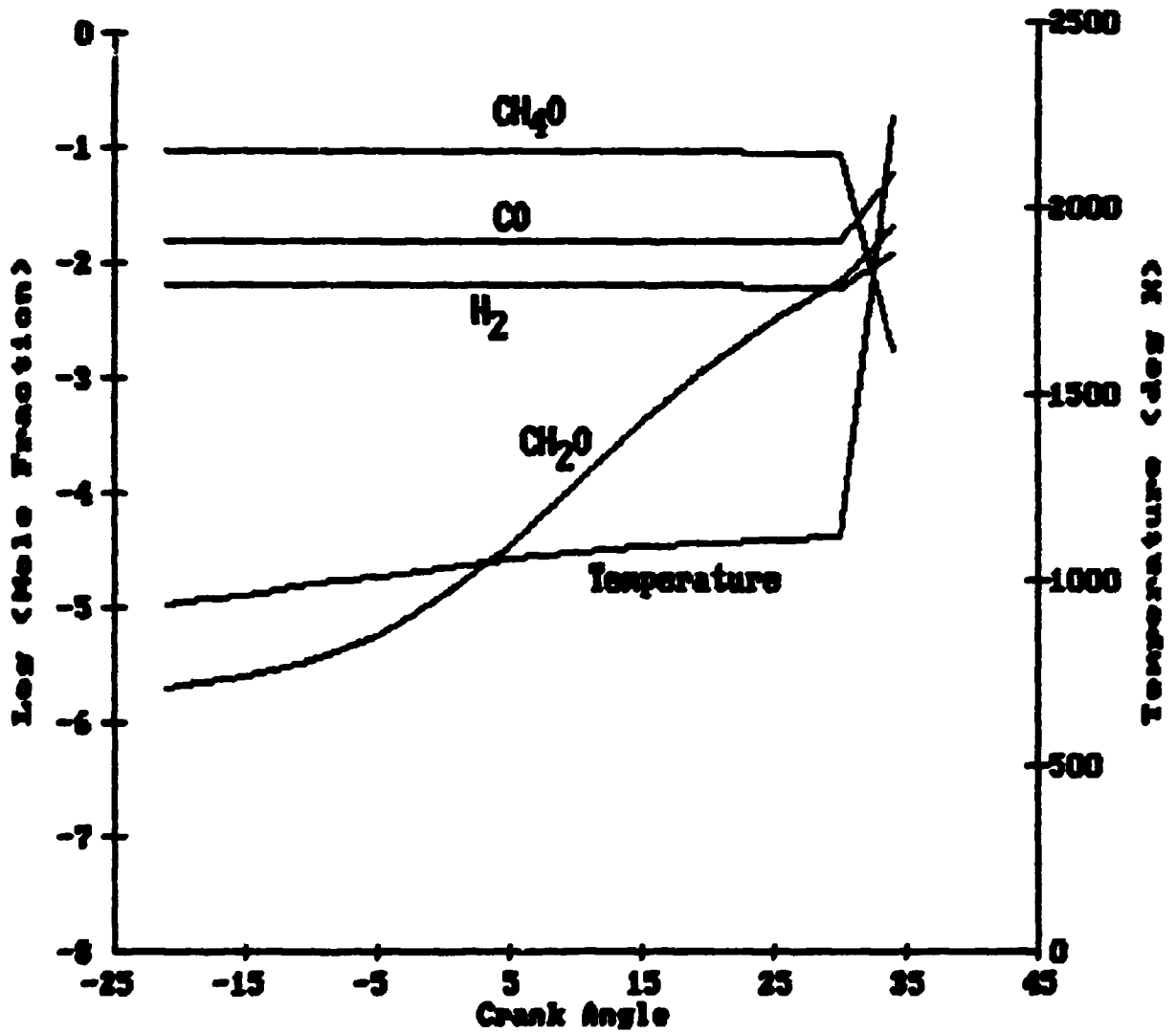
**Figure 2: Comparison of Predicted with Experimental Mass Fraction Burned (See Table II for Engine Conditions)**



**Figure 3: Pressure versus Crank Angle after Adjusting Model for Burn Rate and Heat Transfer (See Table II for Engine Conditions)**



**Figure 4: Throttle Effects on Performance Parameters by Mathematical Model (See Table II for Engine Conditions)**



**Figure 5: End Gas Mole Fractions and Temp, Crank Angle for Closed Throttle**

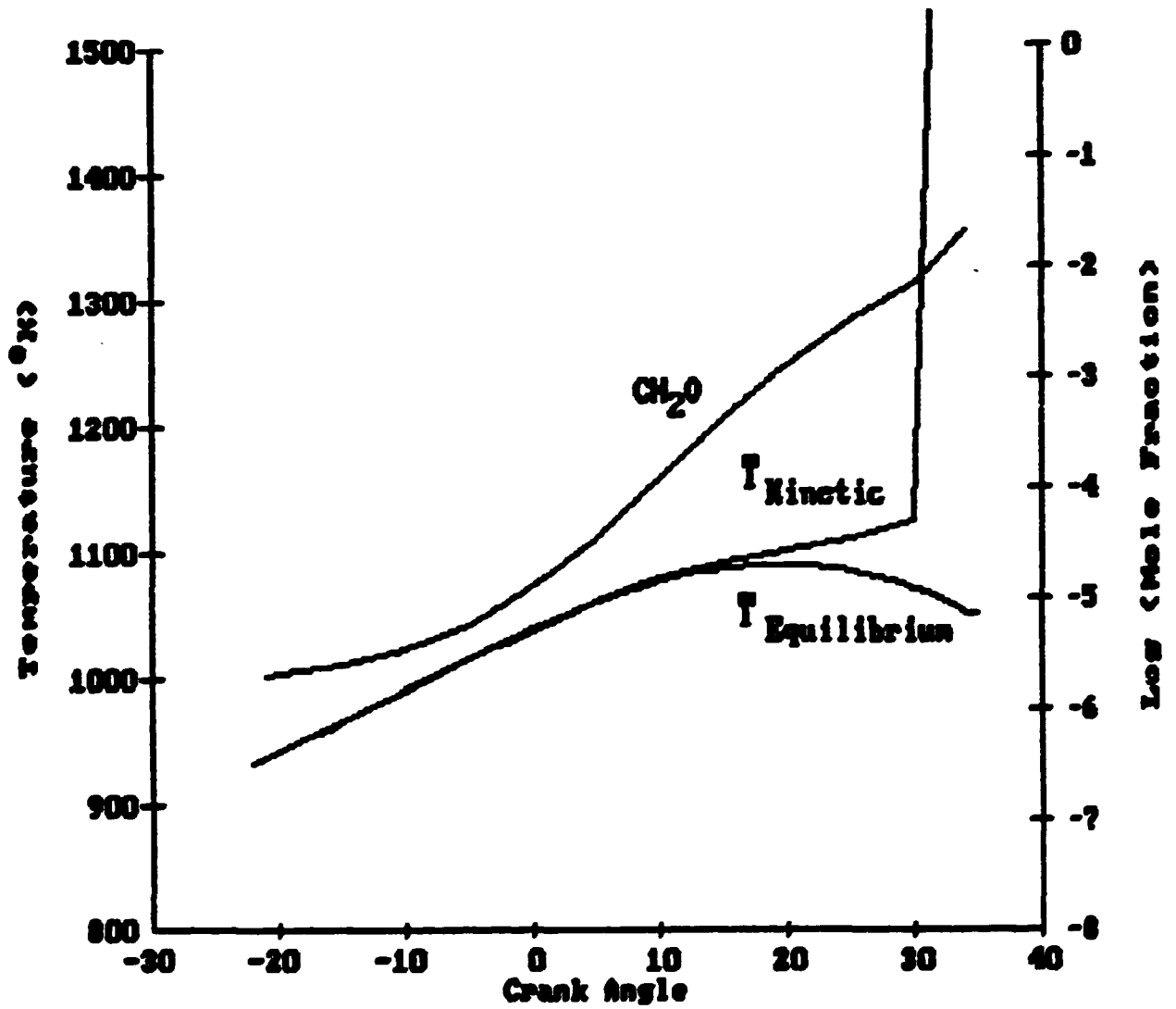


Figure 6: Temperature Contrasts for Chemical Kinetics and Thermal Equilibrium Models versus Crank Angle

TABLE I  
 MASS AND ENERGY ACCOUNTING

Node	Nodal Mass (gms)			Nodal Energy (cals)		
	Start	End	Change	Start	End	Change
1	0.022367	0.022270	-0.000098	-6.3113	-6.2860	0.0253
2	0.394830	0.392414	-0.002416	-101.7286	-101.2510	0.4776
3	0.065452	0.065079	-0.000373	-17.9762	-17.8979	0.0783
4u	0.090758	0.090278	-0.000480	-26.6747	-26.5824	0.0923
4b	0.034803	0.034762	-0.000042	-26.9425	-26.9067	0.0358
5	0.115725	0.115591	-0.000133	-82.6557	-82.4668	0.1889
6	0.895365	0.892420	-0.002945	-598.9126	-600.9518	-2.0392
7	0.011950	0.011923	-0.000027	-8.1026	-8.1408	-0.0382
	-----	-----	-----	-----	-----	-----
	1.631251	1.624738	-0.006513	-869.3041	-870.4834	-1.1794



TABLE II  
TEST ENGINE SPECIFICATIONS

Type	Bajaj Chetak 150
Bore, cm	5.70
Stroke, cm	5.70
Clearance Volume, cc	22.727
Compression Ratio	7.40
Crankcase Volume (min), cc	274.55
Exhaust Port Area, cm <sup>2</sup>	5.40
Exhaust Opens/Closes, °B/ABDC	68.0/68.0
Transfer Port Area, cm <sup>2</sup>	6.30
Transfer Opens/Closes, °B/ABDC	54.1/54.1
Intake Port Area, cm <sup>2</sup>	3.255
Intake Opens/Closes, °A/BBDC	64.0/130.5
Spark Energy, mJ	50.0
Spark Timing, °BTDC	22.0
Throttle Opening, cm <sup>2</sup>	2.27
Fuel Used	Liquid Methanol
Air/Fuel Ratio	5.7310
Ambient Pressure, atm	0.9370
Ambient Temperature, °K	290

TABLE III  
MODEL TUNING COMPARISONS

	Experimental	Predicted*	Percent** Difference
Fuel Type	M-90	M-100	
Engine Speed, rpm	4000	4000	
Indicated Horsepower	6.29	6.40	+1.7
ISFC, gm/ihp-hr	629.6	571.2	-10.2
Equivalence Ratio	1.122	1.122	
Scavenging Ratio	58.9%	53.7%	-9.7
<b>Emissions (dry):</b>			
CO	3.9%	4.3%	+10.3
CO <sub>2</sub>	10.2%	10.7%	+4.9
O <sub>2</sub>	5.3%	1.1%	-29.3
UBF	3.7%	3.1%	-19.4

\* Thermofluids model only

\*\* (Predicted - Experimental) x 100% / Experimental

TABLE IV  
HIGH TEMPERATURE REACTION SET

Reaction	Log <sub>10</sub> A <sub>j</sub>	n <sub>j</sub>	E <sub>j</sub>
M + CH <sub>2</sub> O	18.00	0.00	67.961
CH <sub>3</sub> + CH <sub>2</sub> O	11.26	0.00	9.817
O + CH <sub>2</sub> O	12.23	0.00	2.285
H + CH <sub>2</sub> O	13.11	0.00	5.306
OH + CH <sub>2</sub> O	14.48	0.00	5.962
CH <sub>2</sub> OH + O <sub>2</sub>	10.70	0.00	0.007
M + CH <sub>2</sub> OH	14.40	0.00	29.013
CH <sub>4</sub> + OH	14.78	0.00	12.499
CH <sub>4</sub> + H	4.35	3.00	8.744
CH <sub>4</sub> + O	13.32	0.00	9.061
CH <sub>3</sub> + O	14.00	0.00	0.000
CH <sub>3</sub> + O <sub>2</sub>	10.30	0.00	0.000
CH <sub>2</sub> O + O <sub>2</sub>	14.73	0.00	6.299
CH <sub>2</sub> O + OH	13.13	0.00	3.756
CH <sub>2</sub> O + H	13.70	0.00	4.570
M + CH <sub>2</sub> O	14.00	0.00	36.763
HCO + OH	14.00	0.00	0.000
HCO + H	14.30	0.00	0.000
HCO + O	14.00	0.00	0.000
M + HCO	14.70	0.00	19.017
H <sub>2</sub> + OH	14.46	0.00	10.989
OH + HO <sub>2</sub>	12.78	0.00	0.000
O + H <sub>2</sub>	14.51	0.00	14.983
H + O <sub>2</sub>	14.64	0.00	16.792
OH + OH	13.74	0.00	6.995
CO + OH	14.60	0.00	40.000
H + HO <sub>2</sub>	14.40	0.00	1.888
H + OH	21.92	-2.00	0.000
H + O <sub>2</sub>	15.18	0.00	-0.994
N + NO	13.49	0.00	0.334
N + O <sub>2</sub>	9.81	1.00	6.250
N + OH	13.51	0.00	0.000
H + N <sub>2</sub> O	13.48	0.00	10.800
O + N <sub>2</sub> O	13.56	0.00	24.000
O + N <sub>2</sub> O	13.70	0.00	24.000
N + O	16.81	-0.50	0.000
M + N <sub>2</sub> O	15.30	0.00	57.640
NO + HO <sub>2</sub>	13.00	0.00	0.000
NO <sub>2</sub> + H	14.86	0.00	1.930
O + NO <sub>2</sub>	13.28	0.00	1.060
Nu <sub>2</sub> + CO	12.28	0.00	29.260
N + N	14.85	0.00	0.000
H <sub>2</sub> + NO <sub>2</sub>	9.30	0.00	18.000
NO + O	15.04	0.00	-1.870

$k_j = A_j T^{n_j} \exp(-E_j/RT)$  moles/cc/sec  
E<sub>j</sub> in kcal/s/mole

TABLE V  
 LOW TEMPERATURE REACTION SET

Reaction	$\log_{10} A_j$	$n_j$	$E_j$
M + CH <sub>2</sub> O <=> CH <sub>3</sub> + OH	18.50	0.00	80.000
CH <sub>2</sub> O + O <sub>2</sub> <=> CH <sub>2</sub> OH + HO <sub>2</sub>	13.60	0.00	50.900
CH <sub>2</sub> O + OH <=> CH <sub>2</sub> OH + H <sub>2</sub> O	12.60	0.00	2.000
CH <sub>2</sub> O + O <=> CH <sub>2</sub> OH + OH	12.20	0.00	2.300
CH <sub>2</sub> O + H <=> CH <sub>2</sub> OH + H <sub>2</sub>	13.50	0.00	7.000
CH <sub>2</sub> O + H <=> CH <sub>3</sub> + H <sub>2</sub> O	12.70	0.00	5.300
CH <sub>2</sub> O + CH <sub>3</sub> <=> CH <sub>2</sub> OH + CH <sub>4</sub>	11.30	0.00	9.800
CH <sub>2</sub> O + HO <sub>2</sub> <=> CH <sub>2</sub> OH + H <sub>2</sub> O <sub>2</sub>	12.80	0.00	19.400
M + CH <sub>2</sub> OH <=> CH <sub>2</sub> O + H	13.40	0.00	29.000
CH <sub>2</sub> OH + O <sub>2</sub> <=> CH <sub>2</sub> O + HO <sub>2</sub>	12.00	0.00	6.000
M + CH <sub>4</sub> <=> CH <sub>3</sub> + H	11.10	0.00	88.400
CH <sub>4</sub> + H <=> CH <sub>3</sub> + H <sub>2</sub>	14.10	0.00	11.900
CH <sub>4</sub> + OH <=> CH <sub>3</sub> + H <sub>2</sub> O	3.50	3.08	2.000
CH <sub>4</sub> + O <=> CH <sub>3</sub> + OH	13.20	0.00	9.200
CH <sub>4</sub> + HO <sub>2</sub> <=> CH <sub>3</sub> + H <sub>2</sub> O <sub>2</sub>	13.30	0.00	18.000
CH <sub>3</sub> + HO <sub>2</sub> <=> CH <sub>2</sub> OH + OH	13.20	0.00	0.000
CH <sub>3</sub> + OH <=> CH <sub>2</sub> O + H <sub>2</sub>	12.60	0.00	0.000
CH <sub>3</sub> + O <=> CH <sub>2</sub> O + H	14.10	0.00	2.000
CH <sub>3</sub> + O <sub>2</sub> <=> CH <sub>3</sub> O + O	13.40	0.00	29.000
CH <sub>3</sub> + HCO <=> CH <sub>4</sub> + CO	11.50	0.50	6.000
CH <sub>3</sub> + HO <sub>2</sub> <=> CH <sub>4</sub> + O <sub>2</sub>	12.00	0.50	0.000
M + CH <sub>3</sub> O <=> CH <sub>2</sub> O + H	13.70	0.00	0.400
CH <sub>3</sub> O + O <sub>2</sub> <=> CH <sub>2</sub> O + HO <sub>2</sub>	12.00	0.00	21.000
M + CH <sub>2</sub> O <=> HCO + H	11.84	0.00	301.000
CH <sub>2</sub> O + OH <=> HCO + H <sub>2</sub> O	14.00	0.00	17.000
CH <sub>2</sub> O + H <=> HCO + H <sub>2</sub>	13.52	0.00	18.000
CH <sub>2</sub> O + O <=> HCO + OH	13.62	0.00	17.000
CH <sub>2</sub> O + HO <sub>2</sub> <=> HCO + H <sub>2</sub> O <sub>2</sub>	12.00	0.00	33.000
CH <sub>2</sub> O + CH <sub>3</sub> <=> HCO + CH <sub>4</sub>	10.00	0.00	8.000
HCO + OH <=> CO + H <sub>2</sub> O	14.00	0.00	0.000
M + HCO <=> H + CO	14.20	0.00	19.000
HCO + H <=> CO + H <sub>2</sub>	14.30	0.00	0.000
HCO + O <=> CO + OH	14.00	0.00	0.000
HCO + HO <sub>2</sub> <=> CH <sub>2</sub> O + O <sub>2</sub>	14.00	0.00	3.000
HCO + O <sub>2</sub> <=> CO + HO <sub>2</sub>	12.50	0.00	7.000
CO + OH <=> CO <sub>2</sub> + H	7.10	1.30	-0.800
CO + HO <sub>2</sub> <=> CO <sub>2</sub> + OH	14.00	0.00	23.000
CO + O <=> CO <sub>2</sub> + M	15.80	0.00	4.100
CO <sub>2</sub> + O <=> CO + O <sub>2</sub>	12.40	0.00	43.800
H + O <sub>2</sub> <=> O + OH	14.30	0.00	16.800
H <sub>2</sub> + O <=> H + OH	10.30	1.00	8.900
H <sub>2</sub> O + O <=> OH + OH	13.50	0.00	18.400
H <sub>2</sub> O + H <=> H <sub>2</sub> + OH	14.00	0.00	20.300
H <sub>2</sub> O <sub>2</sub> + OH <=> H <sub>2</sub> O + HO <sub>2</sub>	13.00	0.00	1.800
M + H <sub>2</sub> O <=> H + OH	16.30	0.00	105.100
H + O <sub>2</sub> <=> HO <sub>2</sub> + M	15.20	0.00	-1.000
HO <sub>2</sub> + O <=> OH + O <sub>2</sub>	13.70	0.00	1.000
HO <sub>2</sub> + H <=> OH + OH	14.40	0.00	1.900
HO <sub>2</sub> + H <=> H <sub>2</sub> + O <sub>2</sub>	13.40	0.00	0.700
HO <sub>2</sub> + OH <=> H <sub>2</sub> O + O <sub>2</sub>	13.70	0.00	1.000

TABLE V (Con't)  
LOW TEMPERATURE REACTION SET

Reaction				$\text{Log}_{10}A_j$	$n_j$	$E_j$
$\text{H}_2\text{O}_2$	+ $\text{O}_2$	$\rightleftharpoons$	$\text{HO}_2 + \text{HO}_2$	13.60	0.00	42.600
M	+ $\text{H}_2\text{O}_2$	$\rightleftharpoons$	$\text{OH} + \text{OH}$	17.10	0.00	45.500
$\text{H}_2\text{O}_2$	+ H	$\rightleftharpoons$	$\text{HO}_2 + \text{H}_2$	12.20	0.00	3.800
O	+ H	$\rightleftharpoons$	$\text{OH} + \text{M}$	16.00	0.00	0.000
M	+ $\text{O}_2$	$\rightleftharpoons$	$\text{O} + \text{O}$	15.70	0.00	115.000
M	+ $\text{H}_2$	$\rightleftharpoons$	$\text{H} + \text{H}$	14.30	0.00	96.000
H	+ NO	$\rightleftharpoons$	$\text{N} + \text{OH}$	14.35	0.00	50.500
O	+ NO	$\rightleftharpoons$	$\text{N} + \text{O}_2$	9.37	1.00	38.650
O	+ $\text{N}_2$	$\rightleftharpoons$	$\text{N} + \text{NO}$	14.26	0.00	76.250
NO	+ NO	$\rightleftharpoons$	$\text{N}_2\text{O} + \text{O}$	12.11	0.00	67.200
M	+ $\text{N}_2\text{O}$	$\rightleftharpoons$	$\text{N}_2 + \text{O}$	14.15	0.00	51.280
NO	+ H	$\rightleftharpoons$	$\text{HNO} + \text{M}$	15.73	0.00	-0.600
HNO	+ H	$\rightleftharpoons$	$\text{H}_2 + \text{NO}$	11.48	0.50	2.400
HNO	+ OH	$\rightleftharpoons$	$\text{H}_2\text{O} + \text{NO}$	12.48	0.50	2.400
M	+ $\text{NO}_2$	$\rightleftharpoons$	$\text{NO} + \text{O}$	16.04	0.00	65.000
$\text{NO}_2$	+ O	$\rightleftharpoons$	$\text{NO} + \text{O}_2$	13.00	0.00	0.596
NO	+ $\text{HO}_2$	$\rightleftharpoons$	$\text{NO}_2 + \text{OH}$	13.15	0.00	1.400
$\text{NO}_2$	+ H	$\rightleftharpoons$	$\text{NO} + \text{OH}$	14.54	0.00	1.470

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 $k_f = A_j T^{n_j} \exp(-E_j/RT)$  moles/cc/sec  
 $E_j$  in kcal/mole

## VI. REFERENCES

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