Multidimensional Simulation of Flow Evolution, Mixture Preparation and Combustion in a 4-Valve SI Engine

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ABSTRACT

The multidimensional computational fluid dynamics code system FIRE, consisting of a finite volume mean flow method coupled with a Monte Carlo PDF combustion model, is employed to investigate the flow evolution, mixture preparation and flame propagation process in a 4-valve spark ignition engine. The engine compression ratio is 10.3 : 1, and the study pertains to the operating condition of part load and an engine speed of 1000 rpm. The pre-combustion flow and charge composition distribution were obtained through complete simulation of the gas exchange and compression stroke, taking into account pressure wave induced back flow of in-cylinder charge into the intake port during valve overlap.

The results show the fuel deposition before intake valve opening to produce a regularily-mixed charge distribution in large areas of the combustion chamber at the time of ignition. The calculation further reveals that the flow pattern at spark timing is predominantly determined by the remnant of the induction flow, generating large vortex structures with their rotational axis parallel to the symmetry plane of the combustion chamber. These vortices, inducing areas of high turbulence intensity during compression, persist throughout a significant portion of the combustion process, strongly interacting with the turbulent flame front and exerting enduring influence on its propagation characteristics.

INTRODUCTION

Multi-valve spark ignition engines, both conventional and lean-burn, offer a great potential in increasing engine power and further reducing fuel consumption and pollutant emissions [1]. Substantial experimental development experience, however, has shown the part load performance of 4-valve engines to be critically dependent on the in-cylinder charge motion and, in the case of lean-burn concept, on the mixture composition distribution, both strongly influenced by the induction process [2, 3]. In engine development the steady flow test method has been used to investigate the geometric aspects of the gas exchange characteristics and to optimise the intake system for best filling efficiency. This practice, however, provides scant or even no information about the details of the charge composition distribution evolution, the characteristic features of tumbling motion generating mechanisms [4] and both their impact on combustion performance under realistic engine operating conditions.

Owing to the realisation of insufficient knowledge of the important features of the in-cylinder flow structure, mixture composition evolution and turbulent flame propagation, and their dependence on port design, injection timing and the gas dynamic behaviour of the intake system, theoretical investigations of these processes have become the subject of increasing interest and attention [5]. The last decade has seen a number of applications of multidimensional CFD codes to the simulation of in-cylinder flow, charge mixing and premixed engine combustion in two stroke as well as in four stroke cycle engines [6 - 10]. Although useful for gaining more fundamental knowledge of the important features and major underlying interactions of the governing processes, the computational methods adopted so far suffered from the limited geometric flexibility in modelling complex engine geometries with moving parts and from the lack of real predictive capability of

the applied combustion models. The latter can mainly be attributed to more or less crude assumptions regarding the impact of turbulence on the mean reaction rate, thus requiring adjustment of empirical constants according to experimental combustion data for the case under investigation. In the recent past a lot of effort has been spent on the development of more fundamentally based and thus more predictive models [11 - 16]. Currently the most promising approach for practical application is that solving a transport equation for the single-point probability density function distribution of scalar species concentrations [16]. PDF methods, as they are usually referred to, offer the great advantage of providing a complete statistical description of the quantities under consideration, fully accounting for turbulence / chemistry interactions and thus obviating the need for any prior assumptions as to whether one or the other process is controlling the mean rate of reaction.

The present paper describes the extension of a computational fluid dynamics method, the FIRE code system, to modelling of turbulent inhomogeneous charge combustion, adopting a Monte Carlo PDF approach, and its application to the study of flow evolution, mixture preparation and flame propagation in a 4-valve spark ignition engine. The engine has a compression ratio of 10.3 : 1, and the calculation pertains to the operating conditions of part load and an engine speed of 1000 rpm. The in-cylinder flow and charge distribution prior to combustion were obtained through multidimensional simulation of the complete gas exchange and subsequent compression processes in which resort was made to an unsteady gas dynamic and cycle calculation method to provide the initial and boundary conditions for the multidimensional calculation under the operating condition of interest. This procedure enables incorporation of all data pertinent to the operating engine into the multidimensional calculation, including the important pressure wave oscillations in the intake system.

THE CALCULATION METHOD

The Mathematical Framework

The method solves the density-weighted ensemble averaged differential conservation equations of mass, momentum and stagnation enthalpy, in addition to the transport equations of the k-ε turbulence model in three space dimensions and time. In the case of inhomogeneous, partially-mixed reactive flows, additional conservation equations are solved, in order to determine the charge composition, thermodynamic state and heat release rate.

The Combustion Model

The complex hydrocarbon oxidation process is expressed, in accordance with the current practice [6, 7], by a single-step irreversible combustion reaction in which fuel and oxidizer are completely converted into combustion products.

In order to represent the reactive system the present mathematical method solves partial differential equations for the mixture fraction f and the probability density function of a reaction progress variable c, whose solution, with the aid of auxiliary relations, enables determination of the composition and thermodynamic state of the charge. The conservative scalar variable f is equivalent to the total (burnt + unburnt) fuel mass-fraction and thus a measure of the mixing between the air and the fuel ($0 \leq f \leq 1$), irrespective of their taking part in the combustion process. Therefore, in the case of homogeneous premixed-charge combustion f is a constant value, independent of space and time. The reaction progress variable c is equivalent to the reaction product mass-fraction normalised by the maximum product mass-fraction that can occur such that either all the fuel or all the oxidant is depleted (or both for stoichiometric mixtures). It can be seen that c is bounded by the values of zero and unity corresponding to the unburnt and burnt states, respectively - regardless of the equivalence ratio.

Adopting the standard gradient diffusion approximation and a stochastic mixing model [17] for modelling turbulent convection in physical and molecular mixing in composition space, respectively, the modelled transport equations for the mixture fraction f and the reaction progress variable probability density function $p_{(c)}$ can be written in the form

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{f}\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{U}_j\tilde{f}-\Gamma_f\frac{\partial \tilde{f}}{\partial x_j}\right)=0 \qquad (1)$$

$$\frac{\partial}{\partial t}\left\{\bar{\rho}\tilde{p}_{(c)}\right\}+\frac{\partial}{\partial x_j}\left\{\bar{\rho}\tilde{U}_j\tilde{p}_{(c)}-\Gamma_c\frac{\partial\tilde{p}_{(c)}}{\partial x_j}\right\}=$$

$$\frac{\partial}{\partial c}\left\{\bar{\rho}\tilde{p}_{(c)}{}^{s}{}_{(c)}\right\}+\bar{\rho}\frac{2C_m}{\tau}\left\{\int_0^c\tilde{p}_{(c-c')}\tilde{p}_{(c+c')}dc'-\tilde{p}_{(c)}\right\} \quad (2)$$

with $p_{(c)}$ being the probability that at location x and time t the quantity c is within the range $c < c < c + dc$. The mean density is then given by

$$\tilde{\rho}=\left\{\int_0^c\frac{\tilde{p}_{(c)}}{\rho_{(c)}}dc\right\}^{-1} \quad (3)$$

In the above, ρ is the mixture density, U_j are components of the velocity vector and $\Gamma_f = \Gamma_c$ (according to the Simple Chemically Reacting System [18]) are mass diffusion coefficients. In the present case of turbulent flow, the mass diffusion coefficients are calculated based upon the solution of the k-ε equations. In equation (2), $\tau = k/\varepsilon$ is the turbulent mixing time and C_m a model constant. The first term on the right hand side of equation (2) represents the effect of chemical reaction and is assumed here to be of the standard Arrhenius type.

The Solution Method

The differential transport / conservation equations are recast into the general curvilinear non-orthogonal form and transformed to an Eulerian-Lagrangian coordinate system, so to enable their solution on a body fitted computational mesh with moving boundaries.

The single-point PDF transport equation for the reaction progress variable c is solved using a Monte Carlo simulation approach in which the continuous probability density function $p_{(c)}$ is represented by an ensemble of notional particles located at the cell centers of the finite volume grid [19]. In order to advance the PDF from time t to $t + \Delta t$, the notional particles are moved across physical and composition space according to the processes of convection, diffusion, reaction and mixing. In the Monte Carlo method these processes are simulated sequentially based on an explicit operator splitting method.

The partial differential equations governing mean fluid motion are discretized adopting the finite volume method. The temporal integration of the governing equations is Euler implicit, in order to ensure unconditional numerical stability, and for approximation of the spatial derivatives a hybrid central/upwind differencing scheme is employed. These discretisation practices lead to coupled algebraic equation systems solved iteratively adopting an optimised version of the SIMPLE algorithm. The solution of each algebraic equation system is effected using the ILU preconditioned conjugate gradient method for unsymmetric problems, ORTHOMIN [20].

The solution of the coupled equation systems is advanced from the initial conditions in a time marching method, updating velocity, pressure and mean scalar fields according to the solution of the Monte Carlo simulation that determines the thermochemical state of the fluid.

THE APPLICATION DETAILS

Engine Simulation Data

The engine under consideration is the BMW M50 6-cylinder production engine. The engine geometric and operation data are given in Table 1.

GEOMETRIC DATA	
Bore	85 mm
Stroke	75 mm
OPERATION DATA	
Engine speed	1000 rpm
Compression Ratio	10.3:1
Load	40 %
Ignition time	26 °BTDC

Table 1 Engine geometric and operation data

The computational mesh of the cylinder / port assembly is illustrated in figure 1. The arrangement of the intake and exhaust ports is symmetrical; thus, the calculation domain is confined to half of the cylinder volume.

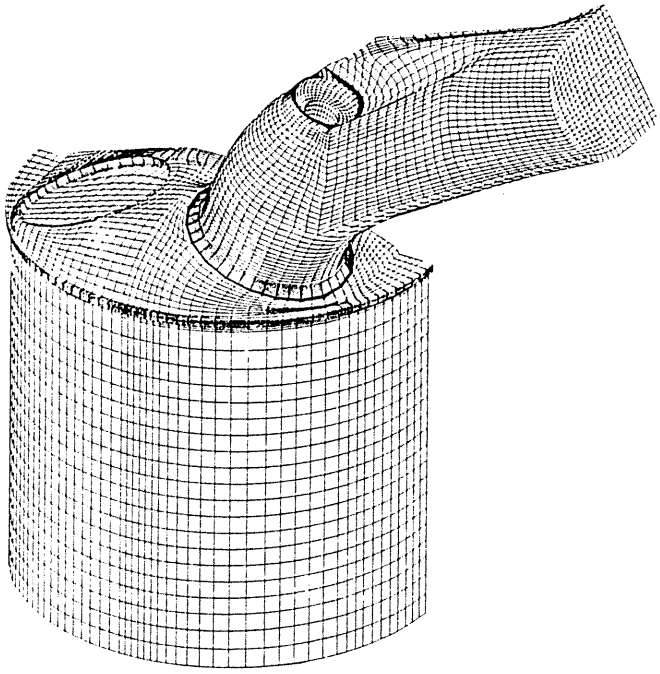

Figure 1 Computational Mesh

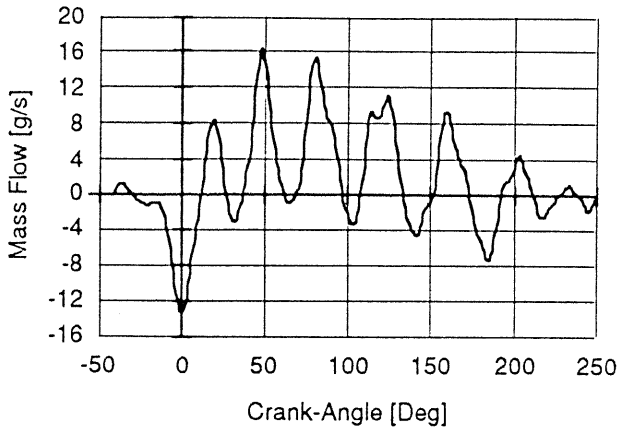

Figure 2 Intake Mass Flow

Initial and Boundary Conditions

The thermodynamic initial conditions and the boundary conditions at the cylinder head entrance and in the exhaust valve gap, in addition to the instantaneous mass flow rate during the induction stroke, were obtained from a prior unsteady gas dynamic calculation. The variation of the intake mass flow rate, pertaining to an engine speed of 1000 rpm is depicted in figure 2. The in-cylinder temperature and pressure at the beginning of the calculation were obtained to T = 823 K and p = 0.98 bar, respectively, temperature and pressure at the intake port were initialised with T = 393 K and p = 0.5 bar; the pressure at the exhaust valve gap was set to 0.95 bar. The boundary conditions at solid walls were the no-slip velocity and constant temperature conditions. The cylinder head and liner were given a temperature of T = 393 K, the piston was assigned a value of T = 473 K. The 'law-of-the-wall' expressions for velocity, temperature and turbulence parameters were employed to bridge the low Reynolds number region near the wall. Fuel deposition was simulated through initialisation of a volume of approximately 40 mm height in the intake port immediately upstream of the intake valve with a rich fuel / air mixture (approximate equivalence ratio of 25), according to the total injected fuel quantity.

Ignition Procedure

The ignition is simulated through prescription of the temporal variation of the reaction progress variable c in a block of computational cells at the spark location, containing approximately 0,25 % of the cylinder total fuel mass. An 's'-shaped variation over a 4 degree crank-angle period has been used in the present calculation. Although the mean value of the progress variable is thus fixed, there exists an infinite number of possible PDF shapes that satisfy this. "Maximum" variance ignition has been used in the present calculation.

Calculation Procedure

The calculation commenced at inlet valve opening and was continued until the complete combustion of the cylinder charge. A computational time-step equivalent to $\Delta\Theta$ = 1/10 degree crank-angle was used throughout the calculations.

RESULTS AND DISCUSSION

Flow, Charge Mixing and Combustion Analysis

At intake valve opening, the pressure difference between combustion chamber and intake system induces a strong back flow of cylinder charge into the intake port. This leads to the establishment of recirculation zones in the port area near the valve and in the vicinity of the valve stem that significantly contribute to the pre-homogenisation of the charge. At CA = 18 deg. after TDC nearly the whole intake port area is oc-

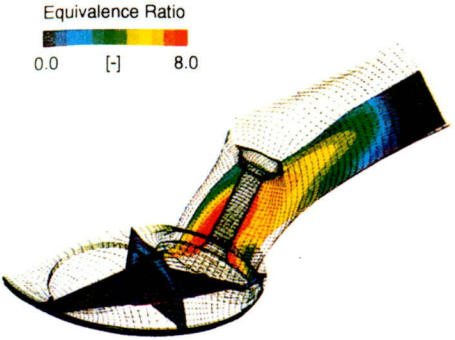

Fig. 3 (a)

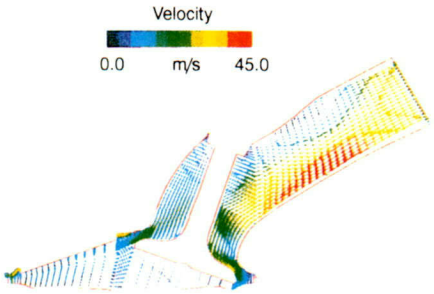

Fig. 3 (b)

Fig. 3 Results at CA = 18°
(a) Mixture Composition
(b) Velocity Field

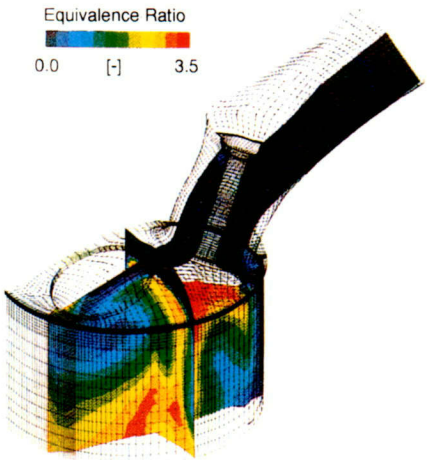

Fig. 4 (a)

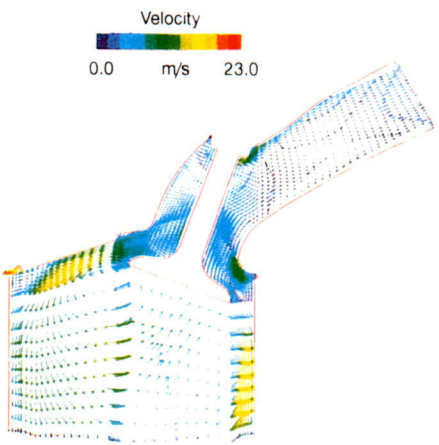

Fig. 4 (b)

Fig. 4 Results at CA = 98°
(a) Mixture Composition
(b) Velocity Field

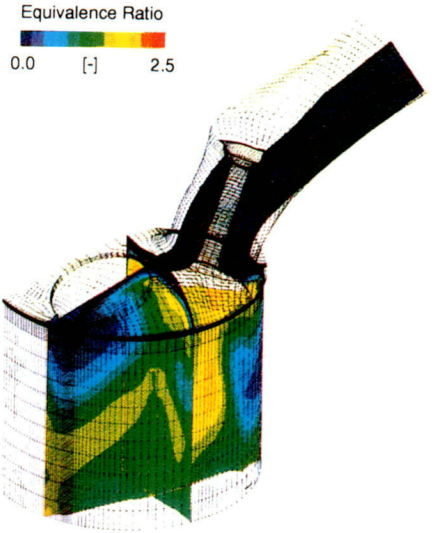

Fig. 5 (a)

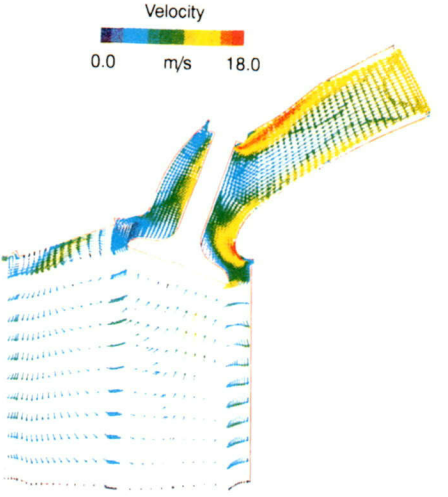

Fig. 5 (b)

Fig. 5 Results at CA = 138°
(a) Mixture Composition
(b) Velocity Field

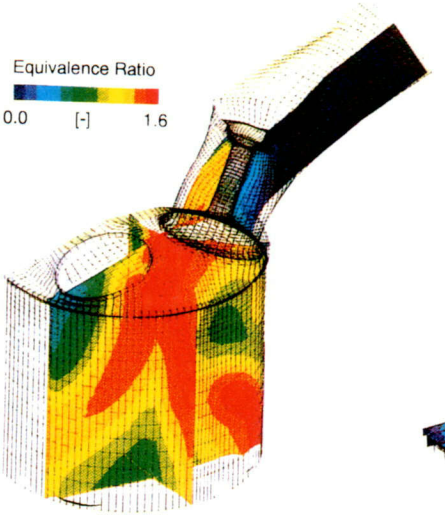

Fig. 6 Mixture Composition at CA = 228°

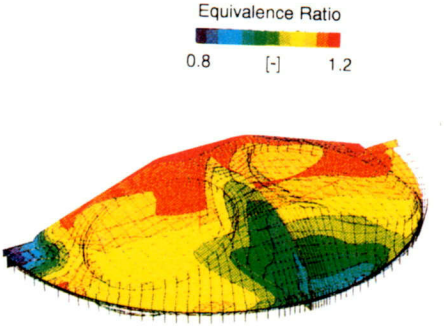

Fig. 7 Mixture Composition at CA = 334°

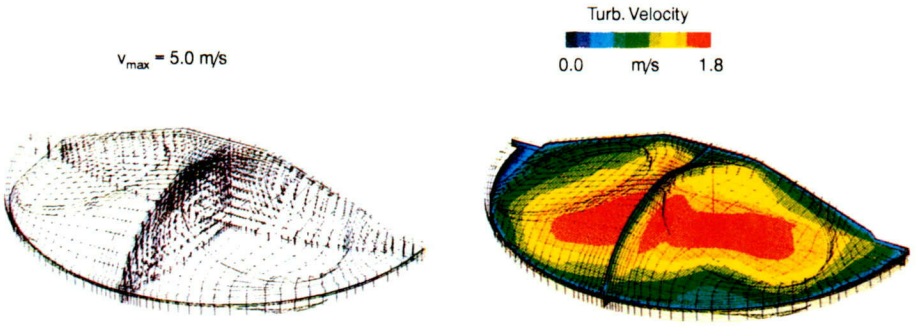

Fig. 8 (a)

Fig. 8 (b)

Fig. 8 Flow Pattern at CA = 334°
(a) Mean Velocity Field
(b) Turbulent Velocity Field

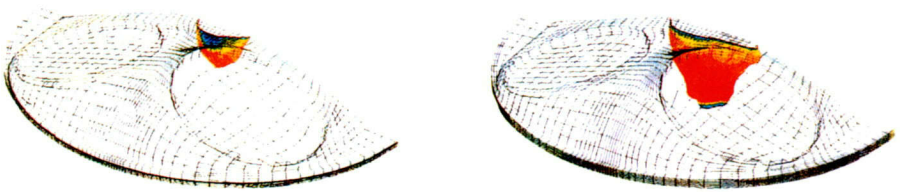

Fig. 9 (a)

Fig. 9 (b)

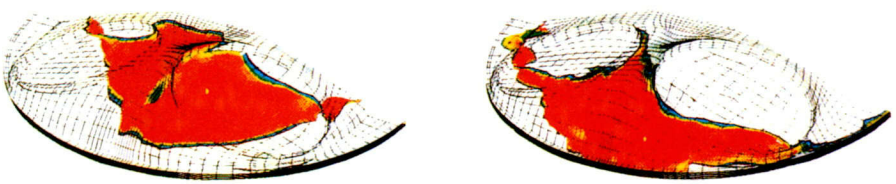

Fig. 9 (c)

Fig. 9 (d)

Fig. 9 Flame Propagation - Isosurface c = 0.5
of Mean Reaction Progress Variable
(a) CA = 342°
(b) CA = 350°
(c) CA = 360°
(d) CA = 368°

cupied by the fuel; simultaneously the maximum fuel / air equivalence ratio in the intake port has decreased by a factor of three compared to its initial value, as shown in figure 3(a). By that time - approximately 40 degrees crank-angle after inlet valve opening - the main flow direction changes and starts to actually contribute to cylinder filling, as depicted in figure 3(b).

Figures 4 and 5 show the charge mixture distribution and the velocity fields at 98 and 138 deg. crank-angle after TDC. The results at CA = 98 deg. correspond to the time at which all the fuel has entered the cylinder. The velocity field at CA = 98 deg. in figure 4(b) shows a complex flow structure with two counter-rotating vortices situated below the intake valve, determining the charge mixture distribution at that time - figure 4(a). Figure 5(b) shows the noticeable alternation of the velocity field at CA = 138 deg. due to the negative mass flow at the cylinder head entrance at that time (see figure 2) caused by pressure the wave oscillations in the intake system. The vortices are convected upward towards the valve disc and are partly sucked back into the valve gap, simultaneously losing angular momentum. Figure 5(a) shows the impact of this back flow onto the in-cylinder charge mixture distribution. It can be seen that the mass flow oscillations during the induction period additionally contribute to the fuel / air homogenisation process; at CA = 138 deg. the maximum fuel / air equivalence ratio has been decreased by a factor of 10 compared to its initial value.

The plots of the fuel / air equivalence ratio in figures 6 and 7 depict the evolution of the spatial distribution of the mixture composition during the compression stroke, from just before inlet valve closure to the time of spark ignition. The charge homogeneity at spark timing (CA = 334 deg.) is evidenced in figure 7 by the variation of the fuel / air equivalence ratio corresponding to an air fuel ratio A/F = 13 - 19, with a near stoichiometric mixture composition in large regions of the combustion chamber.

The fields of mean and turbulent velocity at spark timing (CA = 334 deg.) are presented in figures 8(a) and 8(b). The velocity field in figure 8(a) depicts a flow pattern that does not exhibit a significant tumbling motion as it has been observed in similar 4-valve configurations, but shows a large vortex motion with its rotational axis perpendicular to the cylinder axis and parallel to the symmetry plane of the engine. The results indicate that this characteristic flow structure can mainly be attributed to the geometric details of this specific combustion chamber / port configuration. The turbulence intensity distribution in figure 8(b) shows peak levels in the bulk of the flow that correspond to the regions of large strain rates within the induction remnant flow structure.

The evolution in the combustion process is depicted in figure 9, presenting the plots of the reaction progress variable iso-surface c = 0.5 at the selected crank-angles CA = 342, 350, 360 and 368 deg., respectively, representing the shape and location of the turbulent reaction zone. The result at CA = 342 deg., shown in figure 9(a), corresponds to the time of transition from combustion delay phase to the main combustion period, with the combustion delay defined as the duration between ignition and time of rapid heat release. At this early stage of combustion the spark induced flame kernel exhibits a regular, nearly spherical shape, mainly unaffected by the mean flow. In the later stages starting at at CA = 350 deg., a fully developed turbulent flame has already been established, the characteristic mean flow field starts to exert a strong influence on the turbulent reaction zone, as depicted in figure 9(b). Due to the fact that perpendicular to the symmetry plane the flame propagation is directed against the mean fluid flow, the resulting flame front propagation velocity is remarkably decreased, leading to a delayed combustion in the region in between the valves - figure 9(c). In axial direction, however, flame speed and mean flow velocity add together and lead to a preferential flame propagation towards the piston; in the symmetry plane, where there exists only a weak fluid motion, the flame growths mainly uneffected by the mean flow. Due to this enduring and significant combustion / flow interaction, the flame front exhibits a characteristic evolution in shape that is nearly conserved throughout the whole combustion phase - figure 9(d).

Global Parameters

The data (measurement and results from the gas dynamic and cycle program) and the predicted variations of the volume-averaged mean progress variable (i.e. the fuel mass-fraction burned normalised by the total fuel mass-fraction) and the normalised instantaneous heat release rate are presented in figures 10 and

11, respectively. Figure 10 provides an indication of the overall agreement between the calculations and the data. The discrepancy in agreement in figure 10

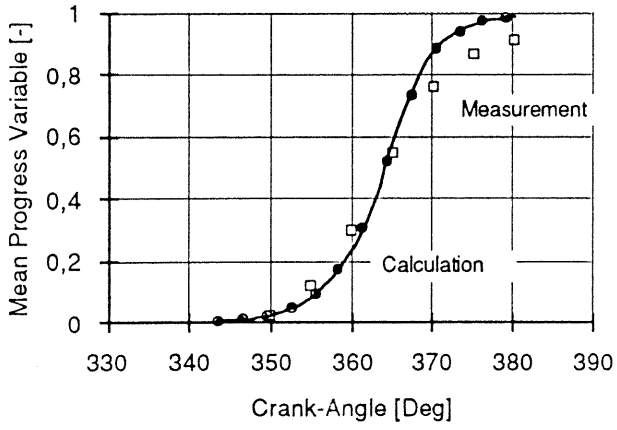

Figure 10 Cylinder Volume-Averaged Mean Progress Variable

could have been improved by further adjustment of the model parameters. The overall extent of agreement, however, is considered to be adequate for the purpose of the present study. The normalised instantaneous heat release rate in figure 11 indicates a short

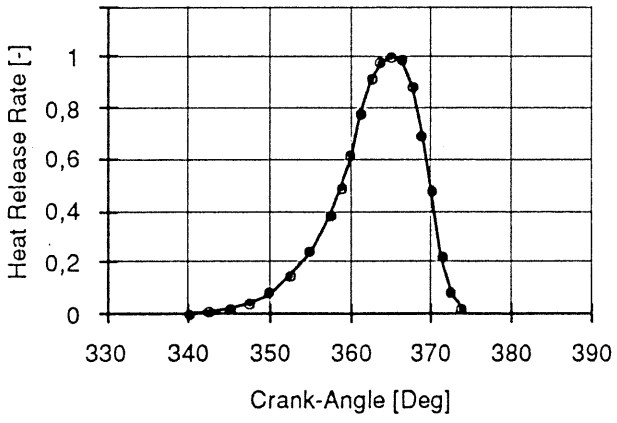

Figure 11 Normalised Heat Release Rate

ignition delay of approximately 10 deg. crank-angles (i.e. CA = 336 - 345 deg.) and a main combustion period of 30 deg. The rapid increase in heat release starts at CA = 345 deg. and attains the peak value at CA = 365; it thereafter rapidly diminishes till completion of combustion at CA = 375 deg. The multidimensional results presented earlier reveal that the concurrent interaction of the flame with the flow is responsible for this rapid combustion development.

The sensitivity of the combustion model adopted in the present study to a variation in the engine operation parameters is presented in figures 12 and 13. Figure 12 shows the dependence of the evolution of the mean progress variable on different fuel/air equivalence ratios. The results provide evidence of the capability of

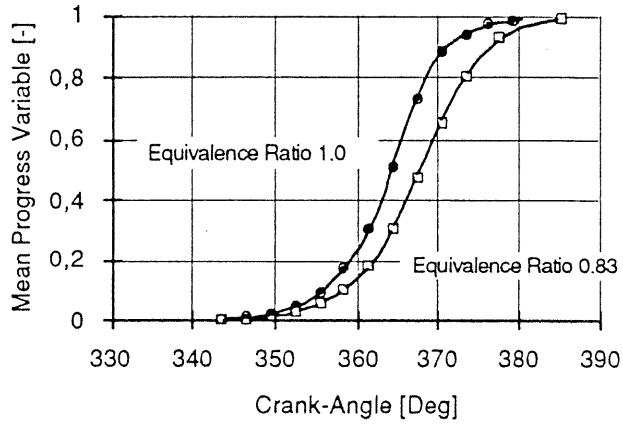

Figure 12 Variation of Cylinder Volume-Averaged Mean Progress Variable with Equivalence Ratio

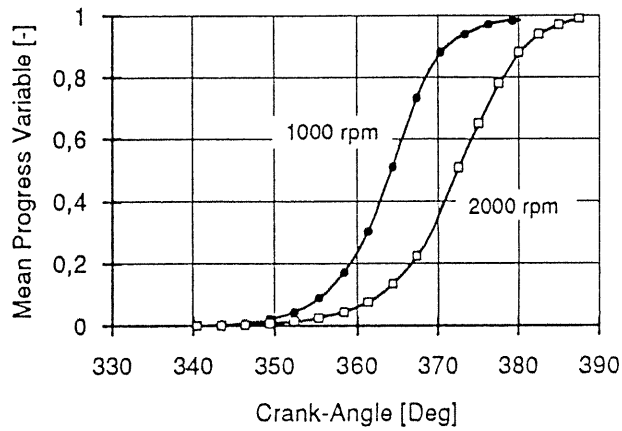

Figure 13 Variation of Cylinder Volume-Averaged Mean Progress Variable with Engine Speed

the model to reflect the impact of lean mixture onto the burning velocity during the initial phase of flame kernel growth - leading to a markedly increased duration of the ignition delay phase - as well as its influence onto the main combustion process that seems to be no lon-

ger purely turbulence controlled in the case of lean mixture, as indicated by the different slopes of the mean progress variable curves in figure 12. The influence of an increase in engine speed on the evolution of the mean progress variable is shown in figure 13. Due to the kinetics controlled nature of the flame formation and initial propagation process the ignition delay expressed in terms of degrees crank-angle increases with an increase in engine speed, while leaving the main combustion phase nearly unaffected; a trend well predicted by the PDF method adopted in the present study.

SUMMARY AND CONCLUSIONS

A multidimensional mathematical method is applied to the investigation of the instationary flow evolution, air / fuel mixing and flame propagation process in a 4-valve spark-ignition engine. The study reveals several notable aspects of the mixture preparation process and the interaction of the intake generated flow with the flame front, some of which appear to be specific to this engine. These can be summarised as follows:

i) The flow and charge mixture distribution at the time of ignition are predominantly characterised by the evolution of the induction flow.

ii) The fuel deposition before intake valve opening produces a regularly-mixed charge distribution in large areas of the combustion chamber at spark-timing.

iii) During the intake process, large vortex structures with their rotational axis parallel to the symmetry plane of the combustion chamber are formed.

iv) The vortices produced in the course of the intake process generate areas of high turbulence intensity during compression.

v) The flow structure at spark-timing persists throughout a significant portion of the combustion process, strongly interacting with the turbulent flame front and exerting enduring influence on its propagation characteristics.

The above results show the induction process to be an important and integral part of the numerical simulation of flow and combustion processes in reciprocating engines. The present study further indicates that the Monte Carlo PDF model for turbulent combustion in spark ignition engines overcomes the limitations of models adopted so far and shows the FIRE-code to offer a unique means for investigation of the characteristic features of flow, mixture preparation and flame propagation in 4-valve spark ignition engines.

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