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MODELLING OF A FOUR STROKE DIESEL ENGINE OPERATED WITH HYDROGEN BLENDED FUEL

A Thesis

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BY

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جمهورية العراق

وزارة التعليم العالي

والبحث العلمي

جامعة بابل

نمذجة محرك ديزل رباعي الاشواط يعمل بخلط وقود الهيدروجين

رسالة

مقدمة إلى كلية الهندسة في جامعة بابل

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بكالوريوس هندسة ميكانيكية

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١٤٢٧هـ ٢٠٠٦م

بسم الله الرحمن الرحيم

نَرْفَعُ دَرَجَـتٍ مَنْ نَشَاءُ وَفَوْقَ
كُلِّ ذِي عِلْمٍ عَلِيمٌ۞

صدق الله العلي العظيم

سورة يوسف الاية-(٧٦)

الأهـداء

الـــى مــن أحــبهم قلبـــي.. رمــز المثــابرة وعنــوان التضحية

والديّ العزيزين .. بـراً واحساناً

الــى من شدوا أزري وساندوني.. رمز الايثار

أخوتي و أخواتي .. محبةً وعرفاناً

والـــى كل من يسره نجاحي

..امتناناً واعتزازاً

أهــدي هــذا الجــهد

محمد فاضل ثابت

٢٠٠٦/١/٢٢

الخلاصة

نتيجة للتوسع الهائل في أستخدام وسائط النقل المختلفة وتوليد الطاقة الكهربائية وفي الصناعة, أتجهت البحوث الحالية الى الاهتمام المتزايد بتصميم وتطوير محركات الاحتراق الداخلي لتحقق أعلى كفاءة وأفضل اداء للمحرك, وأقل انبعاث للملوثات, وكذلك لتقليل استهلاك الوقود لمعالجة مشكلة نضوب الطاقة. كذلك أهتم عدد من الباحثين بالبحث عن أنواع اخرى من الوقود غير القابل للنضوب, ويكون ملوثات قليلة عند الاحتراق, ويحسن كفاءة وأداء المحرك وأن هذا يمثل الاتجاه الحديث في مجال تطوير محركات الاحتراق الداخلي. يعتبر الهيدروجين في الوقت الحالي الوقود البديل المثالي لمحركات الاحتراق الداخلي وخلايا الوقود, حيث لايخلف انبعاثات كاربونية ويمتاز بخواص فيزيائية وكيميائية تؤهله للعمل كوقود جيد في محركات الديزل و البترول.

تضمن هذا البحث دراسة تاثير أضافة الهايدروجين بنسب وزنية مختلفة الى وقود الديزل على أداء و ملوثات محرك ديزل رباعي الاشواط يعمل بالانضغاط. وذلك بأعداد برنامج حسابي بلغة فورتران يعتمد على نموذج رياضي شبه بعدي متعدد المناطق.

يتم في هذا البرنامج حساب الضغط داخل الاسطوانة, درجة الحرارة لكل منطقة, معدل الطاقة المتحررة لكل منطقة, لثلاثة انواع من الوقود هي ديزل فقط, خليط من الديزل والهيدروجين, وهيدروجين فقط.

و تم في هذا البرنامج دراسة تاثير التفكك ومركبات التفاعل على تركيز نواتج الاحتراق في غازات العادم وعلى أداء المحرك.

لقد وجد من النتائج ان اضافة(١٢) ٪ من الهيدروجين تمثل القيمة المثالية والتي ادت الى رفع (قيم الضغط, الحرارة لكل منطقة والطاقة المتحررة) العظمى وهذا بسبب زيادة في كتلة الوقود المحترق ولهذا يقل الوقت اللازم لانهاء عملية الاحتراق.

ولقد وجد من النتائج ايضا ان اضافة (١٢) ٪ من الهيدروجين يؤدي انخفاض في تركيزي السناج و احادي اوكسيد الكاربون في غازات العادم. ان اضافة (١٢) ٪ من الهيدروجين اعطت اعظم انخفاض في تركيز السناج بنسبة (٣٣) ٪ وبنسبة (٦٥) % في تركيزاحادي اوكسيد الكاربون. وهذا منسوب الى انخفاض في تركيز ذرات الكاربون في غازات العادم. وكذلك ادت اضافة (١٢) ٪ الهيدروجين الى ارتفاع في تركيز اكاسيد النتروجين وهذا يعود الى الارتفاع في درجة الحرارة و الانخفاض في الوقت اللازم لتفكك اكاسيد النتروجين الى اوكسجين ونتروجين.

وبشكل عام, ان اضافة(١٠) % من الهيدروجين سببت زيادة في القدرة والكفاءة وسببت انخفاضا في معدل استهلاك الوقود بنسبة (٦٠)%. وقد أعطت هذه الدراسة تقارب كبير مقارنةً بالنتائج العملية والنظرية لعدد من الباحثين.

ABSTRACT

Considering energy crises and pollution problems today, investigations have been concentrated on reducing fuel consumption and lowering toxic component concentration in exhaust gases by using alternative sources of energy and/or alternative fuels. At present, hydrogen gas ($H_{٢}$) is being explored for use in internal combustion engines and fuel-cell. It is considered as the future fuel which is characterized with no unburnt hydrocarbon, carbon oxides or carbon particulate emissions. It is can be used either pure or mixed with gasoline or diesel fuels.

In the present work, the effect of hydrogen addition on the performance and emission of a Diesel engine has been studied. A multizone combustion model to simulate a four-stroke cycle of a Diesel engine fueled with hydrogen-Diesel mixture is developed. The effect of dissociation of combustion products and rate kinetics is accounted for in this model. A computer program written in Fortran ٩٠ Language has been accomplished to calculate the performance and emission levels in diesel engine working with three types of alternative fuels, i.e. Diesel, Diesel-hydrogen mixture and hydrogen fuel.

It is found that the addition of (١٢)% by mass of hydrogen is an optimum hydrogen/Diesel ratio. The addition of hydrogen causes an increase in the maximum (pressure, zonal temperature, and rate of heat release). This is due to the increase in the rate of mass burning, therefore, the time required to complete the combustion is reduced.

It is also found that the addition of (١٢)% by mass of hydrogen causes reduction in the soot and CO concentrations in the exhaust gases. The addition of (١٢)% of hydrogen produces the maximum reduction in soot (٣٣)% and CO (٦٥)%. This is attributed to the reduction in the carbon atoms concentration in the mixture of hydrogen-Diesel fuel. However, the NO_X concentration was increased due to the increase in the peak zonal temperature level caused by faster heat release and the reduction in the time required to dissociate NO to $N_{٢}$ and $O_{٢}$. However, operating engine with different lean mixtures was used to reduce the increase in the NOx concentration.

In general, the addition of (١٠)% of hydrogen by mass gives a maximum improvement in the power and efficiency and a maximum reduction in specific fuel consumption (٦٠)%. A very good agreement was obtained between the results and the available theoretical and experimental results of other researchers.

CERTIFICATATION

I certify that this thesis entitled **"MODELLING OF A FOUR STROKE DIESEL ENGINE OPERATED WITH HYDROGEN BLENDED FUEL "** was prepared by Mr. **MOHAMED FADHIL** under my supervision at **BABYLON UNIVERSITY** in partial fulfillment of the requirements for the degree of **Master of Science in Mechanical Engineering/ Power Engineering.**

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Nomenclature

The following symbols are used generally throughout the text. Others are defined as when used.

Symbol	Description	Units
A	Total Area of Cylinder	$m^{٢}$
B	Cylinder Bore	*mm*
C_D	Discharge Coefficient	-
d_n	Nozzle Diameter	*mm*
d_{32}	Sauter Mean Diameter	μm
dS/dt	Velocity of Zone	*m/sec*
dE_{comp}	Step Change of Internal Energy during Compression stage	*kJ*
$dE_{\exp}$	Step Change of Internal Energy during Expansion Stage	*kJ*
d_S	Soot Particle Diameter	*m*
dW	Step Change of Work in the system during Time Step	*kJ*
E	Total Internal Energy	*kJ*
E_{Sf}	Activation Energy of Soot Formation	*kJ/kmol*
E_{So}	Activation Energy of Soot Oxidation	*kJ/kmol*
$F_{i,j}$	Fuel Fraction in Zone (I,J)	-
h_c	Heat Transfer Coefficient	$W/m^{٢}.K$
kp	Equilibrium Constant	*atm*
L	Connecting rod Length	*mm*
Lr	Radiation Path Length	*mm*

m_f	Mass of Fuel in a Zone	*kg*
$m_{f,v}$	Mass of Fuel Vapor	*kg*
m_m	Mass of Entrainment Mixture in the Zone	*kg*
M_{NO}	Molecular Weight of NO	*g/mole*
N_d	Number of Droplets Contained within a Zone	-
P	Cylinder Pressure	*bar*
P_{ox}	Partial Pressure of Oxygen	*atm*
ΔP	Pressure Drop across the Injector Nozzle	*Mpa*
Q	Total Heat Transfer Rate	*kW*
Q_w	Heat Transfer Rate to the Cylinder Wall	*kW*
Q_{fg}	Total Heat Transfer Rate to the Liquid Fuel Droplets	*kW*
$Q_{radiation}$	Radiation Heat Transfer Rate	*kW*
$Q_{convection}$	Convection Heat Transfer Rate	*kW*
r_Z	Zonal Radius	*mm*
RRp	Heat Release during Premixed Combustion Phase	*J/degree*
RRm	Heat Release during Diffusion Combustion Phase	*J/degree*
S_t	Stroke	*mm*
T_l	Liquid Fuel Temperature	*K*
T_Z	Zonal Temperature	*K*
V_{Cyl}	Volume of Cylinder	$m^{۳}$
X_{fv}	Mass Fraction of Fuel Vapor	-
X_{ox}	Mass Fraction of Oxygen	-
Z	Correction Factor of Boundary Layer	-

Greek Symbols

Symbol	Description	Units
ε	Total Emissivity.	-
$\varepsilon_{\text{CO٢}}$	Gas Emissivity of Carbon Dioxide.	-
$\varepsilon_{\text{H٢O}}$	Gas Emissivity of Water Vapor.	-
ε_{s}	Soot Emissivity.	-
α	Spray Angle.	*degree*
β	Zonal Angle.	*degree*
ΔG_T	Change in Gibbs Free Energy of Formation per. mole at T and P.	*kJ*
τ	Ignition Delay.	*ms*
λ	Percent of Hydrogen Added.	*Kmol*

λ_f	Specific Heat of Vaporization of Liquid Fuel.	$kJ/Kmol$
ρ_S	Soot Density.	g/cm^3
μ_m	Mixture Viscosity.	$kg/ m.s$
μ_l	Viscosity of Liquid Fuel.	$kg/ m.s$
μ_a	Viscosity of Ambient Gas.	$kg/ m.s$
ϕ	Equivalence Ratio.	-
$\partial\phi/\partial t$	Equivalence Ratio Gradient.	$\sec^{-1}$
w	Local average gas velocity in the cylinder.	$[m/sec]$
δ	Stephan-Boltzman constant.	$W/m^{٢}. K^{٤}$
σ_f	Surface Tension of Fuel.	N/m
θ	Crank Angle.	*degree*
η_{th}	Thermal Efficiency.	-

SUBSCRIPTS

a	Air
b	Burned
c	Clearance
$C.V$	Control Volume
$comp$	Compression
cyl	Cylinder
d	Droplet
$disp$	Displacement
eq	Equilibrium

exp	Expansion
f	Fuel
fg	Gaseous Fuel
fv	Fuel Vapor
g	Gas Phase
H.t	Heat Transfer
i	Number of zone in the Axial Direction
ign	Ignition
inj	Injection
j	Number of zone in the Radial Direction
l	Liquid Phase
m	Mean
P	Products
R	Reactants
s	Soot Concentration
sf	Soot Formation
so	Soot Oxidation
stoi	Stoichiometric
tot	Total
u	Unburned
v	Vapor
w	Wall
z	Zone

SUPERSCIPTS

C	Exponent of pressure in equation (٣.٩٠)
j	Order of polynomial coefficient
o	Standard condition
.	Differentiating with respect to time.

ABBREVIATIONS

Comb.D.	Combustion Duration
DI	Direct Injection
Deg.	Degree
Eff.	Efficiency
LHV	Lower Heating Value
NTP	Conditions at Normal Temperature and Pressure
Nu	Nusselt Number
Pr	Prandtl number
Re	Reynolds Number
RR_P	Heat Release during Premixed Combustion Phase
RR_m	Heat Release during Mixing Controlled Combustion Phase
Sc	Schmidt Number
Sh	Sherwood Number
SMD	Sauter Mean Diameter
We	Weiber Number

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MOHAMED

January , ٢٠٠٦

EXAMINING COMMITTEE CERTIFICATE

We certify that we have read the thesis entitled "**MODELLING OF A FOUR STROKE DIESEL ENGINE OPERATED WITH HYDROGEN BLENDED FUEL"** and as an examining committee, examined the student **"MOHAMED FADHIL THABIT**", in its contents and that in our opinion it meets the standard of a thesis for the degree of Master of Science in Mechanical Engineering / Power Engineering.

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CHAPTER ONE

INTRODUCTION

١.١ General

Internal combustion engines have been in use for more than a century and have undergone tremendous changes in design, materials used and operating characteristics. Never once during their long history of development have they lost their importance as the planet ́s most widely used prime movers. It is a well-known fact that Diesel engine is one of the most fuel-efficient power producing units in use today. Hence, the importance of this type of engine has been long recognized, particularly in heavy duty engine applications. In the past few decades, research efforts have been focused largely on better engine design, from the perspective of reducing the pollutant emissions without sacrificing performance and fuel economy. Another driving force behind the need to design engines amenable to operate on non-conventional fuels is the rapid depletion rate of currently used fossil fuels.

The world reserves of primary energy and of raw materials are obviously limited. The enormous growth of the world population during the last decades and the strongly increased technical development and standard of living in the industrial nations has led to an intricate situation in the field of energy supply. It might be mentioned here that more than ninety percent of the present worlds energy demand is still supplied by the exhaustible fossil fuels (natural gas, oil, coal). It is well known that combustion of fossil fuel degrades the human environment causing air pollution in cities, acid rains buildup of carbon dioxide and changing the heat balance of the earth, etc------.

Anything can be done to save our environment is important, such as the substitution of fossil fuel in part or totally by a number of alternative energy sources, specially in automobiles. Several alternative fuels such as methyl alcohol, natural gas, bio gas, and hydrogen are being tried as possible substitutes for the Diesel fuel in compression ignition engine or petrol in spark ignition engine. The operation of diesel engines with alternative fuels, can be classified into two modes, multi-fuel and dual fuel. It's perhaps instructive to state the difference between the two. A multi-fuel engine is one in which two fuels may be separately used to produce power. On the other hand, in a dual fuel engine, two fuels are simultaneously employed.

Research on engines operating on alternative fuels has followed different directions due to different performance requirements and operation constrains. In this respect, regulations on emissions, which have become increasingly tough over the years, have provided renewed impetus to the search for practical alternative fueling concepts. However, the inability to achieve performance characteristics similar to those of traditional Diesel or gasoline engines under all operating conditions have imposed an important constraint on the potential for use of alternative fuels, because many alternative fuels have been tested for both petrol and Diesel engines with variable degree of success. Diesel engines owing to the typically high compression ratios employed, posses the potential to achieve high fuel conversion efficiencies and are ideally suited for operation on several alternative fuels.

The use of alternative fuels as an auxiliary fuel in Diesel engine such as methanol, ethanol, and biogas appear to promise significant improvement in NOx emissions and the combustion took place without misfiring or knocking. The combustion was smoother, with lower noise than with usual combustion with Diesel. The thermal efficiency was maintained at the same level as in conventional Diesel operation. But these fuels contain carbon atoms in its structure; hence carbon emissions are still in the exhaust gases.

Hydrogen is the most abundant in the universe. Over ٩٠ percent of all atoms in existence are hydrogen, but on earth, free hydrogen is rare. It is almost always bound together with atoms of other elements to make a wide variety of compounds. These include hydrocarbons like natural gas and, of course $H_{٢}O$-water.

Hydrogen gas ($H_{٢}$) is being explored for use in internal combustion engines and fuel-cells. It is considered as the future fuel without carbon oxides emissions. This fuel is very attractive substance for the role of the energy vector in many practical applications. While conventional energy sources such as natural gas, oil and coal are non renewable, hydrogen can be coupled to renewable energy sources. This fuel is nearly ideally suited as energy carrier because of its physical and chemical properties. It can be produced by several techniques. The use of hydrogen fuel as supplemental automotive fuels appears to promise a significant improvement in performance of diesel engine and reduces the emissions of Greenhouse gases, nitrogen oxide, and smoke.

For the prediction of the performance of an engine, which is fuelled with hydrogen-diesel mixture, it is; therefore essential to employ either combustion modeling techniques which takes into consideration the effect of the presence of hydrogen or experimental techniques. One of the major areas of development in the internal combustion engine is the development of computer simulations of various types of engine. Their economic value is the reduction of time and costs for the development of new engines and their technical value is the identification of areas, which require specific attentions as the design study evolves. Computer simulations of internal combustion engine cycle are desirable because of the aid they provide in design studies, in predicting trends, in serving as diagnostic tools, in giving more data than are normally obtained from experiments, and in helping to understand the complex processes that occur in the combustion chamber.

١.٢ Hydrogen as a Fuel in I.C.E.

Hydrogen has been used extensively in the space program since it has the best energy to weight ratio of any fuel. Liquid hydrogen is the recommended fuel for rocket engines [٥٨], and has been utilized in the upper stages of launch vehicles on space missions. In the recent years, the concern for cleaner air, along with stricter air pollution regulation and the desire to reduce the dependency on fossil fuels have rekindled the interest in hydrogen as a vehicular fuel. There are a number of unique features associated with hydrogen that make it remarkably well suited to principle, to engine applications. Some of these most notable features that contribute to its use as a combustible fuel are the following [٥٨,٣٦]:

١. Hydrogen has a wide flammability range in comparison with all other fuels. As a result, hydrogen can be burnt in internal combustion engines over a wide range of fuel-air mixtures. A significant advantage of this is that lean mixtures of hydrogen can be burnt.

٢. Hydrogen, over wide ranges of temperature and pressure, has very high flame propagation rates within the engine cylinder in comparison with other fuels. These rates remain sufficiently high even for very lean mixtures that are well away from stoichiometric region. The associated energy release is also so fast that the combustion duration tends to be short and contributes towards producing high power output, and high rate of pressure rise following ignition.

٣. One of the most important features of hydrogen engine operation is that it is associated with less undesirable exhaust emissions than for operation on other fuels. As far as the contribution of the hydrogen fuel to emissions, there are no unburnt hydrocarbons, carbon monoxide, carbon dioxide, and soot emissions. Only the oxides of nitrogen and water vapor are the main product of combustion emitted. Also with lean operation the level of NOx tends to be significantly smaller than those encountered with operation on other fuels.

٤. Hydrogen has a very high diffusivity and therefore its dispersion in air is considerably greater than Diesel or gasoline fuels for the following two advantageous. Firstly, it facilitates the formation of a uniform mixture of fuel and air. Secondly, if a hydrogen leakage is developed, the hydrogen disperses rapidly. Thus, unsafe conditions can either be avoided or minimized.

٥. The high flame speed of hydrogen makes hydrogen engine to operate more closely to the ideal thermodynamic cycle.

٦. Hydrogen has a relatively high auto ignition temperature. This is an important implication when a mixture of hydrogen and air is subjected to a high compression ratio. In fact, the auto ignition temperature is an important factor in determining the compression ratio to be used, since the temperature rise during compression process is related to the compression ratio.

١.٣ The Present Work

The aim of the present work is to study the performance and emissions of a single cylinder diesel engine with hydrogen blending. Consequently a computer program has been constructed and written by using a Quasi Dimensional multi-zone model with a set of semiemprical equations to simulate the combustion process.

The model is used to predict the following performance parameters during each power cycle;

* Cylinder pressure.
* Zonal Temperature.
* Zonal Composition.
* Zonal Heat release rate.
* Emission of pollutants of exhaust gases.
* Engine performance.

A parametric study is presented in order to determine the effect of several influencing parameters on the performance and emissions of diesel engine.

١.٤ Layout of the Thesis

This thesis consists of six chapters. After this introductory chapter, chapter two is concerned with a brief literature review and a back ground of some observed aspects of hydrogen production, storage in vehicles and its usage as a fuel in internal combustion engine. Chapter three is devoted to the theoretical analysis that leads to the estimation of power cycle parameters. Chapter four is concerned with computational procedure and computer program, which is wrote to perform all calculation, based on the theoretical analysis. Chapter five is devoted to the presentation of results and the discussion of these results. Chapter six presents the conclusions drawn from this work in addition to some future suggestions to develop this work further.

CHAPTER TWO

LITERATURE REVIEW

٢.١ Introduction

The hope of the technology is to provide utility and comfort with no damage to the user or to the surroundings. For many years now, petroleum products and other fossil fuels have given us utility and comfort in a variety of areas, but are blamed for such disasters as lung disease and global warming **[٢٣]**. Also, the fears of depleting the petroleum supply demand that a new technology be developed to take its place. With the use of alternative energy sources , a large step is being made to reduce emissions and to improve the efficiency of power production

٢.٢ Alternative Fuels

The importance of reduced pollution, scarcity of existence of petroleum in some countries, fears of fuel shortage, energy crises and cost increases of the petroleum fuels have generated intense interest in alternative fuels, especially non petroleum fuels.

Alternative fuels are fuels that have the capability of yielding energy security and environmental benefits **[٦٠]**. There are different types of alternative fuels for automobiles, such as CNG, LPG, biodiesel, methanol, ethanol, and Hydrogen.

Takemi [٥٥] investigated the use of methanol as an auxiliary fuel in diesel engine. The effect of proportion and timing of auxiliary fuel injection and the main injection timing on engine performance and on emissions were investigated. The result showed that with ٥٪ methanol energy substitution of total energy input, combustion took place without misfiring or knocking. The combustion was smokeless, smoother, with lower NO_x and lower noise than with usual combustion with diesel. The thermal efficiency was maintained at the same level as in conventional diesel operation.

Thyagarajan V. [٥٦] made an investigation for a dual fuel direct injection diesel engine in which the biogas is supplied through the inlet manifold and the diesel fuel through the fuel injection system. This work is based on two steps. In the first step it is assumed that the fuel spray consisting of fuel droplets travel from the tip of the injector to the cylinder wall and the fuel preparation and burning rates are computed for the diesel fuel. In the second step, the surrounding medium consisting of air and biogas are assumed to enter the diesel fuel spray and burn along with the diesel. The entrainment rates of air and biogas are calculated on the basis of the spray penetration and taking swirl into consideration. From this study, it is noticed that introduction of biogas reduces the rate of combustion due to the presence of carbon dioxide and hence brings down the engine performance. This could be improved by having scrubbers to absorb the carbon dioxide so that the calorific value of the biogas could enhanced when it is supplied to the engine.

Ismail I. [٣١] investigated in his work the main characteristic of the combustion process and soot formation in diesel engine in the case of using a diesel fuel and a mixture of diesel fuel and methanol. The latter is the modern trend in the field of internal combustion engine research in the last decades in order to reduce the diesel fuel consumption. Experiments have been conducted on a single cylinder direct injection diesel engine with different operating parameters such as the injection advance angle, engine speed, and load. The experiments were realized using two kinds of fuel a single diesel fuel, and blending of diesel with methanol. The following results were obtained **[٣١]**:

١. The percentage of methanol addition (at different running conditions of engine) has no effect on the rate of burning, up to percentage of methanol equal to ٣٠ percent.

٢. As the percentage of methanol increases, the soot concentration and hence the smoke level decreases.

Abdul-Kadhim M. [١] studied in his research the performance of single cylinder, diesel engine that was fueled with mixture of diesel fuel and ethanol. The cumulative heat release and temperature variation of the cylinder contents were studied as the percentage of ethanol in the mixture was varied from (٠-٢٠) % percent. The following results were obtained:

١. The maximum power output decreases at medium and high range of speed, but it was nearly the same as that of straight gas oil at low speed range.

٢. Little effect is noticed on brake thermal efficiency and break specific fuel consumption at low and medium ranges of load.

٣. The decrease in (air-fuel) ratio with increase engine speed for the dual fuel was less compared to that of straight gas oil.

٤. The maximum rate of heat release increases during the first stage of combustion, and decreases during the ٢nd stage of combustion.

٥. The cumulative heat release and maximum temperature of combustion was reduced.
٦. The addition of more than ٢٠٪ ethanol causes knock.

Krishnan S.R. and Biruduganti M. [٣٨] made an investigation to study the influence of engine operating variables on the performance, emissions and heat release rate in a diesel engine operating on normal diesel and dual fuel modes (with natural gas fueling). Substantial reductions in NO_X emissions were obtained with dual fuel operation. There was a corresponding decrease in unburned hydrocarbon emissions as the substitution of natural gas was increased. Brake specific energy was decreased with natural gas substitution at high loads, but it increased at low loads. Experimental results at fixed pilot injection timing have also established the importance of intake manifold pressure and temperature in improving dual fuel performance and emission at part load.

Keyu P. and Cheung C.S. [٣٩] have carried out experiments on a single cylinder diesel engine and alight duty vehicle with a ٤-cylinder diesel engine, fueled with ultra low sulpher diesel oil blended with different percentages of Dimethyl carbonate (DMC). The blending ratio of (DMC) affects the fuel properties, the injection properties and hence the combustion process and the emission. An analysis of the in-cylinder pressure obtained from the single cylinder diesel engine indicates that with an increase in the blending ratio of (DMC), there is a corresponding increase in ignition delay, peak rate of pressure rise, peak heat release rate and the proportion of fuel burned in the premixed mode. Tests carried out on the single cylinder showed, with an increase in ratio of (DMC), significant decrease in submicron particles in the exhaust. Coupled with this there is an increase in HC and a reduction in NOx.

Tests carried out on the diesel vehicle showed a reduction in power output at fixed fuel pump setting, due to the lower calorific value of the blended fuel. Also with an increase in ratio of (DMC), there is a significant reduction in smoke opacity and CO concentration, but an increase in both HC and NOx, per unit of the measured maximum power.

Srinivasan K. and Krishnan S.R. [٥٢] investigated the performance and emissions of a single cylinder natural gas engine using a pilot ignition strategy. Small diesel pilots (٢-٣) % on energy basis, when used to ignite homogeneous natural gas-air mixture indicated a potential for reduced NO_X emissions while maintaining good engine performance. The effects of pilot injection timing, intake charge pressure, and charge temperature on engine performance and emissions were studied. Total unburned hydrocarbon (HC) emissions were higher with natural gas operation. The nature of combustion under these conditions was analyzed by using heat release schedules predicted from measured cylinder pressure data. The importance of pilot injection timing and inlet conditions on the stability of engine operation and knock are also discussed.

٢.٣ Effect of Hydrogen Addition on the Engine Performance and Emission of Exhaust Gas Pollutants.

Considering energy crises and pollution problems today, investigation have been concentrated on decreasing fuel consumption by using alternative fuels and on lowering the concentration of toxic components in the exhaust gases. Hydrogen is considered as an ideal alternative fuel. It is available in abundance in nature in compounds. It may be considered as a promising fuel of the future.

Two methods of using hydrogen in diesel engines can be investigated. The first method is to mix hydrogen with diesel and the second is to use hydrogen as a pure fuel.

According to the hydrogen supplemented fuel concept, conventional compression ignition engines fueled with hydrogen and diesel can operate with lean fuel/air mixtures, thus improving fuel economy and reducing HC, NO_x and CO emissions **[٢٣]**. Another advantage of this method is that it requires a smaller quantity of hydrogen, which considerably reduces the problem of hydrogen storage in the automobile.

Hydrogen combustion engine emits practically no pollutants, especially in lean operation. However the only possible toxic products of combustion of hydrogen are nitric oxides. Hydrogen engines could therefore represent a possible alternative prime-mover, which are non-polluting and independent of petroleum.

Ikengami M. [٣٢] investigated the possibility of establishing a hydrogen fueled compression ignition engine experimentally by using a conventional swirl chamber diesel engine. Two different systems were used. An air aspirated compression ignition engine is used in the first system and an argon-oxygen mixture is charged in the compression ignition engine is used in the second system. It has been suggested that both pilot injection and fuel leakage from the injector can aid ignition of the hydrogen fuel, bringing about a smooth operation **[٣٢]**. The result has indicated that ignition and engine operation are satisfactory without any ignition aid. A considerable gain has also been proved in the thermal efficiency when argon mixture is used.

Gopal G. [١٩] studied the use of hydrogen in a diesel engine. In his work, a conventional single cylinder, four-stroke diesel engine has been converted to work on the dual-fuel principle with hydrogen as the inducted fuel. The main objectives of the investigation were to determine the optimum proportions between hydrogen and diesel oil under various engine-operating conditions. The results showed that very satisfactory dual-fuel operation with hydrogen is possible. The thermal efficiencies obtained were comparable with pure diesel operation up to about half the engines energy requirement is derived from hydrogen. The main problem noticed is that knock setting is noticed well before the Stoichiometric hydrogen-air ratio.

Rao H.B. [٤٨] made an attempt to burn hydrogen in a diesel engine that was operated on a dual-fuel principle. Hydrogen was supplied along with intake air in small proportions and ignition was initiated by injecting diesel fuel in the conventional manner. The engine was operated at different loads. Such operation resulted in an increase in thermal efficiency at full load, a reduction in exhaust temperature and an increase in maximum pressure. Nitrogen oxides in the exhaust were observed to increase. Also the effect of hydrogen blending on the flame propagation velocities was studied. This study showed that increasing the proportion of hydrogen in the hydrogen-hydrocarbon-air mixture was observed to increase the flame velocity **[٤٨]**.

Varde K.S. [٦٣] made an experimental study to investigate the possibility of reducing diesel emissions in the exhaust by aspirating small quantities of gaseous hydrogen in the intake of a diesel engine. A single cylinder, direct injection type diesel engine was used in the experiments. Hydrogen flow rates equivalent to about ١٠٪ of the total energy input substantially reduced smoke emissions at part loads **[٦٣]**. At the full rated load, reduction in smoke levels was limited. It is believed that this is due to the lower amounts of excess air available in the cylinder **[٦٣]**. It was found that the engine thermal efficiency was dependent on the proportion of hydrogen energy out of the total input energy supplied to the engine. There was no significant change in the hydrocarbon emissions but oxides of nitrogen in the exhaust increase with the increase of hydrogen energy.

Fukuma T. [١٦] studied in his work the hydrogen combustion characteristics in a late injection (near TDC) hot surface ignition engine. As a supplemental experiment, the mode of combustion was observed in a constant volume combustion chamber by the schlieren method. It was observed that the flame propagation initiated by a hot surface through heterogeneous hydrogen jets, was not the same as that of diesel engine. The experimental results on the test engine showed that the optimum number of injection holes is six and the intake air swirl gives better mixture formation. It was observed that the combustion was frequently accompanied by non-negligible combustion pressure vibration at all engine-operating conditions. The experimental result suggested that, besides the vibrations in the air column between pressure sensor and the combustion chamber, the cylinder gas knocked at a characteristic frequency corresponding to the cylinder size.

Harold.C.Hampton.[٢٥] made an investigation to determine whether a sufficient amount of hydrogen could be efficiently burned in a compression ignition engine to compensate the increase of lift in air ship due to the consumption of the fuel oil. The performance of a single cylinder four stroke cycle compression ignition engine operating on fuel oil alone was compared with its performance when various quantities of hydrogen were included with the inlet air. Engine performance data, indicator cards and exhaust gas samples were obtained for each change in engine operating condition. The result of this study showed that:

١. Hydrogen could be burned satisfactory at compression ratios of ١٣.٤ and ١٥.٦ in sufficient quantities to compensate the increase in lift due to the consumption of the fuel oil.

٢. In the cruising range the mixture of fuel oil and hydrogen burned more efficiently than the fuel oil alone.

The engine always stopped firing when the fuel oil was cutoff. Throughout the limits of the test conditions, it was never possible to auto-ignite the various mixtures of hydrogen and air but the injection of even a minute quantity of fuel oil would cause the mixture to burn. The engine showed that no ill effects from the use of hydrogen and no change in engine operation was apparent.

Jing Ding L.[٣٤] made an experimental study of burning hydrogen fuel, and hydrogen-diesel oil mixture to improve the combustion process. He showed **[٣٤]**:

١. CO and HC emissions are lower compared to that of diesel fuel.

٢. In diesel engine operated with heterogeneous mixture, the amount of smoke depends on mode of mixture formation and the combustion process, especially on the injection lag and relative quantities of fuel injected before ignition occurs.
٣. Smoke decrease with increasing hydrogen ratio in mixed fuels.
٤. The effect of hydrogen added to diesel oil is to reduce the quantity of smoke and this reduction will be greater and greater as the engine speed is reduced. Thus for an automotive diesel engine, good reduction in smoke under low-speed and, high-load conditions will be gained by using diesel oil-hydrogen mixed fuels.

Tomita E. [٥٧] made an investigation to study the effect of inducting hydrogen from intake port in to the cylinder of a diesel engine. Light oil was injected through the main injection system. The heat release was determined from the pressure history in the cylinder. The relation between the heat release and the exhaust emissions are discussed. As a result, when hydrogen is mixed with the inlet air, exhaust emissions such as smoke, hydrocarbon, CO, $CO_{٢}$, and NO_x are reduced simultaneously while brake thermal efficiency is slightly reduced.

Milos P. [٤٣] has used an advanced numerical methods to model hydrogen fueled engine. A sensitivity study of the influence of main engine parameters on NOx formation has been performed using the GT-power code. A general CFD algorithm based on the previously published Advanced Multizone Eulerian model has been adapted to detailed simulation of in-cylinder phenomena of the hydrogen engine. Procedure of the model parameter identification according to experimental data has been verified. Combination of the model with complex description of chemical kinetics of both fast reaction and slow ones is shown. Possibilities of the chemical kinetics application to the semi-empirical model parameter estimation are discussed. The results of this study showed that:
١. The simplified combustion model based on experimental data splits connection between stiff chemistry and turbulence model.
٢. The hydrogen combustion chemistry solution shows that the reaction zone should be very thin, because of the very fast chemistry.
٣. The CFD model predicts that NOx are formed in post flame region only.

Schefer R. [٥١] has studied the combustion process of hydrogen when blended with traditional hydrocarbon fuels in gas turbine combustors. The objectives of this work are **[٥١]**:
١. Effect of the amount of hydrogen on flame stability, combustor acoustics, emissions and efficiency.

٢. Establish a scientific and technological database for lean combustion of hydrogen-enriched fuels.
٣. Establish the numerical simulation capabilities that will facilitate design optimization of lean premixed swirl burner.
The approach was used to design and fabricate a lean premixed swirl burner that simulate the basic features of gas turbine combustors as shown in **Fig.(٢.١).**
The results of study showed that ultra-lean premixed combustion is an effective approach to NOx emissions reduction from gas turbine engines. Hydrogen blended with traditional hydrocarbon fuels significantly improves flame stability during lean combustion and allows stable combustion at low temperature needed to minimize NOx production.

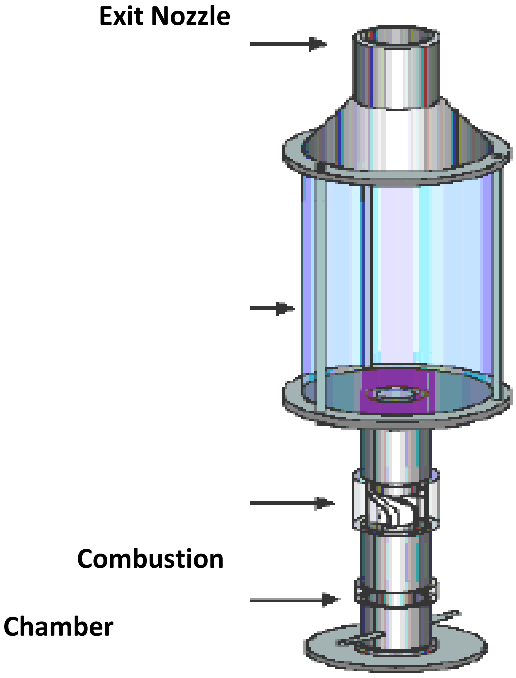


Fig.(٢.١) Lean Premixed Swirl Burner [٥١].

Mather H.B. [٤٤] made an experimental investigation to study the effect of small percent of hydrogen energy substitution on the performance of direct injection diesel engine. He used a single cylinder, water–cooled, direct injection type small diesel engine. Helium as diluents was found to control the engine knock, but the thermal efficiency and optimum percentage of hydrogen energy substitution exhibited no positive gain. Nitrogen showed the best influence on engine performance and knock-limited power output improvement. Water induction, in small concentrations, demonstrated the highest percentage of hydrogen energy substitution at full load, although the engine thermal efficiency and knock limited power output were marginally affected.

Frankfort J. and Garner J.[١٧] tested four gaseous fuel vehicles as a part of their alternative fuelled vehicle fleet. One vehicle, a dodge ram wagon van, operating initially on compressed natural gas (CNG) and latter on a blend of (CNG) and hydrogen. The other three vehicles, one was fuelled with pure hydrogen and two were fuelled with a blend of CNG and hydrogen. The primary objective of the test was to evaluate the safety and reliability of operating vehicles on pure hydrogen and blended hydrogen fuel and the interface between the vehicle and the hydrogen fueling infrastructure. A secondary objective was to quantify vehicle emission, cost and performance. No safety issues were found and also significant reductions in emissions were achieved by adding hydrogen to the fuel. This report presents results of ٢٢,٨١٦ miles of testing for the dodge ram wagon van, operating on CNG fuel, blended with ١٥٪ hydrogen.

Ma J., Yongkang S. & Zhang Z. [٤٥] have made a comprehensive computer simulation to predict the performance of hydrogen engine vehicles. The effect of various operating parameters, such as compression ratio, excessive air parameter and ignition advancing, on the engines performance were calculated and then the optimal parameters of the engine structure were determined. The simulation and analysis showed several meaningful results:

١. Hydrogen engine may operate on lean combustion.

٢. The cylinder pressure will increase quickly, as the proportion of hydrogen in the mixture is increased.

٣. The thermal efficiency will decline and has a higher thermal efficiency in the range (٣٥-٥٠) %.

٤. The thermal efficiency grows with the increase of compression ratio.

٥. An optimal value for the cylinder bore is in the range (.٠٧-.٠٩) m.

٢.٤ Closing Remarks

From the scope of literature review, a number of points can be drawn:

١. The use of hydrogen fuel as supplemental automotive fuels appears to promise a significant improvement in performance and emissions of diesel engine.

The model of **Jung D. & Assanis D. [٣٨]** proved to be more reliable due to the implication of multizone procedure for the spray formation. Therefore; it will be used in this study.

CHAPTER THREE

THEORETICAL ANALYSIS

٣.١ Introduction

The operating cycle of an internal combustion engine can be broken down into a sequence of processes, namely intake, compression, combustion, expansion and exhaust. The structure of this type of engine simulation is indicated in **Fig. (٣.١)**

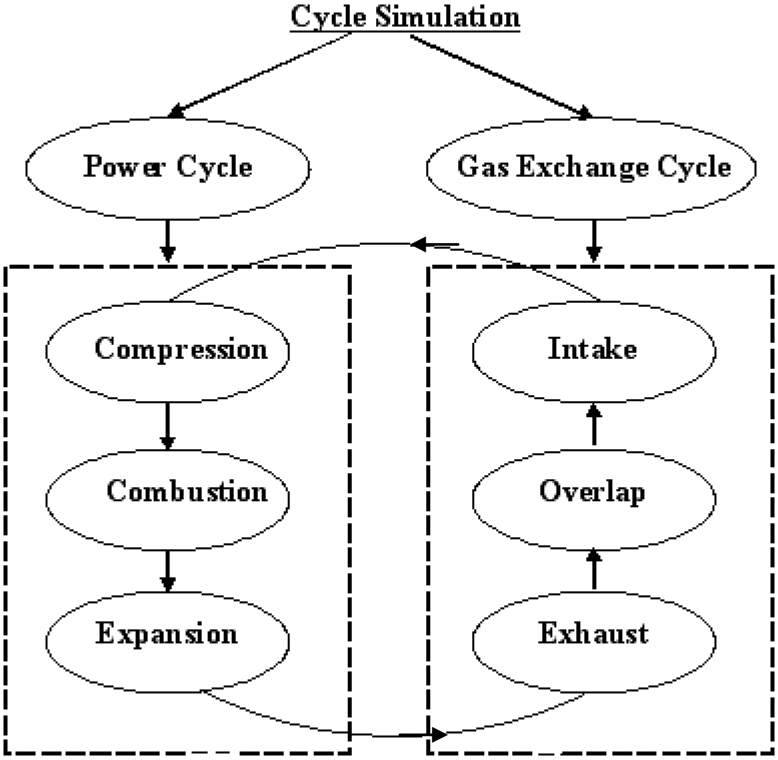


Fig. (٣.١) Sequence of Processes Followed by Cycle related Engine Simulations [١١].

A mathematical model has to be developed in the present work, to study the effect of hydrogen addition on engine performance and pollutants emission.

٣.٢ The Present Mathematical Model

٣.٢.١ The Scope of the Model

Diesel engine simulation models can be classified into three categories, zero-dimensional single zone models, quasi-dimensional multizone model (which is used in the present study) **[٣٥]**, and multi-dimensional models. Zero-dimensional single-zone models assume that cylinder charge is uniform in composition and temperature at all time during the cycle, see **Fig (٣.٢.a)**. Single zone models cannot be used to account for fuel spray evolution and spatial variation in mixture composition and temperature, which are essential to predict exhaust emission. In addition to single zone models there is the two zone model in which there are unburnt zone and burnt zone. Inspite of the differences in the nature of combustion process in S.I. and C.I. engines, the two zone model can still be used for both types since it is basically a zero dimensional model that considers only burned and unburned zones without any consideration of the spatial location of such zones see **Fig. (٣.٢.b).** On the other hand, multi-dimensional models **[٦]** resolve the space of cylinder on a fine grid, thus providing a formidable amount of special information. However, phenomenological sub-models describing fuel spray processes are still included in these models, and the result cannot be always guaranteed. Further more, the computational time and storage constrain still restrain these codes from routine use for design purposes. As an intermediate step between zero-dimensional and multi-dimensional models, quasi-dimensional multizone model which can be effectively used to model diesel engine combustion systems.

The objective of this study is to develop a more physically-based, quasi-dimensional multizone spray model and implement it into a full cycle diesel engine simulation so as to predict engine performance, fuel economy and pollutant emissions using blended fuel.

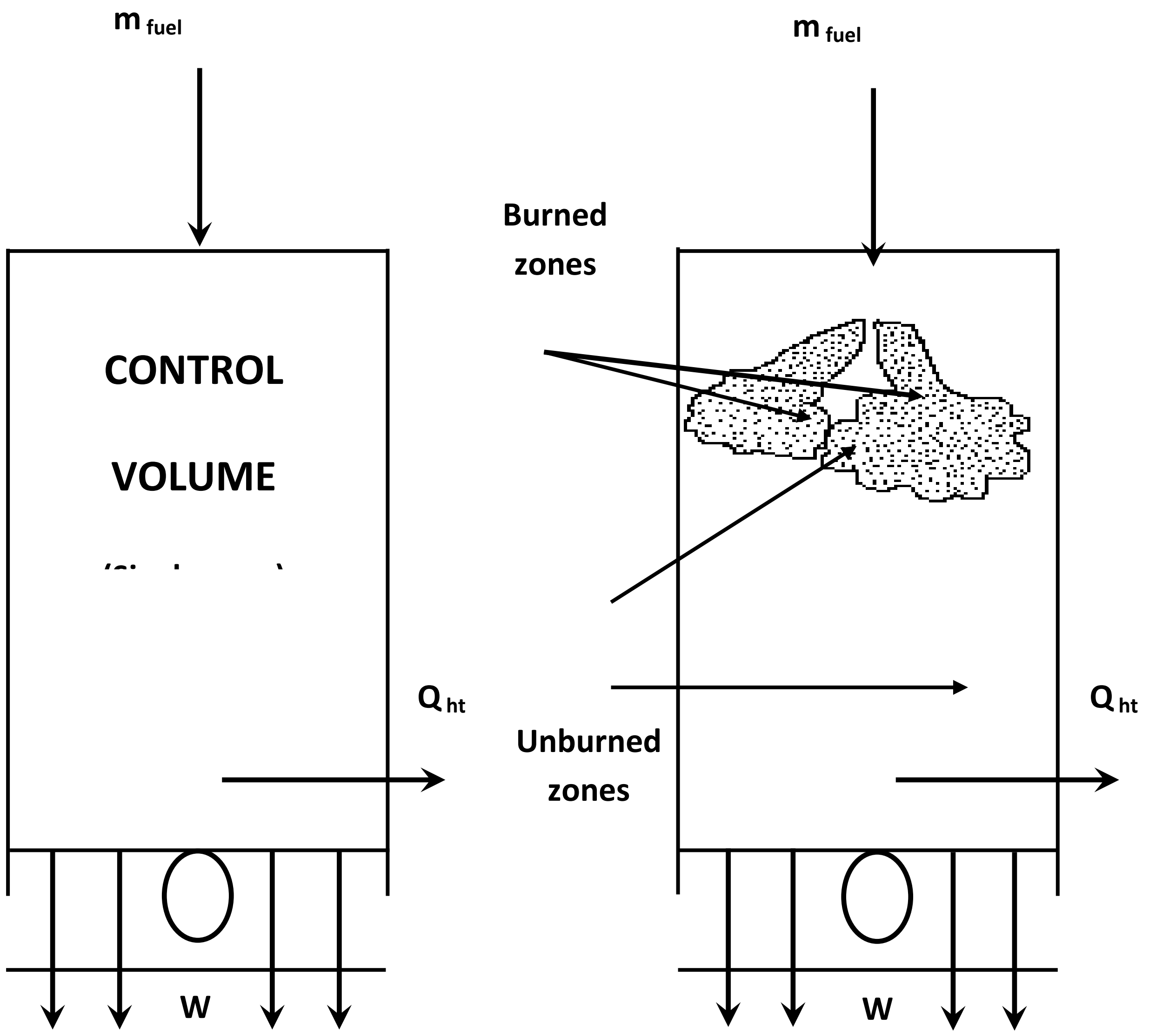
The zonal spray combustion model should be able to:

١. Predict the detailed spray evolution with acceptable fidelity.

٢. Incorporate a heat release model that can explicitly account for both premixed and diffusion controlled combustion phases.

٣. Predict both convection and radiation heat transfer rates.

٤. Cover a wide range of engine operating conditions without losing accuracy.



(a) (b)

Fig.(٣.٢) a: Schematic of the Single Zone Combustion Model [٥٢].

b: Schematic of the Two Zone Combustion Model [٥٢].

٣.٢.٢ Assumptions

The following assumptions were considered in the present analysis:

١. The analysis is based on the quasi dimensional multizone model.

٢. The pressure is assumed to be uniform in the chamber.

٣. The zones in each parcel are assumed to contain the same mass of fuel.

٤. Number of zones in the radial direction is ١٠ zones, which is fixed regardless of the amount of fuel injected or the time step used.

٥. No mixing or passing among zones is permitted.

٦. Following breakup, it is assumed that the fuel spray is atomized to fine droplets, each with a diameter equal to the sauter mean diameter (SMD).

٧. The effect of droplet size distribution in a spray parcel is neglected.

٨. No spray impingement on cylinder walls and piston.

٩. Due to the symmetry about spray axis only half spray was considered.

١٠. The flow leakage through valves and past the piston rings are neglected.

Figure (٣.٣) shows the division of spray into parcels and zones at a certain instance.

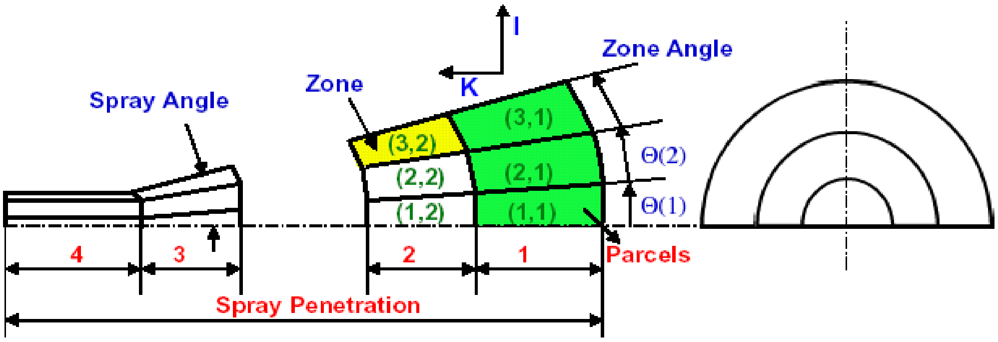


Fig. (٣.٣) Division of Spray into Parcels and Zones at a Certain Instance [١٤].

٣.٣ The State of the Cylinder Contents during Combustion Process

The optimum equivalence ratio for a Diesel engine is that which gives the required power output with the lowest fuel consumption, consistent with smooth and reliable operation.

In practice, the constraints of emission control may dictate a different equivalence ratio. The relative proportions of fuel and air that provide the lowest fuel consumption, smooth reliable operation, and to satisfy the emission requirements, at the required power level, depend on engine speed and load **[٢]**.

The following information is useful to study different case studies of different fuels with the assumptions of no dissociation and NOx formation.

At first the following symbol definitions are noted;

n : Number of carbon atoms in hydrocarbon fuel.

m : Number of hydrogen atoms in hydrocarbon fuel.

X : Number of Kmoles of Oxygen for one Kmol of fuel and it is equal to;

λ : Mole ratio of hydrogen added.

$E1$: Number of Kmoles of CO٢ from the combustion of ١ Kmol of fuel.

$E2$: Number of Kmoles of H٢O from the combustion of ١ Kmol of fuel.

$E3$: Number of Kmoles of N٢ from the combustion of ١ Kmol of fuel.

$E4$: Number of Kmoles of O٢ from the combustion of ١ Kmol of fuel.

$E5$: Number of Kmoles of CO from the combustion of ١ Kmol of fuel.

<u>CASE ١, Pure hydrocarbon fuel.</u>

A-Perfect Combustion (ϕ=١.٠)

$$C_nH_m + XO_2 + 3.76XN_2 \rightarrow E1.CO_2 + E2.H_2O + E3.N_2$$

...(٣.١)

The atomic balance of C, O, N and H gives;

$$E1 = n$$ **...(٣.٢)**

$$E2 = m/2$$

...(٣.٣)

$$E3 = 3.76X$$

...(٣.٤)

B- Complete Combustion (ϕ<١.٠)

$$C_nH_m + XO_2 + 3.76XN_2 \rightarrow E1.CO_2 + E2.H_2O + E3.N_2 + E4.O_2$$

...(٣.٥)

The atomic balance of C, O, N and H gives;

$E1 = n$

...(٣.٦)

$E2 = m/2$

...(٣.٧)

$E3 = 3.76X$

...(٣.٨)

$E4 = X - n - m/4$ **...(٣.٩)**

C-Incomplete Combustion (ϕ>١.٠)

$$C_nH_m + XO_2 + 3.76XN_2 \rightarrow E1.CO_2 + E2.H_2O + E3.N_2 + E5.CO$$

...(٣.١٠)

The atomic balance of C, O, N and H gives;

$E1 = 2X - m/2 - n$

...(٣.١١)

$E2 = m/2$ **...(٣.١٢)**

$E3 = 3.76X$

...(٣.١٣)

$E5 = 2n + m/2 - 2X$

...(٣.١٤)

CASE ٢, Mixture of hydrocarbon fuel and hydrogen fuel.

A- Perfect Combustion (ϕ= ١.٠)

$$[(1-\lambda)C_nH_m+\lambda H_2]+XO_2+3.76XN_2\rightarrow E1.CO_2+E2.H_2O+E3.N_2$$

...(٣.١٥)

The atomic balance of C, O, N and H gives;

$$E1=n(1-\lambda)$$

...(٣.١٦)

$$E2=(m/2).(1-\lambda)+\lambda$$

...(٣.١٧)

$$E3=3.76X$$

...(٣.١٨)

B- Complete Combustion (ϕ < ١.٠)

$$[(1-\lambda)C_nH_m+\lambda H_2]+XO_2+3.76XN_2\rightarrow E1.CO_2+E2.H_2O+E3.N_2+E4.O_2$$

...(٣.١٩)

The atomic balance of C, O, N and H gives;

$$E1=n(1-\lambda)$$

...(٣.٢٠)

$$E2=(m/2).(1-\lambda)+\lambda$$

...(٣.٢١)

$$E3=3.76X$$ **...(٣.٢٢)**

$$E4=X-(m/4).(1-\lambda)-n(1-\lambda)$$

...(٣.٢٣)

C- Incomplete Combustion (ϕ > ١.٠)

$$[(1-\lambda)C_nH_m+\lambda H_2]+XO_2+3.76XN_2\rightarrow E1.CO_2+E2.H_2O+E3.N_2+E5.CO$$

...(٣.٢٤)

The atomic balance of C, O, N and H gives;

$$E1=2X-(m/2).(1-\lambda)-\lambda-n.(1-\lambda)$$

...(٣.٢٥)

$$E2=(m/2).(1-\lambda)+\lambda$$

...(٣.٢٦)

$$E3=3.76X$$

...(٣.٢٧)

$$E5=2n.(1-\lambda)+\lambda+(m/2).(1-\lambda)-2X$$

...(٣.٢٨)

<u>CASE ٣, Pure hydrogen fuel.</u>

A- Perfect Combustion (ϕ= ١.٠)

$$H_2+XO_2+3.76XN_2\rightarrow E2.H_2O+E3.N_2$$

...(٣.٢٩)

The atomic balance of O, N and H gives;

$$E2=1$$

...(٣.٣٠)

$$E3=3.76X$$

...(٣.٣١)

B- Complete Combustion ($\phi <$ ١.٠)

$$H_2 + XO_2 + 3.76XN_2 \rightarrow E2.H_2O + E3.N_2 + E4.O_2$$

...(٣.٣٢)

The atomic balance of O, N and H gives;

$$E2 = 1$$

...(٣.٣٣)

$$E3 = 3.76X$$

...(٣.٣٤)

$$E4 = X - (1/2)$$

...(٣.٣٥)

The total number of moles of residual gas, hydrogen, and air in the cylinder at trapped condition;

$$N_m = \frac{P_{cyl}.V_{cyl}}{R_{mol}.T_{cyl}} \qquad \text{[Kmol]}$$

...(٣.٣٦)

Where; P_{cyl} Cylinder pressure at trapped condition [kpa].

T_{cyl} Cylinder temperature at trapped condition [K].

V_{cyl} Cylinder volume [m^{٣}].

R_{mol} Universal gas constant ٨.٣١٤٣ [kJ/Kmol. K].

For any of the previous cases, the composition of the charge at trapped conditions is calculated as follows;

$N_{H_2} = \lambda.CM$ [Kmol]

...(٣.٣٧)

$N_{CO_2} = E1.CD$ [Kmol]

...(٣.٣٨)

$N_{H_2O} = E2.CD$ [Kmol]

...(٣.٣٩)

$N_{N_2} = 3.79X + E3.CD$ [Kmol]

...(٣.٤٠)

$N_{O2} = X + E4.CD$ [Kmol]

...(٣.٤١)

$N_{CO} = E5.CD$ [Kmol]

...(٣.٤٢)

Where CM and CD are scale factors reducing the mole numbers to the proper size to fit in the engine.

$$CM = \frac{N_m - N_x}{N_{mo}}$$ ...(٣.٤٣)

$$CD = \frac{N_x}{N_{po}}$$

...(٣.٤٤)

Heywood [٢٦], showed that the typical residual fractions in diesel engines range from (٣-٦) %. In the present work residual fraction is taken as ٦٪.

٣.٤ Thermodynamic Properties of Mixtures

٣.٤.١ Internal Energy and Specific Heats.

The internal energy is defined as;

$$e = e(T) + e_O \qquad \text{[kJ/Kmol]}$$

...(٣.٤٥)

Where; $e(T)$ Specific Internal energy at temperature T [kJ/Kmol].

e_o Specific Internal energy at the absolute zero [kJ/Kmol].

The specific internal energy $e(T)$ for gas i is given by **Benson [١٠]** as;

$$e_i(T) = R_{mol} \cdot \left[\left(\sum_{J=1}^{J=5} U_{i,j} . T^j \right) - T \right] \qquad \text{[kJ/Kmol]}$$

...(٣.٤٦)

The coefficients $U_{i,j}$ are given in **Appendix (A)**

The total internal energy E is given by the following equation;

$$E = E(T) + E_O \qquad \text{[kJ]}$$

...(٣.٤٧)

Where;

$$E(T) = \sum_{i=1}^{i=n} N_i . e_i(T)$$ **...(٣.٤٨)**

$$E_O(T)=\sum_{i=1}^{i=n} N_i.(e_O)_i$$

...(٣.٤٩)

N_i is the total number of moles of gases i .

Hence the total internal energy for a gas mixture of n species is;

$$E=R_{mol}\sum_{i=1}^{i=n} N_i.\left[\left(\sum_{J=1}^{J=5} U_{i,j}.T^j\right)+\frac{(e_O)_i}{R_{mol}}-T\right] \qquad \text{[kJ]}$$

...(٣.٥٠)

Through the power cycle of internal combustion engine there are three processes, namely compression, combustion and expansion process.

In compression process, the combustion chamber contains a mixture of H_2, O_2, N_2 and residual gases which are CO_2, H_2O .The internal energy of the mixture during compression process given by **[١٠]**;

$$E_{COMP}=R_{mol}.\sum_{i=1}^{i=n}(N_{COMP})_i\left[\left(\sum_{j=1}^{j=5} U_{i,j}.T_{COMP}^j\right)+\frac{(e_O)_i}{R_{mol}}-T_{COMP}\right] \qquad \text{[kJ]}$$

...(٣.٥١)

Where; T_{COMP} Cylinder temperature throughout compression stroke [K].

$(N_{COMP})_i$ Number of moles of gas (i) throughout compression stroke [Kmol].

In combustion process the fuel spray is divided into number of zones. Unburned zones and burned zones. The concentration of species in the unburned zones is a mixture of H_2, O_2, N_2, residual gases which are

CO_2, H_2O and unburned fuel. The internal energy in theses zones E_u is given by **[١٠]**;

$$E_u = R_{mol} \cdot \sum_{i=1}^{i=n} (N_u)_i \left[\left(\sum_{j=1}^{j=5} U_{i,j} . T_u^j \right) + \frac{(e_O)_i}{R_{mol}} - T_u \right] \qquad [\mathrm{kJ}]$$

...(٣.٥٢)

Where; T_u. Unburned zone temperature [K].

$(N_u)_i$ Number of moles of gas(***i***) in the Unburned zone [Kmol].

The concentration of species in the burned zones is mixture of products of combustion such as ($CO_2, H_2O, CO, NO, OH, N_2, O_2, O, N, H, H_2, soot, Ar$)

The internal energy in the burned zones E_b is given by **[١٠]**;

$$E_b = R_{mol} \cdot \sum_{i=1}^{i=n} (N_b)_i \left[\left(\sum_{j=1}^{j=5} U_{i,j} . T_b^j \right) + \frac{(e_O)_i}{Rmol} - T_b \right]$$

...(٣.٥٣)

Where; T_b Burned zone temperature [K].

$(N_b)_i$ Number of moles of gas (i) in the burned zone [Kmol].

During expansion process, the cylinder contains a mixture of products gases which are ($CO_2, H_2O, CO, NO, OH, N_2, O_2, O, N, H, H_2, soot, Ar$) and the internal energy $E_{\exp}$ is given by **[١٠]**;

$$E_{\exp} = R_{mol} \cdot \sum_{i=1}^{i=n} (N_{\exp})_i \left[\left(\sum_{j=1}^{j=5} U_{i,j} . T_{\exp}^j \right) + \frac{(e_O)_i}{R_{mol}} - T_{\exp} \right]$$

...(٣.٥٤)

Where; $T_{\exp.}$ Cylinder temperature throughout expansion stroke [K].

$(N_{\exp})_i$ Number of moles of gas (i) throughout expansion stroke [Kmol].

The other important properties are the specific heats, and are calculated as follows;

$$C_v(T)=\frac{de(T)}{dT} \qquad \text{[kJ/Kmol. K]}$$

…(٣.٥٥)

Thus

$$C_v(T)=\frac{1}{N_T}.\frac{dE}{dT} \qquad \text{[kJ/Kmol. K]}$$

…(٣.٥٦)

Where $\{N_T=\sum N_i\}$ Total number of moles of the mixture.

By differentiating equation (٣.٥٠) with respect to temperature T at constant volume and combining with equation (٣.٥٦), the following equation can be obtained;

$$C_V(T)=R_{mol}\sum_{i=1}^{i=n}\frac{(N_i)}{N_T}\left[\left(\sum_{j=1}^{j=5} j.U_{i,j}.T^{j-1}\right)-1\right]$$

…(٣.٥٧)

For compression process, the specific heat at constant volume can write;

$$C_{v_{comp}}(T_{comp}) = R_{mol} \sum_{i=1}^{i=n} \frac{(N_{comp})_i}{N_T} \left[\left(\sum_{j=1}^{j=5} j.U_{i,j}.T_{comp}{}^{j-1} \right) - 1 \right]$$

...(٣.٥٨)

For combustion process the chamber is divided into number of zones in which the specific heat at constant volume is;

$$C_{v_Z}(T_Z) = R_{mol} \sum_{i=1}^{i=n} \frac{(N_Z)_i}{N_T} \left[\left(\sum_{j=1}^{j=5} j.U_{i,j}.T_Z{}^{j-1} \right) - 1 \right]$$

...(٣.٥٩)

During expansion process the specific heat at constant volume is;

$$C_{v_{\exp}}(T_{\exp}) = R_{mol} \sum_{i=1}^{i=n} \frac{(N_{\exp})_i}{N_T} \left[\left(\sum_{j=1}^{j=5} j.U_{i,j}.T_{\exp}{}^{j-1} \right) - 1 \right]$$

...(٣.٦٠)

The specific heat at constant pressure is defined as;

$$C_p(T) = C_v(T) + R_{mol} \qquad \text{[kJ/Kmol. K]}$$

...(٣.٦١)

Hence for compression process the specific heat at constant pressure is;

$$C_{p_{comp}}(T_{comp}) = C_{v_{comp}}(T_{comp}) + R_{mol}$$

...(٣.٦٢)

For combustion process there are n zones

$$C_{p_Z}(T_Z) = C_{v_Z}(T_Z) + R_{mol}$$

...(٣.٦٣)

Finally during expansion process the specific heat at constant pressure is;

$$C_{p_{\exp}}(T_{\exp}) = C_{v_{\exp}}(T_{\exp}) + R_{mol}$$

...(٣.٦٤)

٣.٤.٢ Equilibrium Constant

The equilibrium constant k_p for any chemical reaction is given by **Benson [١٠]** as;

$$\ln k_p = \frac{-\Delta G_T}{R_{mol}.T}$$

...(٣.٦٥)

Where ΔG_T Gibbs free energy of formation [kJ] at temperature T [K] and a unit pressure P [Pa] hence;

$$\ln k_p = \left[\sum \left(\frac{v_i.g_i(T)}{R_{mol}.T} + \frac{v_i.g_o}{R_{mol}.T} \right)_R - \sum \left(\frac{v_i.g_i(T)}{R_{mol}.T} + \frac{v_i.g_o}{R_{mol}.T} \right)_P \right]$$

...(٣.٦٦)

Where v_i Stoichiometric coefficient of gas i.

$g_i(T)$ Specific Gibbs free energy function at temperature T [kJ/Kmol].

g_o Specific Gibbs free energy function at absolute zero [kJ/Kmol].

The term $\left(\frac{g_i(T)}{R_{mol}.T} \right)$ is given by **Benson [١٠]** as;

$$\frac{g_i(T)}{R_{mol}.T} = U_{i,1} - (\ln T) - \sum_{j=2}^{j=5} \frac{U_{i,j}}{j-1}.T^{j-1} - U_{i,6}$$

...(٣.٦٧)

The equilibrium constant k_p for the following stoichiometric reaction;

$$v_a.A + v_b.B \leftrightarrow v_c.C + v_d.D$$

...(٣.٦٨)

is expressed as;

$$k_p = \left(\frac{X_c^{vc}.X_d^{vd}}{X_a^{va}.X_b^{vb}} \right).P^{vc+vd-va-vb}$$

...(٣.٦٩)

Where v the Stoichiometric coefficient

X_i molar fraction

P total pressure in atmospheres divided by reference pressure.

Equations (٣.٦٦) and (٣.٦٩) are used to determine the mole fraction X_i for each species.

٣.٥ Heat Transfer Model

Heat transfer affects engine performance, efficiency, and emissions. For a given mass of fuel within the cylinder, the higher heat transfer to the combustion chamber walls will reduce the average temperature and pressure of the combustion gas, and reduce also the work transfer to the piston **[٧]**. Changes in gas temperature due to the heat transfer has an impact on emission formation processes, both within the engine cylinders and in the exhaust system. Therefore, a certain compromise is necessary between heat transfer rate and limitation of the combustion chamber wall material. Therefore, the engine heat transfer is of obvious importance to the engine designer.

The total heat transfer is the sum of the heat transfer to the cylinder wall via convection and radiation and heat transfer to the liquid fuel droplets during the evaporation process. Therefore, the heat transfer rate term $\frac{dQ}{dt}$ is expressed as $\frac{dQ}{dt} = -\frac{dQ_w}{dt} - \frac{dQ_{fg}}{dt}$

...(٣.٧٠)

Heat transfer rate to the wall $\frac{dQ_w}{dt}$ is given as;

$$\frac{dQ_w}{dt} = \frac{dQ_{Convection}}{dt} + \frac{dQ_{Radiation}}{dt}$$

...(٣.٧١)

The convective heat transfer from the gas to cylinder wall interface will depend on the temperature gradient in the boundary layer at the surface. However, due to the inherent difficulties in calculating the details of turbulent fluid motion in the combustion chamber during the operating cycle of the engine, the convective heat transfer rate is usually expressed as;

$$\frac{dQ_{Convection}}{dt} = h_C . A . \left(T_g - T_w\right)$$

...(٣.٧٢)

Where T_g gas temperature [K].

T_w wall temperature [K].

A surface area for heat transfer [m٢].

h_C heat transfer coefficient [W/m٢. K].

For convection term **Woschni [٦٤]** developed the following empirical correlation;

$$Nu_s = 0.035\mathrm{Re}^{0.8}$$

...(٣.٧٣)

Where $Nu_s = \frac{h_C.B}{k}$ Nusselt number.

...(٣.٧٤)

$\mathrm{Re} = \frac{\rho.w.B}{\mu}$ Reynolds number.

...(٣.٧٥)

B Cylinder bore taken as the characteristic length [m].

w Local average gas velocity in the cylinder [m/sec].

k Thermal conductivity [W/m. K].

Assuming $k \propto T, \mu \propto T, and P = \rho RT$, the above correlation can be rewritten;

$$h_C = 3.26B^{-0.2}.T^{-.55}.P^{0.8}.w^{0.8}$$ [W/m٢.K]

...(٣.٧٦) During compression process, **Woschni [٦٤]** argued that the average gas velocity should be proportional to the mean piston speed. During combustion and expansion processes he attempted to account directly for the gas velocities induced by the change in density that results from combustion. The following expression is used;

$$w=\left[C_1u_p+C_2\left(\frac{V_{disp}}{V_{cyl}}\right).\left(\frac{P(\theta)-P_{motor}(\theta)}{P_{cyl}}\right).T\right] \quad \text{[m/s]}$$

...(٣.٧٧)

Where u_p mean piston speed [m/s].

V_{disp} displacement volume [m^{٣}].

V_{cyl} cylinder volume [m^{٣}].

$P(\theta)$ Cylinder pressure [bar].

$P_{motor}(\theta)$ Motoring pressure [bar].

C_1 and C_2 are model constant, which are specified as:

For the gas exchange period: C_1=٦.١٨; C_2 =٠

For the compression period: C_1=٢.٢٨; C_2=٠

For the combustion and expansion period: C_1=٦.١٨; C_2=٣.٢٤*١٠$^{-٣}$

Unit of C_2 is [١/K].

The heat transfer area is a function of time in the heat transfer model. The formula suggested by **Heywood [٢٦]** is used in the present work assuming a flat top piston;

$$A=A_{Piston}+A_{Head}+\pi.B.P_{disp}+\frac{4V_C}{B}$$

...(٣.٧٨)

where

$$P_{disp} = L + \frac{St}{2}.(1-\cos(\theta)) - \sqrt{\left(L^{2} + \frac{St^{2}}{4}.\left(\cos^{2}(\theta-1)\right)\right)}$$

...(٣.٧٩)

A Total area of the combustion chamber [m^{٢}].

A_{Piston} Piston area [m^{٢}].

A_{Head} Cylinder head surface area [m^{٢}].

V_C Is clearance volume [m^{٣}].

Detailed specifications of engine test are given in the **Appendix (B)**.

The total cylinder volume at any crank angle position θ is given by **Ferguson C.R. [١٨]** as;

$$V(\theta)=V_C+\left[\frac{V_{cyl}-V_C}{2}\right]\left[\frac{L}{ar}+1+\cos(\theta)-\sqrt{\left(\left(\frac{L}{ar}\right)^{2}-\sin^{2}(\theta)\right)}\right]$$

...(٣.٨٠)

Where ar is the crank radius [m].

The primary sources of radiative heat transfer in a Diesel engine are the high temperature burned gases and the soot particles which are formed in the turbulent, diffusion controlled diesel flame. In general, the radiant heat flux depends on the location of the combustion chamber surface, engine load, and engine design. Due to the complexity of the problem, accepted prediction models for radiant heat flux in a diesel engine are not available. The instantaneous radiant heat flux is expressed as **[٣,٥٣]**:

$$\frac{dQ_{Radiation}}{dt} = \varepsilon\ .\delta.A.\left(T_g^4 - T_w^4\right)$$

...(٣.٨١)

Where ε total emissivity.

δ **Stephan-Boltzman** constant (٥.٦٧*١٠$^{-٨}$ W/m^{٢}.°K^{٤}).

This equation assumes that each zone radiates to the whole combustion chamber surface area without any radiative interactions between zones.

Radiation in Diesel engine is due to luminous (soot) and non-luminous (gaseous) radiation. Thus, the total emissivity may be given approximately by **[٥٣]**:

$$\varepsilon = \varepsilon_g + \varepsilon_S - \varepsilon_g.\varepsilon_S$$

...(٣.٨٢)

Where the subscripts g and s stand for gas and soot respectively.

The non-luminous radiation from combustion gasses is primarily due to emission contribution from the molecules of carbon dioxide, and water vapor. Thus, the total gas emissivity may be calculated by the following approximation **[٥٣]**:

$$\varepsilon_g = \varepsilon_{H_2O} + \varepsilon_{CO_2} - \varepsilon_{CO_2}.\varepsilon_{H_2O}$$

...(٣.٨٣)

The gas emissivities of carbon dioxide, and water vapor were obtained by the following empirical relations **[٥٣]**:

$$\varepsilon_{CO_2} = 0.711\left(P_{CO_2}.Lr\right)^{1/3} / \left(T_Z/100\right)^{1/2}$$

...(٣.٨٤)

And

$$\varepsilon_{H_2O} = 0.707(P_{H_2O}.Lr)^{1/3}/(T_Z/100)^{1/2}$$

...(٣.٨٥)

Where

P_{H_2O} & P_{CO_2} partial pressure of H_2O & CO_2 respectively [bar].

T_Z zonal temperature [°K].

Lr radiation path length [m].

With sufficient accuracy the mean path length for a volume V and area A is given by **[٥٣]**:

$$Lr = 0.9 * \frac{4.V_Z}{A_Z}$$

...(٣.٨٦)

The truncated zonal volume and surface area can be simply calculated from radius of zone and spray penetration as;

$$V_Z = \frac{\pi}{3}.r_Z{}^2.S$$

...(٣.٨٧)

$$A_Z = 2\pi.r_Z.dr_Z$$ **...(٣.٨٨)**

Where

$$r_Z = S.\tan(nr.\beta)$$ **...(٣.٨٩)**

β : accumulated zonal angle in degree.

nr : zonal division in the radial direction.

S : zonal Spray tip penetration.

A detailed explanation for grid generation and zonal volume calculation is given in chapter four-section **(٤.٤)**.

The soot emissivity was obtained from the following equation, derived by **[٥٣]**:

$$\varepsilon_s = 1 - \exp\left\{P^C \ln\left[1 - \varepsilon_{go}\left(\frac{0.09}{\left(\tau^2 - sg^2 + 0.35sg - 0.38\right)} + 6.8sg - 5.95\right)\right]\right\}$$

...(٣.٩٠)

Where subscript o on the gas emissivity term refers to the gas emissivity at atmospheric pressure

τ air to fuel ratio (defined as $(1/\phi)$)

sg specific gravity of the fuel

The exponent of the pressure P is given by the following expression:

$$C = 4.95/(\tau + 1.5) - 0.25$$

...(٣.٩١)

The total heat transfer to the liquid fuel droplets is given by **[٣٨]**;

$$\frac{dQ_{fg}}{dt} = \sum_{i=zones} q_i$$ **...(٣.٩٢)**

The total heat transfer rate given by equation (٣.٧٠) is distributed to each zone by weighting its components with zonal mass and temperature, as follows **[٣٥]**;

$$\frac{dQ_i}{dt} = -q_i \frac{m_i T_i}{m_m T_m + m_i T_i} - \frac{dQ_{Convection}}{dt} . \frac{m_i T_i}{\sum_{i=zones} m_i T_i} - \frac{dQ_{Radiation}}{dt} . \frac{m_i T_i^4}{\sum_{i=zones} m_i T_i^4}$$

...(٣.٩٣)

In terms of crank angle degree Eq.(٣.٩٣) becomes:

$$\frac{dQ_i}{d\theta} = \frac{dQ_i}{dt} . \frac{1}{360.rps}$$ **...(٣.٩٤)**

Where: rps is the engine speed in revolution per second.

٣.٦ The Power Cycle Model

In a conventional compression ignition engine air alone is compressed through the intake valve into the cylinder, where mixing with residual gas takes place. Then it is raised to a high temperature during the compression stroke, so that rapid instantaneous ignition of fuel is possible after it has been injected in to the combustion chamber **[١٠]**. Then, expansion stroke begins and continues until the exhaust valve opening. Each of the processes is discussed to complete engine power cycle simulation.

٣.٦.١ Compression Process

The compression starts at the trapped condition, and ends after delay period process. The state of gas during the process is derived by using a perfect mixing model for the fresh charge and residuals from the previous cycle **[٤]**. The first law of thermodynamic for a closed system is;

$$\frac{dQ_w}{d\theta}=\frac{dE_{comp}}{d\theta}+\frac{dW}{d\theta}$$ [kJ/Degree]

...(٣.٩٥)

Where

dQ_w heat transfer rate to the cylinder wall [kJ], and is computed as in section (٣.٥)

dE_{comp} change of internal energy of the system [kJ], and is computed from internal energy section (٣.٤.١).

dW work transfer to the system [kJ].

$$\frac{dW}{d\theta}=P.\frac{dV}{d\theta}$$

...(٣.٩٦)

And from definition of internal energy and specific heat;

$$\frac{dE_{comp}}{d\theta}=N_{comp}.C_{v_{comp}}\left(T_{comp}\right).\frac{dT_{comp}}{d\theta}$$

...(٣.٩٧)

A combination of equations (٣.٩٥), (٣.٩٦) and (٣.٩٧) after rearrangement gives;

$$\frac{dQ_w}{d\theta}=N_{comp}.C_{v_{comp}}\left(T_{comp}\right).\frac{dT_{comp}}{d\theta}+P\frac{dV}{d\theta}$$

...(٣.٩٨)

By differentiating the state equation

$\left(P.V = N_{comp}.R_{mol}.T_{comp}\right)$ with respect to crank angel θ, the following equation is obtained to calculate the change in temperature during the time step;

$$\frac{dT_{comp}}{d\theta} = T_{comp}.\left[\frac{1}{P}.\frac{dP}{d\theta} + \frac{1}{V}.\frac{dV}{d\theta}\right]$$

...(٣.٩٩)

By combination equation (٣.٩٨) with (٣.٩٩) the following equation is obtained to calculate the change in pressure during the time step

$$\frac{dP}{d\theta} = \left[-\left(1 + \frac{R_{mol}}{C_{v_{comp}}\left(T_{comp}\right)}\right).P.\frac{dV}{d\theta} + \frac{R_{mol}}{C_{v_{comp}}\left(T_{comp}\right)}.\frac{dQ_w}{d\theta}\right]/V$$

...(٣.١٠٠)

Equations (٣.٩٩) and (٣.١٠٠) are solved by Runge-Kutta method to calculate the cylinder temperature and pressure respectively during each time step.

٣.٦.٢ Injection and Combustion Processes

A-Fuel Injection

The timing and rate of fuel injection into the combustion chamber affect the spray dynamics and combustion characteristic. If the pressure up stream of the injector is known, and assuming the flow through each nozzle is quasi-steady, incompressible, and one dimensional, the mass flow rate of fuel injected through the nozzle, m_i is given by **Heywood [٢٦]**;

$$m_{i} = C_D.A_n.\sqrt{2\rho_l.\Delta P}$$

...(٣.١٠١)

Where C_D discharge coefficient equal to ٠.٦٦.

A_n nozzle area [m^{٢}].

ρ_l density of liquid fuel [kg/m^{٣}].

ΔP pressure drop across the injector nozzle [N/m^{٢}].

Since

$$\dot{m}_i = \rho_l . A_n . u_i$$ **...(٣.١٠٢)**

The fuel injection velocity at the nozzle tip, u_i can be expressed as:

$$u_i = C_D . \sqrt{2\Delta P / \rho_l}$$

...(٣.١٠٣)

B-Fuel Spray Penetration

Unlike multi-dimensional models in which the combustion chamber is taken as the computational domain, only the fuel spray is divided into a number of zones in the multizone model. The control volume of each zone is treated as open system, the mass and energy equations are solved for each zone. Instead of solving the full momentum equation, which is one of the dominant reasons for the computational inefficiency of multi-dimensional models. In the multizone model a simplified momentum equation is applied based on prescribed spray penetration and mass of fuel injected. Utilizing this method, quasi-dimensional models can offer the fastest and least expensive means of generating the spatial information required to predict emission products. Since the multizone model depends on empirical correlations for spray evolution, the fidelity of the spray penetration is crucial for accuracy. **Fig.(٣.٤)** shows the main parameters that express the aspect of a spray.

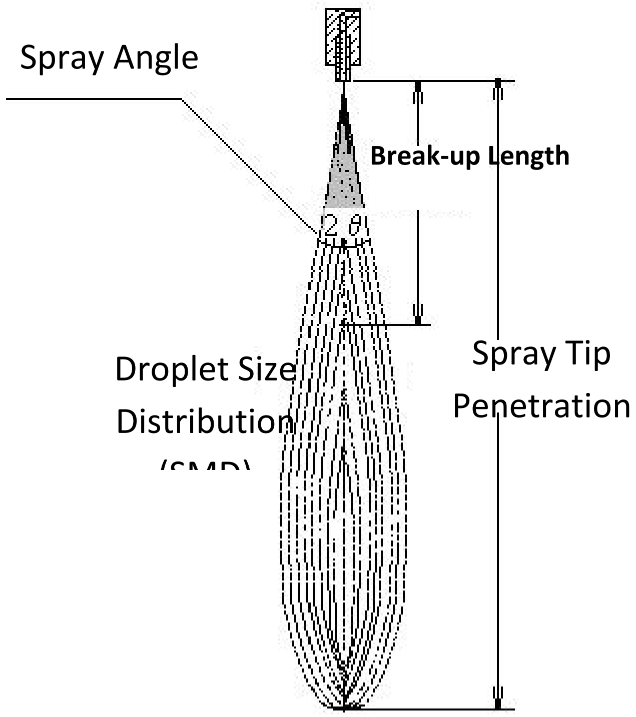


Fig.(٣.٤) Schematic of Diesel Fuel Spray Defining Its Major Parameters [٢٧].

Hiroyasu and Arai [٢٨] proposed the following correlations for spray penetration before and after breakup;

Before breakup, $0 < t < t_b(l)$

$$S = 0.39\left(\frac{2.\Delta P}{\rho_l}\right)^{0.5}.t$$

...(٣.١٠٤)

After breakup, $t \geq t_b$

$$S = 2.95\left(\frac{\Delta P}{\rho_a}\right)^{0.25}(d_n.t)^{0.5}$$

...(٣.١٠٥)

Where t_b is breakup time given as:

$$t_b = 28.65\frac{\rho_l.d_n}{(\rho_a.\Delta P)^{0.5}}$$

...(٣.١٠٦)

S spray penetration [m].

ΔP pressure drop through the nozzle hole [N/m٢].

ρ_l density of fuel [kg/m٣].

d_n nozzle hole diameter [m].

And subscript l and a denote liquid fuel and ambient gas respectively.

The value used in equations (٣.١٠٤) and (٣.١٠٥) for the discharge coefficient of the nozzle was ٠.٣٩ **[٣٥]**. However, the discharge coefficient depends on the nozzle geometry which is in modern diesel engine usually ranges between ٠.٦ and ٠.٨. To generalize the **Hiroyasu** correlations, and to allow for values of discharge coefficient other than ٠.٣٩, their correlation is modified as follows **[٢٨]**:

Before breakup, $0 < t < t_b(l)$

$$S = C_D\left(\frac{2\Delta P}{\rho_l}\right)^{0.5}.t$$

...(٣.١٠٧)

After breakup, $t \geq t_b$

$$S = 2.95\left(\frac{\Delta P}{\rho_a}\right)^{0.25} .(d_n.t)^{0.5}$$

...(٣.١٠٨)

Where breakup time, t_b, is

$$t_b = 4.351\frac{\rho_l.d_n}{C_D{}^2(\rho_a.\Delta P)^{0.5}}$$

...(٣.١٠٩)

A detailed derivation of the above correlation is given in the **Appendix (C)**.

C-Spray Angle

One of the most used correlations for spray angle calculations is that suggested by **Hiroyasu and Arai [٢٨]**. This correlation is used in this work.

$$\alpha = 0.025\left(\frac{\rho_a.\Delta P.dn^2}{\mu_a^2}\right)^{0.25}$$

...(٣.١١٠)

Where μ_a is the viscosity of ambient gas.

D-Droplet Diameter after Breakup

Following breakup, all droplets in a zone are assumed to have same initial diameters, which is equal to the Sauter mean diameter (SMD), thus, neglecting droplet size distribution and the details of the atomization process.

The following equations **[٢٩]** which are commonly used in the multizone model, give the sauter mean diameter d_{32} in the zone located along spray center line, with the radial SMD assumed to be fixed. However, allowance is made for droplet size variations from one fuel parcel to the next depending on the operating conditions

$$\frac{d_{32}}{d_n} = MAX\left(\left(\frac{d_{32}}{d_n} \right)_1, \left(\frac{d_{32}}{d_n} \right)_2 \right)$$

...(٣.١١١)

Where

$$\left(\frac{d_{32}}{d_n} \right)_1 = 4.12 \mathrm{Re}_i^{0.12} . We_i^{-0.75} . \left(\frac{\mu_l}{\mu_m} \right)^{0.45} . \left(\frac{\rho_l}{\rho_m} \right)^{0.18}$$

...(٣.١١٢)

$$\left(\frac{d_{32}}{dn} \right)_2 = 0.38 \mathrm{Re}_i^{0.25} . We_i^{-0.32} . \left(\frac{\mu_l}{\mu_m} \right)^{0.37} . \left(\frac{\rho_l}{\rho_m} \right)^{-0.47}$$

...(٣.١١٣)

$$\mathrm{Re}_i = \frac{\rho_l . u_i . d_n}{\mu_m}$$

...(٣.١١٤)

$$We_i = \frac{u_i^2 . d_n . \rho_l}{\sigma_f}$$

...(٣.١١٥)

σ_f is the surface tension of fuel.

By using the above equations and assuming normal distributions, initial diameter of liquid fuel droplets right after the breakup time in each zone is calculated. Therefore; the number of droplets in each zone can be determined knowing the sauter mean diameter and the mass of fuel injected.

E-Mixture Entrainment

Mixture entrainment (hydrogen+air) rate into a given zone is controlled by the conservation of momentum applied to that zone. It is assumed that the initial momentum imparted in a zone upon nozzle exit is equal to the momentum of the zone at any subsequent distance traveled **[٣٥]**, i.e.

$$m_f . u_i = \left(m_f + m_m\right)\left(\frac{dS}{dt}\right)$$

...(٣.١١٦)

Where $\left(\frac{dS}{dt}\right)$ is the velocity of zone (m/sec)

m_f mass of fuel in a zone.

m_m mass of mixture entrainment in the zone.

Therefore; the amount of entrained mixture in a zone is proportional to the decrement in the zone velocity. Equation (٣.١١٣) can be rewritten as;

$$m_m = m_f \left(\frac{u_i}{\frac{dS}{dt}} - 1\right)$$

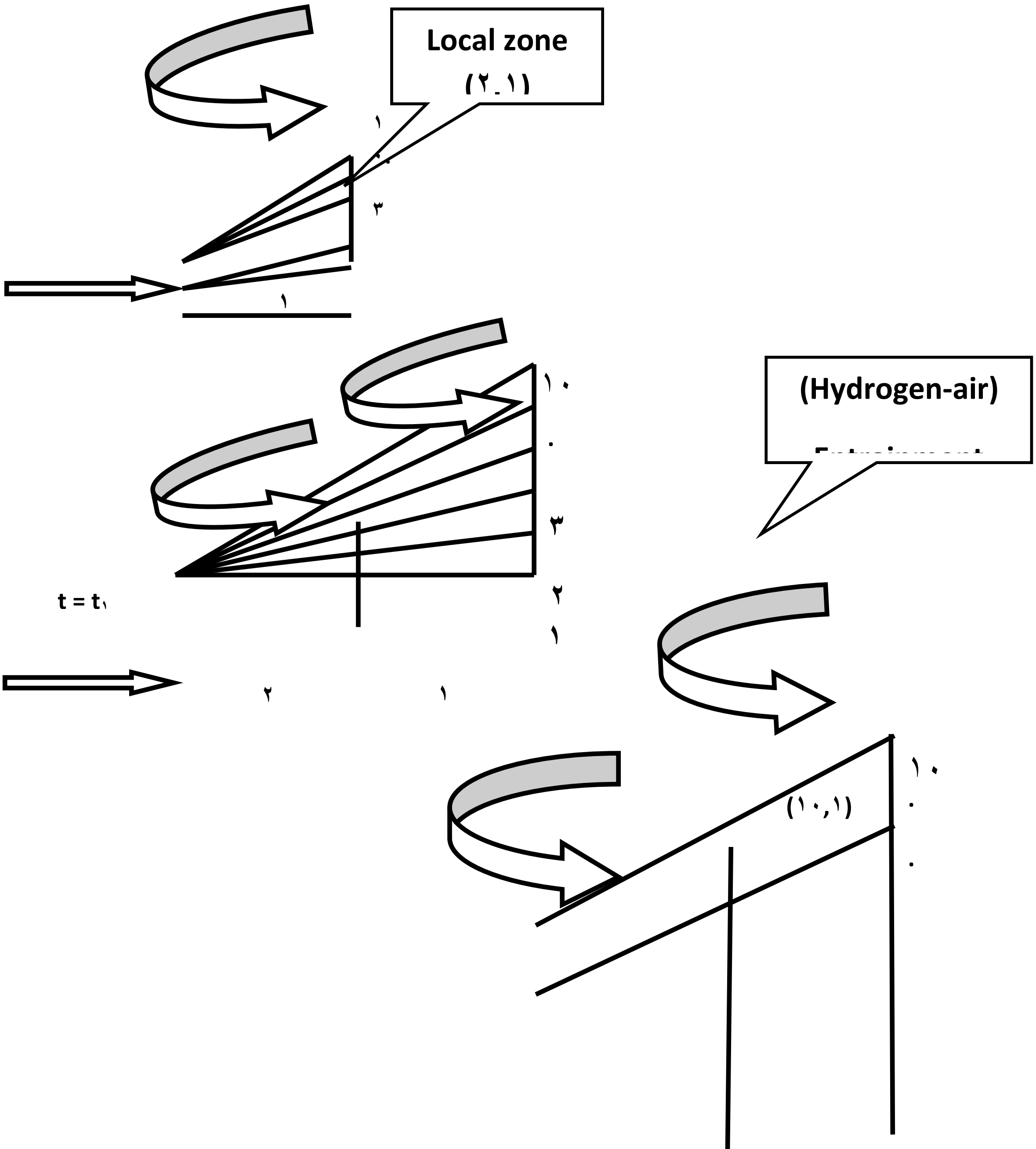
...(٣.١١٧)

By differentiating equation (٣.١١٧) with respect to time, the mixture entrainment rate can be obtained as;

$$\frac{dm_m}{dt} = -\frac{m_f . u_i}{\left(\frac{dS}{dt}\right)^2} . \frac{d^2S}{dt^2}$$

...(٣.١١٨)

The schematic of parcel development and mixture entrainment during fuel injection is shown in **Fig.(٣.٥)**



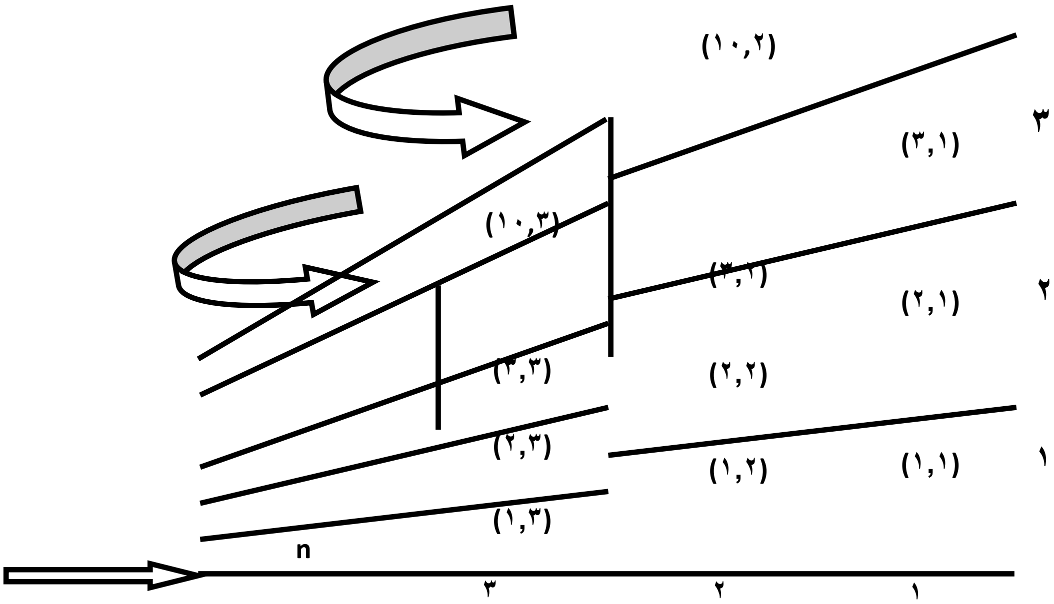


Fig.(٣.٥) Schematic of Parcel Development and Mixture Entrainment During Fuel Injection [٤٠].

F-Fuel Evaporation

Following the breakup period, its postulated that liquid fuel in zones is atomized into fine droplets of size equal to the (SMD). Each individual zone has its own initial SMD. Together with the amount of fuel contained in the zone, the initial droplet size gives the number of droplets, N_d contained within a zone **[٣٥]** ;

$$N_d = \frac{m_{i,j}}{\pi d_{32}^3 . \rho_l / 6}$$

...(٣.١١٩)

Where $m_{i,j}$ is the fuel mass injected into a local zone

The number of droplets in a zone is not changed. However; the diameter of all droplets within a zone decreases during the process due to evaporation. At any instance, the mean diameter of droplets d_l in a zone is given by **[٣٥]** :

$$d_l = \left[6\left(m_{l,i} - \int dm_{fg}\right) / \pi N_d \rho_l\right]^{1/3}$$

...(٣.١٢٠)

Where m_{fg} is the mass of gaseous fuel

The rate of evaporation is determined by combining equations governing mass diffusion and heat transfer. The rate of diffusion of vapor away from the droplet is given by **[٨]**:

$$\frac{dm_{fg}}{dt} = -\frac{dm_l}{dt}$$

$$= \pi . d_l . N_d . D_v . Sh \frac{P_t}{R_v . T_m} . \ln\left(\frac{P_t}{P_t - P_{sat.f}}\right)$$

...(٣.١٢١)

Where

$$T_m = \frac{T_a + T_l}{2}$$

...(٣.١٢٢)

D_v mass diffusivity.

P_t total pressure.

R_v specific gas constant.

T_a ambient gas temperature.

The partial pressure of fuel vapor at droplet surface $P_{sat.f}$ is equal to the saturation pressure corresponding to the temperature of the droplet **[٦٥]**.

During the evaporation process convective heat transfer from the hot gas to liquid fuel droplets in a zone is modeled following the methodology of **Gosman and Johns [٢٠]**.

$$q = \pi . d_l . N_d . K_m (T_g - T_l) . Nu . f_b \qquad \text{...(٣.١٢٣)}$$

Where T_g & T_l are bulk temperature of gas and liquid droplet respectively.

K_m mean thermal conductivity that is defined as;

$$K_m = (1 - P_{sat.f} / 2P_t) K_a + (P_{sat.f} / 2P_t) K_v$$

...(٣.١٢٤)

Where K_a thermal conductivity of ambient gas.

K_v thermal conductivity of vaporized fuel.

Expression for the Nusselt number are obtained from the following correlations proposed by **[٣٥]** for a single droplet;

$$Nu = 2 + 0.6 \mathrm{Re}_d^{1/2} . \mathrm{Pr}^{1/3}$$

...(٣.١٢٥)

The Reynolds and Prandtl numbers are defined as follows;

$$\mathrm{Re}_d = \frac{\rho_m . u . d_l}{\mu_m}$$

...(٣.١٢٦)

$$\Pr = \frac{C_{p_m}\mu_m}{K_m}$$

...(٣.١٢٧)

The mean values in the above expressions are:

$$\rho_m = \frac{Pt.M_m}{R_{mol}.T_m}$$

...(٣.١٢٨)

$$M_m = (1 - P_{sat.f}/2Pt).M_a + (P_{sat.f}/2Pt).M_v$$

...(٣.١٢٩)

$$\mu_m = (1 - P_{sat.f}/2Pt).\mu_a + (P_{sat.f}/2Pt).\mu_v$$

...(٣.١٣٠)

$$C_{p_m} = (1 - P_{sat.f}/2Pt).C_{p_a} + (P_{sat.f}/2Pt).C_{p_v}$$

...(٣.١٣١)

Where subscript a & v denote ambient gas and fuel vapor respectively.

Expression for the Sherwood numbers is obtained from the following correlations proposed by **[٣٥]** for a single droplet;

$$Sh = 2 + 0.6\,\mathrm{Re}_d^{1/2}.Sc^{1/3}$$

...(٣.١٣٢)

The Reynolds and Schmidt numbers are defined as follows;

$$Sc = \frac{\mu_m}{\rho_m.D_v}$$ **...(٣.١٣٣)**

$D_v, \mu_a, \mu_v, K_a, K_v, C_{p_a}, C_{p_v}$ are evaluated at temperature T_m while $P_v, \rho_l and C_{p_l}$ are evaluated at T_l. To correct these effects of boundary layer thickening due to mass transfer, the heat transfer coefficient in equation (٣.١٢٣) is multiplied by a factor f_b which is given by **[٢٠]**;

$$f_b = \frac{Z}{(\exp(Z) - 1)}$$

...(٣.١٣٤)

$$Z = \frac{C_{p_v} . \frac{dm_{f,g}}{dt}}{\pi d_l N K_m Nu}$$

...(٣.١٣٥)

The resulting rate of liquid fuel temperature rise is given by the energy balance as:

$$\frac{dT_l}{dt} = \frac{1}{m_l . C_{p_l}} \left(q - \lambda_f \frac{dm_{f,g}}{dt} \right)$$

...(٣.١٣٦)

Where λ_f specific heat of vaporization of liquid fuel given in **Appendix (D)**.

G-Ignition Delay

Ignition delay period can be calculated as the difference between the time at which the ignition starts t_{ign}, and the time at which injection starts t_{inj}.

In general, the ignition delay is a complicated function of mixture temperature, pressure, equivalence ratio, and fuel properties. For the purpose of diesel combustion simulations, a simplified Arrhenius expression has been used **[٦٥]**.

$$\tau = 3.45P^{-1.02}\exp\left(\frac{2100}{T}\right)$$

...(٣.١٣٧)

Where P gas pressure at the moment of injection [atm].

T gas temperature at the moment of injection [K].

٣.٦.٣ Combustion Process

٣.٦.٣.١ Conservation of Mass

The rate of change of total mass in any open system is equal to the sum of the flow rates into and out of the system **[٣]**.

$$\dot{m}_i = \sum \dot{m}_{i,j}$$

...(٣.١٣٨)

Where $\dot{m}_i$ mass flow rate in parcel of fuel i

$\dot{m}_{i,j}$ mass flow rate in local zone

During the intake and compression processes only (hydrogen-air) zone which is considered as a closed system, exits inside the cylinder. Once the fuel is injected, spray zones are generated inside the cylinder. Each zone is considered as an open system. Mixture entrainment is the mass flow for each spray zone. In particular conservation of the fuel species can be expressed as;

$$m^{\cdot}_{fi} = \sum m^{\cdot}_{fi,j}$$

...(٣.١٣٩)

Where $m^{\cdot}_{fi}$ denotes the fuel content in parcel i. Defining the fuel fraction, F_i in the system as **[٣]**;

$$F_i = \frac{m_{fi}}{m_i}$$ **...(٣.١٤٠)**

Where m_i is the total mass in the parcel i

m_{fi} is mass of fuel in the parcel i

Equation (٣.١٣٩) can be rewritten as:

$$\frac{d(m_i F_i)}{dt} = \sum m^{\cdot}_{i,j} F_{i,j}$$

...(٣.١٤١)

Where $F_{i,j}$ denotes the fuel fraction in local zone. Differentiating the left hand side of equation (٣.١٤١) and substituting for $m^{\cdot}_i$ from equation (٣.١٣٨) results in a differential equation for the change in the fuel fraction of the open system i.e.

$$\dot{F_i} = \frac{\sum \dot{m}_{i,j}}{m_i}\left(F_{i,j} - F_i\right)$$ **...(٣.١٤٢)**

An average fuel-air equivalence ratio, ϕ, for the content of the open system can be defined as:

$$\phi = \frac{\left(m_f / m_a\right)_{act}}{\left(m_f / m_a\right)_S}$$

...(٣.١٤٣)

Expressing the equivalence ratio in terms of the fuel fraction and differentiating with respect to time, an equation for the rate of change of the equivalence ratio of the zone is obtained **[٣]**;

$$\dot{\phi_i} = \frac{1}{\left(m_{fi} / m_{ai}\right)_S} \cdot \frac{\dot{F_i}}{\left(1 - F_i\right)^2}$$

...(٣.١٤٤)

٣.٦.٣.٢ Conservation of Energy

The first law of thermodynamic supplemented with a heat transfer model can be applied to yield cylinder pressure and temperature of the spray zones and (hydrogen- air) zone. Treating the contents of each zone as an ideal gas, with thermodynamic properties that are functions of temperature, pressure and fuel-air equivalence ratio an equation for the time rate of change of pressure is obtained **[٣]**:

$$\frac{dP}{dt}=\frac{\rho}{d\rho/dP}\left(-\frac{V^{\cdot}}{V}-\frac{1}{\rho}\frac{dP}{dT}\frac{dT}{dt}-\frac{1}{\rho}\frac{d\rho}{d\phi}\frac{d\phi}{dt}+\frac{m^{\cdot}}{m}\right)$$

...(٣.١٤٥)

In terms of crank angle degree

$$\frac{dP}{d\theta}=\frac{dP}{dt}.\frac{1}{360.rps}$$

...(٣.١٤٦)

And

$$mCp\frac{dT}{dt}=\sum m^{\cdot}_{j}h_{j}+\frac{dQ}{dt}+\left(V-C_{T}\right)\frac{dP}{dt}-mC_{\phi}\frac{d\phi}{dt}-m^{\cdot}h$$

...(٣.١٤٧)

The first term in equation (٣.١٤٧) is the net rate of influx of enthalpy, $\frac{dQ}{dt}$ is the total heat transfer rate to the system and it is computed as in section (٣.٢.٥). Heat release due to combustion is treated as the difference of enthalpy of products and the enthalpy of reactants.

By substituting for $\frac{dP}{dt}$ from equation (٣.١٤٦) an equation for the rate of change of temperature that does not explicitly depend on the rate of change of pressure of the system is obtained;

$$\frac{dT}{dt}=\frac{B}{A}\left[\frac{m^{\cdot}}{m}\left(1-\frac{h}{B}\right)-\frac{V^{\cdot}}{V}-\frac{C}{B}\frac{d\phi}{dt}+\frac{1}{Bm}\left(\sum_{j}m^{\cdot}_{j}h_{j}+\frac{dQ}{dt}\right)\right]$$

...(٣.١٤٨)

Where

$$A = Cp + \frac{(d\rho/dT)}{(d\rho/dP)}\left(\frac{1}{\rho} - C_T\right)$$

...(٣.١٤٩)

$$B = \frac{1}{(d\rho/dP)}(1 - \rho C_T)$$

...(٣.١٥٠)

$$C = C_\phi + \frac{(d\rho/d\phi)}{(d\rho/dP)}\left(\frac{1}{\rho} - C_T\right)$$

...(٣.١٥١)

And in terms of crank angle degree

$$\frac{dT}{d\theta} = \frac{dT}{dt}.\frac{1}{360.rps}$$ **...(٣.١٥٢)**

A detailed derivation of equations (٣.١٤٦) and (٣.١٤٨) are given in **Appendix (E)**. The energy equation for each zone as an open thermodynamic system can be expressed from equation (٣.١٤٧) as **[٣٥]**;

$$m_i Cp_i \frac{dT_i}{dt} = \sum \dot{m}_{i,j} h_{i,j} + \frac{dQ_i}{dt} + (V_i - C_{Ti})\frac{dP_i}{dt} - m_i C_{\phi i}\frac{d\phi_i}{dt} - \dot{m}_i h_i$$

...(٣.١٥٣)

Or

$$\frac{dT_i}{dt} = \left[\ \sum \dot{m}_{i,j} h_{i,j} + \frac{dQ_i}{dt} + (V_i - C_{Ti})\frac{dP_i}{dt} - m_i C_{\phi i}\frac{d\phi_i}{dt} - \dot{m}_i h_i\ \right] / \dot{m}_i Cp_i$$

...(٣.١٥٤)

Equations (٣.١٤٦), and (٣.١٤٨), are solved by Runge-Kutta method to calculate the cylinder pressure and zonal temperature respectively during each time step.

٣.٧ Heat Release during Premixed and Diffusion Combustion Phases

During the ignition delay period, some of the injected fuel is evaporated and mixed with mixture of air and hydrogen, forming a combustible mixture. Following ignition, the first phase of combustion occurs under premixed conditions at a rate RRp given by the following Arrhenius type kinetic equation **[٤٦]**;

$$RRp = B1.\rho_{mix}^{2}.X_{fv}.X_{ox}\exp\left(-\frac{1200}{T_Z}\right).V_Z$$

...(٣.١٥٥)

Where $B1$ frequency factor equal to ١.٥ given by **[٣٥]**

ρ_{mix} is the density of mixture [kg/m^{٣}]

X_{fv} mass fraction of fuel vapor.

X_{ox} mass fraction of oxygen.

T_Z zonal temperature [K]

V_Z volume of the zone (truncated cone) [m^{٣}]

Equation (٣.١٥٥) is assumed to be valid until the amount of fuel evaporated during the ignition delay period has been consumed. After this stage, the combustion is assumed to proceed to the mixing controlled and late combustion phases. Accordingly, the combustion model is formulated so that it can handle both mixing and kinetics limited combustion. Under normal conditions the combustion during the second phase is mixing limited, so it proceeds at a rate limited by the availability of fuel vapor and air entrainment. In this situation, the combustion kinetics rate is so rapid that it provides no additional limit on the combustion process. However; when the gas temperature becomes low, the combustion kinetics slow down exponentially and at some point become the limiting factor. This can occur at the latter parts of the expansion process. The kinetics can also slow down when the mixture is very lean. It is therefore proposed that the combustion rate for the mixing-controlled and late combustion phases, RRm is governed by the following expression **[٤٦]**;

$$RRm = B2.m_{f,v}.\frac{P_{ox}}{P} P^{2.5} \exp\left(-\frac{2500}{T_Z}\right)$$

...(٣.١٥٦)

Where $B2$ is constant equal to ٨٠٠ **[٣٥]**.

$m_{f,v}$ mass of fuel vapor [kg]

P_{ox} partial pressure of oxygen [kpa]

P total pressure [kpa]

٣.٨ Modeling of Combustion Products

This section covers the estimation of composition of combustion products. The calculation with complete chemical equilibrium starts from the equation of combustion of the Hydrocarbon, Hydrogen and Air which is represented by:

$$ae\left((1-\lambda).C_nH_m+\lambda H_2\right)+\frac{ae}{\phi}\left(n.(1-\lambda)+\left((m.(1-\lambda)+2\lambda)/4\right)\right).\left[O_2+\frac{78}{21}N_2+\frac{1}{21}Ar\right]\rightarrow X_{H2O}H_2O+X_{H2}H_2+X_{OH}OH+$$
$$X_HH+X_{N2}N_2+X_{NO}NO+X_NN+X_{CO2}CO_2+X_{CO}CO+X_{O2}O_2+X_OO+X_{Ar}Ar+Soot$$

...(٣.١٥٧)

The composition is calculated in terms of molar fractions of these species denoted by X_i. The equation assumes that one mole of the total products is generated from ae mole of fuel plus ($١/\phi$) times the stoichiometric quantity of air. The number of carbon atoms in one mole of fuel is $\{n(1-\lambda)\}$ and the number of hydrogen atoms in one mole of the fuel is $\{m(1-\lambda)+2\lambda\}$.

The equilibrium distribution of these species can be fully described by the following seven reactions **[٢٦]**.

(١) $\frac{1}{2}H_2 \leftrightarrow H$

...(٣.١٥٨)

(٢) $\frac{1}{2}O_2 \leftrightarrow O$

...(٣.١٥٩)

(٣) $\frac{1}{2}N_2 \leftrightarrow N$ **...(٣.١٦٠)**

(٤) $2H_2O \leftrightarrow 2H_2+O_2$ **...(٣.١٦١)**

(٥) $H_2O \leftrightarrow OH + H$ **...(٣.١٦٢)**

$$(٦)\quad CO_2 + H_2 \leftrightarrow H_2O + CO$$

...(٣.١٦٣)

$$(٧)\quad H_2O + \frac{1}{2}N_2 \leftrightarrow H_2 + NO$$

...(٣.١٦٤)

The equilibrium constants for these reactions are;

$$(١)\quad k_{p1} = \frac{X_H}{\sqrt{XH_2}}.\sqrt{P}$$

...(٣.١٦٥)

$$(٢)\quad k_{p2} = \frac{X_O}{\sqrt{XO_2}}.\sqrt{P}$$

...(٣.١٦٦)

$$(٣)\quad k_{p3} = \frac{X_N}{\sqrt{XN_2}}.\sqrt{P}$$

...(٣.١٦٧)

$$(٤)\quad k_{p4} = \frac{X_{O_2}}{b^2}.\sqrt{P}$$

...(٣.١٦٨)

$$(٥)\quad k_{p5} = \frac{X_{OH}}{b^2\sqrt{XH_2}}.\sqrt{P}$$

...(٣.١٦٩)

$$(٦)\quad k_{p6} = \frac{b.X_{CO}}{X_{CO_2}}$$

...(٣.١٧٠)

(٧) $k_{p7} = \frac{X_{NO}}{b\sqrt{XN_2}}.\sqrt{P}$

...(٣.١٧١)

Where ratio of water vapor mole fraction to hydrogen mole fraction is given by **[٢].**

$$b = \frac{X_{H2O}}{X_{H2}}$$

...(٣.١٧٢)

The equilibrium constants k_p for these reactions are calculated by the method described in section (٣.٢.٤.٢).

There are ١٣ unknowns in equation (٣.١٥٧), namely ١٢ mole fractions X_i and the total number of moles of fuel ae. Seven equations are available (٣.١٦٥-٣.١٧١), therefore five more equations are needed for the solution.

One of these is:

$$\sum_{i=1}^{i=12} X_i = 1$$

...(٣.١٧٣)

The remainders are the atomic balances for carbon, hydrogen, oxygen, and nitrogen. Let the number of atoms of Ar, C, H, O, and N corresponding to ١ mole of fuel by VE, WE, XE, LE, and ZE respectively, and noting that (ae) moles of fuel corresponds to ١ mole of products. Therefore the atomic balance can be made as follows;

Argon: $X_{Ar} = ae.VE$

...(٣.١٧٤)

Carbon: $X_{CO} + X_{CO_2} = ae.WE$

...(٣.١٧٥)

Hydrogen: $2X_{H_2O} + 2X_{H_2} + X_{OH} + X_H = ae.XE$

...(٣.١٧٦)

Oxygen: $X_{H_2O} + X_{OH} + X_{NO} + 2X_{CO_2} + X_{CO} + 2X_{O_2} + X_O = ae.LE$

...(٣.١٧٧)

Nitrogen: $2X_{N_2} + X_{NO} + X_N = ae.ZE$

...(٣.١٧٨)

The values of VE, WE, XE, LE, and ZE are known from fuel-air reaction equation (٣.١٥٧). Noting that ae fuel mole is represented by $((1-\lambda)C_nH_m + \lambda H_2)$ and the zonal equivalence ratio by ϕ , the following relationships are obtained.

$$LE = \frac{1}{\phi}.\left(2n.(1-\lambda) + \frac{m}{2}.(1-\lambda) + \lambda\right)$$

...(٣.١٧٩)

$$WE = n.(1-\lambda)$$ ...(٣.١٨٠)

$$XE = m.(1-\lambda) + 2\lambda$$

...(٣.١٨١)

$$ZE = LE.\frac{78}{21}$$

...(٣.١٨٢)

$$VE = \frac{1}{2}.LE.\frac{1}{21}$$

...(٣.١٨٣)

Values of ae and b are calculated as follows **[٢]**; the first estimate of the parameters (ae) and (b) is made by using the following expressions where ϕ the equivalence ratio, P is the pressure in atmosphere and T is the temperature in Kelvin

For $\phi \geq 1.0$

$$ae = \frac{1.3}{[WE + 0.5XE + 1.863(2WE + 0.5XE)/\phi].\exp(0.13T/1000)}$$

...(٣.١٨٤)

And for $\phi \prec 1.0$

$$ae = \frac{1.3}{[0.25XE + 2.363(2WE + 0.5XE)/\phi].\exp(0.13T/1000)}$$

...(٣.١٨٥)

For temperature T $\succ$ ٣٠٠٠ °K an expression for b is given by **[٢]**

$$b = \exp(10.3 - (3.1 - 0.17Log(P)).T/1000)$$

...(٣.١٨٦)

And for temperature T $\leq$ ٣٠٠٠ °K another expression for b is given by **[٢]**

$$b = \exp(-9.0 - 0.5Log(P) + 30000/T)$$

...(٣.١٨٧)

Adjust b for the following case **[٢]**,

$$BX = 2.0 - 9.0 Log(\phi)$$

...(٣.١٨٨)

If $BX \succ 3.5$

$$BE = \exp(\exp(3.5) + 0.25 Log(P))$$

...(٣.١٨٩)

If $BX \leq 3.5$

$$BE = \exp(\exp(2.0 - 9.0 Log(\phi) + 0.25 Log(P)))$$

...(٣.١٩٠)

If $b > BE$, then use;

$$b = BE$$

...(٣.١٩١)

To evaluate the above ١٢ mole fractions, the following procedure is used.

Using equations (٣.١٦٥), (٣.١٦٩), (٣.١٧٢), and (٣.١٧٦) the mole fraction of hydrogen is obtained;

$$X_{H_2} = \left[\frac{-\left(\frac{k_{p5}}{\sqrt{P}}.b + \frac{k_{p1}}{\sqrt{P}} \right) + \sqrt{\left(\frac{k_{p5}}{\sqrt{P}}.b + \frac{k_{p1}}{\sqrt{P}} \right)^2 + 4(2b+2).ae.XE}}{4(b+1)} \right]^2$$

...(٣.١٩٢)

From equation (٣.١٧٢) the mole fraction of water vapor is obtained;

$$X_{H_2O} = b.X_{H_2}$$

...(٣.١٩٣)

And from equation (٣.١٦٩) the mole fraction of hydroxyl is obtained;

$$X_{OH} = \frac{k_{p5}.b.\sqrt{X_{H_2}}}{\sqrt{P}}$$

...(٣.١٩٤)

From equation (٣.١٦٥) the mole fraction of atomic hydrogen is obtained;

$$X_{H} = \frac{k_{p1}.\sqrt{X_{H_2}}}{\sqrt{P}}$$

...(٣.١٩٥)

By using equation (٣.١٧٠) and (٣.١٧٥) the mole fraction of carbon dioxide is obtained;

$$X_{CO_2} = \frac{ae.WE}{\left[\frac{k_{p6}}{b}+1\right]}$$

...(٣.١٩٦)

From equation (٣.١٧٥) the mole fraction of carbon monoxide is obtained;

$$X_{CO} = ae.WE - X_{CO_2}$$

...(٣.١٩٧)

Using equation (٣.١٦٧), (٣.١٧١), and (٣.١٧٨) the mole fraction of nitrogen is obtained;

$$X_{N2} = \left[\frac{ -\left(\frac{k_{p7}}{\sqrt{P}}.b + \frac{k_{p3}}{\sqrt{P}} \right) + \sqrt{ \left(\frac{k_{p7}}{\sqrt{P}}.b + \frac{k_{p3}}{\sqrt{P}} \right)^2 + 8.ae.ZE } }{4} \right]^2$$

...(٣.١٩٨)

From equation (٣.١٦٧) the mole fraction of atomic nitrogen is obtained;

$$X_N = \frac{k_{p3}.\sqrt{X_{N_2}}}{\sqrt{P}}$$

...(٣.١٩٩)

And from equation (٣.١٧١) the mole fraction of nitric oxide is obtained;

$$X_{NO} = \frac{k_{p7}.b.\sqrt{X_{N_2}}}{\sqrt{P}}$$

...(٣.٢٠٠)

And from equation (٣.١٦٨) the mole fraction of oxygen is obtained;

$$X_{O_2} = \frac{k_{p4}.b^2}{P}$$

...(٣.٢٠١)

And from equation (٣.١٦٦) the mole fraction of atomic oxygen is obtained;

$$X_O = \frac{k_{p2}.\sqrt{X_{O_2}}}{\sqrt{P}}$$

...(٣.٢٠٢)

Finally from equation (٣.١٧٤) the mole fraction of argon is obtained;

$$X_{Ar} = ae.VE$$

...(٣.٢٠٣)

٣.٩ Modeling of Nitric Oxide Formation

While nitric oxide (NO) and nitrogen dioxide (NO_2) are usually grouped together as (NO_X) emissions, NO is predominant in diesel engines **[٢٦]**. Therefore; only NO formation is considered in the present study. The principle reactions governing the formation of NO from molecular nitrogen and its destruction are **[٤١]**: $N + NO \xleftrightarrow{k_{1f}} N_2 + O$

...(٣.٢٠٤)

$$N + O_2 \xleftrightarrow{k_{2f}} NO + O$$

...(٣.٢٠٥)

$$N + OH \xleftrightarrow{k_{3f}} NO + H$$

...(٣.٢٠٦)

Where forward rate constants, k_{1f}, k_{2f} and k_{3f} are:

$$k_{1f} = 7.6 \times 10^{13} \exp\left(-\frac{38000}{T}\right)$$

...(٣.٢٠٧)

$$k_{2f} = 6.4 \times 10^{9} T.\exp\left(-\frac{3150}{T}\right)$$

...(٣.٢٠٨)

$k_{3f} = 4.1 \times 10^{13}$

...(٣.٢٠٩)

These equations are exothermic left to right. The values of k_{1f}, k_{2f} and k_{3f} for the forward reactions are taken from Ref. **[٢٦]**. The reverse rate constant for a particular reaction is simply the forward rate constant divided by the equilibrium constant. Only forward rate reactions are considered in the present work because it has greater effect than backward reaction **[٢٦]**.

This is often called the extended **Zeldovich's** mechanism. **Zeldovich** was the first who suggests the importance of reactions (٣.٢٠٤) and (٣.٢٠٥). **Lavoie et al. [٤٦]** added reaction (٣.٢٠٦) to the mechanism. The rate of change of NO concentration in local zone is expressed as **[٢٦]**:

$$\frac{d[NO]}{d\theta} = \frac{2R1\left\{1-\left([NO]/[NO]_e\right)^2\right\}}{1+\left([NO]/[NO]_e\right)R1/\left(R2+R3\right)} \cdot \frac{1}{rps}$$

...(٣.٢١٠)

Where

$[\ ]$ Denotes species concentration in Kilomoles per cubic meter.

Subscript e means equilibrium.

$R1 = k_{1f}[NO]_e[N]_e$

...(٣.٢١١) $R2 = k_{2f}[NO]_e[O]_e$

...(٣.٢١٢) $R3 = k3f[N]_e[OH]_e$

...(٣.٢١٣)

٣.١٠ Modeling of Soot Formation and Oxidation

Soot is a fine dispersion of black carbon particles in a vapor carrier **[٦٢]**. The main source of soot is from the incomplete hydrocarbon combustion. Soot particles form, grow, and oxidize as a result of chemical reactions that occur during combustion.

Soot forms in the rich unburned-fuel contained in the core of fuel spray, within the flame region, where the fuel vapor is heated by mixing with hot gases.

Soot then oxidizes in the flame zone when it contacts unburned oxygen. Therefore; the concentration of soot in the exhaust is governed by the formation and oxidation of soot during the engine cycle, i.e.

$$\frac{dm_S}{d\theta} = \frac{dm_{Sf}}{d\theta} - \frac{dm_{So}}{d\theta}$$

...(٣.٢١٤)

The general fact that the net soot formation rate is primary affected by pressure, temperature and equivalence ratio. This has been fairly well established. However, the details of the mechanism leading to soot formation are not known **[٥٨]**. Consequently, semi-empirical, two rate equation models have been used to describe the soot dynamics. In particular, the soot formation model proposed by **Hiroyasu et al. [٣٥]** is used in many Multizone models. The formation rate is calculated by assuming a first order reaction of vaporized fuel, $m_{f,g}$, as **[٣٥]**:

$$\frac{dm_{Sf}}{d\theta} = A_f m_{f,g} P^{0.5} \exp\left(\frac{-E_{Sf}}{RT}\right) . \frac{1}{rps}$$

...(٣.٢١٥)

The soot oxidation is predicted by assuming a second order reaction between soot, m_S, and oxygen **[٣٥]**.

$$\frac{dm_{So}}{d\theta} = A_o m_S \frac{P_{ox}}{P} P^{1.8} \exp\left(\frac{-E_{So}}{RT}\right) \cdot \frac{1}{rps}$$

...(٣.٢١٦)

Where

$E_{Sf} = 5.23 \times 10^4$ kJ/Kmol.

$E_{So} = 5.8576 \times 10^4$ kJ/Kmol.

A_f & A_o are constants that are determined by matching the calculated smoke with the measured soot in the exhaust gas **[٣٥],** they are equal to ١٥٠ sec$^{-١}$ and ٢٢٥٠ respectively.

٣.١١ Expansion Process

Once the combustion process is complete, the cylinder is considered as a single zone with a uniform temperature and pressure. The number of moles of each species is calculated during each time step. The calculation ends at exhaust valve opening. This completes the power cycle.

The first law of thermodynamics for an open system is;

$$\frac{dQ_w}{d\theta} = \frac{dE_{\exp}}{d\theta} + \frac{dW}{d\theta}$$

...(٣.٢١٧)

Where

dQ_w Heat transfer rate to the cylinder wall [kJ], it is computed as in section (٣.٢.٥)

$dE_{\exp}$ Change of internal energy in the system [kJ] and it's computed from internal energy section (٣.٢.٤.١).

dW Work transfer from the system [kJ].

$$dW = P.\frac{dV}{d\theta}$$ **...(٣.٢١٨)**

And from definition of internal energy and specific heat;

$$\frac{dE_{\exp}}{d\theta} = N_{\exp}.Cv_{\exp}\left(T_{\exp}\right).\frac{dT_{\exp}}{d\theta}$$

...(٣.٢١٩)

A combination of equations (٣.٢١٧), (٣.٢١٨) and (٣.٢١٩) after rearrangement gives;

$$\frac{dQ_w}{d\theta} = N_{\exp}.Cv_{\exp}\left(T_{\exp}\right).\frac{dT_{\exp}}{d\theta} + P\frac{dW}{d\theta}$$

...(٣.٢٢٠)

By differentiating the state equation

$\left(P.V = N_{\exp}.R_{mol}.T_{\exp}\right)$ with respect to crank angel θ, the following equation is obtained to calculate the change in temperature during the time step;

$$\frac{dT_{\exp}}{d\theta} = T_{\exp}.\left[\frac{1}{P}.\frac{dP}{d\theta} + \frac{1}{V}.\frac{dV}{d\theta}\right]$$

...(٣.٢٢١)

By combination equation (٣.٢٢٠) with (٣.٢٢١) the following equation is obtained to calculate the change in pressure during the time step

$$\frac{dP}{d\theta}=\left[-\left(1+\frac{R_{mol}}{Cv_{\exp}\left(T_{\exp}\right)}\right).P.\frac{dV}{d\theta}+\frac{R_{mol}}{Cv_{\exp}\left(T_{\exp}\right)}.\frac{dQ_{wt}}{d\theta}\right]/V$$

...(٣.٢٢٢)

Equations (٣.٢٢١) and (٣.٢٢٢) are solved by Runge-Kutta method to calculate the cylinder temperature and pressure respectively during each time step.

During expansion stroke the cylinder contains a mixture of ١٢ species, and the calculation starts from the following equation **[٢]**.

$$\begin{bmatrix} X_{H2O}H_2O+X_{H2}H_2+X_{OH}OH+X_HH+ \\ X_{N2}N_2+X_{NO}NO+X_NN+X_{CO2}CO_2+ \\ X_{CO}CO+X_{O2}O_2+X_OO+X_{Ar}Ar \end{bmatrix}_{\theta} \rightarrow \begin{bmatrix} X_{H2O}H_2O+X_{H2}H_2+X_{OH}OH+X_HH+ \\ X_{N2}N_2+X_{NO}NO+X_NN+X_{CO2}CO_2+ \\ X_{CO}CO+x_{O2}O_2+X_OO+X_{Ar}Ar \end{bmatrix}_{\theta+1}$$

...(٣.٢٢٣)

Where (θ) Beginning of step crank angle degree.

$(\theta+1)$ End of step crank angle degree.

The equilibrium distribution of these species is the same as described by equations (٣.١٥٨-٣.١٦٤). Thus the same equations for the equilibrium constants are used (equations (٣.١٦٥-٣.١٧١)).

The atomic balance can be made as follows;

Argon:

$$X_{Ar}(\theta+1)=X_{Ar}(\theta)$$

...(٣.٢٢٤)

Carbon:

$$X_{CO_2}(\theta+1)+X_{CO}(\theta+1)=X_{CO_2}(\theta)+X_{CO}(\theta)$$

...(٣.٢٢٥)

Hydrogen:

$$2X_{H2O}(\theta+1)+2X_{H2}(\theta+1)+X_{OH}(\theta+1)+X_{H}(\theta+1)=2X_{H2O}(\theta)+2X_{H2}(\theta)+X_{OH}(\theta)+X_{H}(\theta)$$

...(٣.٢٢٦)

Oxygen:

$$X_{H2O}(\theta+1)+X_{OH}\ (\theta+1)+X_{NO}(\theta+1)+2X_{CO2}(\theta+1)+2X_{O2}(\theta+1)+X_{O}(\theta)=X_{H2O}(\theta)+X_{OH}(\theta)$$
$$+X_{NO}(\theta)+2X_{CO2}(\theta)+X_{CO}(\theta)+2X_{O2}(\theta)+X_{O}(\theta)$$

...(٣.٢٢٧)

Nitrogen:

$$2XN_2(\theta+1)+X_{NO}(\theta+1)+X_N(\theta+1)=2X_{N_2}(\theta)+X_{NO}(\theta)+X_N(\theta)$$

...(٣.٢٢٨)

To evaluate the above ١٢ mole fractions through the expansion stroke, the following procedure is used. Using equations (٣.١٧١) and (٣.٢٢٥) the mole fraction of carbon dioxide is obtained **[٢]**;

$$X_{CO_2}(\theta+1)=\frac{X_{CO_2}(\theta)+X_{CO}(\theta)}{\left[1+\frac{k_{p6}}{b}\right]}$$

...(٣.٢٢٩)

From equation (٣.٢٢٥) the mole fraction of carbon monoxide is obtained;

$$X_{CO}(\theta+1)=X_{CO_2}(\theta)+X_{CO}(\theta)-X_{CO_2}(\theta+1)$$

...(٣.٢٣٠)

Using equations (٣.١٦٧), (٣.١٧١) and (٣.٢٢٨) the mole fraction of nitrogen is obtained;

$$X_{N2}(\theta+1)=\left[\frac{-\left(\frac{kp7}{\sqrt{P}}.b+\frac{kp3}{\sqrt{P}}\right)+\sqrt{\left(\frac{kp7}{\sqrt{P}}.b+\frac{kp3}{\sqrt{P}}\right)^2+8\left(2X_{N2}(\theta)\right)+X_{NO}(\theta)+X_N(\theta)}}{4}\right]^2$$

...(٣.٢٣١)

From equation (٣.١٦٧) the mole fraction of atomic nitrogen is obtained;

$$X_N(\theta+1)=\frac{k_{p3}\cdot\sqrt{X_{N_2}(\theta+1)}}{\sqrt{P}}$$

...(٣.٢٣٢)

And from equation (٣.١٧١) the mole fraction of nitric oxide is obtained;

$$X_{NO}(\theta+1)=\frac{k_{p7}.b.\sqrt{X_{N_2}(\theta+1)}}{\sqrt{P}}$$

...(٣.٢٣٣)

Using equations (٣.١٦٥), (٣.١٦٩), (٣.١٧٢), and (٣.٢٢٦) the mole fraction of hydrogen is obtained;

$$X_{H2}(\theta+1)=\left[\frac{-\left(\frac{kp5}{\sqrt{P}}.b+\frac{kp1}{\sqrt{P}}\right)+\sqrt{\left(\frac{kp5}{\sqrt{P}}.b+\frac{kp1}{\sqrt{P}}\right)^2+8(b+1).\left(2X_{H2O}(\theta)+2X_{H2}(\theta)+X_{OH}(\theta)+X_{H}(\theta)\right)}}{4(b+1)}\right]^2$$

...(٣.٢٣٤)

From equation (٣.١٧٢) the mole fraction of water vapor is obtained;

$$X_{H_2O}(\theta+1)=b.X_{H_2}(\theta+1)$$

...(٣.٢٣٥)

From equation (٣.١٦٩) the mole fraction of hydroxyl is obtained;

$$X_{OH}(\theta+1)=\frac{k_{p5}.b.\sqrt{X_{H2}(\theta+1)}}{\sqrt{P}}$$

...(٣.٢٣٦)

From equation (٣.١٦٥) the mole fraction of atomic hydrogen is obtained;

$$X_{H}(\theta+1)=\frac{k_{p1}.\sqrt{X_{H2}(\theta+1)}}{\sqrt{P}}$$

...(٣.٢٣٧)

And from equation (٣.١٦٨) the mole fraction of oxygen is obtained;

$$X_{O_2}(\theta+1)=\frac{k_{p4}.b^2}{P}$$

...(٣.٢٣٨)

From equation (٣.٢٢٤) the mole fraction of atomic oxygen is obtained;

$$X_O(\theta+1)=\frac{k_{p2}\cdot\sqrt{X_{O_2}(\theta+1)}}{\sqrt{P}}$$

...(٣.٢٣٩)

Finally from equation (٣.١٧٩) the mole fraction of argon is obtained;

$$X_{Ar}(\theta+1)=X_{Ar}(\theta)$$

...(٣.٢٤٠)

٣.١٢ Engine Performance Calculations

This section covers engine performance parameters which include: indicated mean effective pressure, indicated power, specific fuel consumption, volumetric efficiency and finally thermal efficiency.

The indicated mean effective pressure is given by **[٢٦]**:

$$i.m.e.p=\frac{\oint work}{V_d}$$

...(٢.٢٤١)

Where

$\oint work$ summation of the work during the cycle

V_d stroke volume.

The indicated power is obtained from the following equation **[٢٦]:**

$$I.Power = (i.m.e.p) * V_d * \frac{N}{n}$$ [kW]

...(٢.٢٤٢)

Where

N engine speed rpm.

n number of power stroke and its equal to ٢ for ٤-stroke engine, and ١ for ٢-stroke engine.

A more useful parameter is the indicated specific fuel consumption "I.S.F.C" can be found from **[٢٦]** ;

$$I.S.F.C. = \frac{m^{\cdot}_f \times 3600}{I.Power}$$ [g/kW.h]

...(٣.٢٤٣)

The Indicated thermal efficiency $I.\eta_{th}$ can be defined as the ratio of the Indicated power to the energy content of the fuel supplied;

$$I.\eta_{th} = -\frac{I.Power}{m^{\cdot}_f \times Q_{vt}}$$ **...(٣.٢٤٤)**

Where: Q_{vt} is the summation of lower calorific values of the dual fuels used.

By combining equation (٣.٢٤٣) with equation (٣.٢٤٤), the efficiency can be written as follows **[٢٦]**:

$$I.\eta_{th} = -\frac{3600}{I.S.F.C. \times Q_{vt}}$$ **...(٣.٢٤٥)**

Another performance parameter of importance is the volumetric efficiency, η_V, it is defined as the mass of fuel and air induced into the cylinder divided by the mass that would occupy the displaced volume at the density ρ_i in the intake manifold [٢٦];

$$\eta_V = \frac{(m_a + m_{H_2})}{\rho_m V_d}$$ **...(٣.٢٤٦)**

where

m_a & m_{H2} mass of air and hydrogen inducted into engine respectively [kg].

ρ_m mixture density evaluated at atmospheric conditions outside the engine [kg/m^{٣}].