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Full-cycle firing simulation of a pent-roof spark-ignition engine with visualization of the flow structure, flame propagation and radiative heat flux

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Abstract: A numerical study is made of how the complex geometry of a pent-roof spark-ignition engine influences the flow field, the flame propagation and, novelly, the instantaneous radiative heat flux. The solver integrates a generalized weighted-sum-of-grey-gases-discrete transfer method radiation model into the computational fluid dynamics code KIVA-II also modified to enable the simulation of open ports and canted valves, wave action effects in the exhaust and mixing-controlled combustion.

The full-cycle mean pressure variation is in good agreement with measurements. The overall burning angle of 37° crank angle and peak radiative flux of 210 kW/m^2 are also plausible on the basis of published data. Finally, remarkable insight is gained into how the head geometry and flow structure influence flame propagation and in turn how this governs the spatial and temporal variation in radiative heat flux on the cylinder walls.

Keywords: spark-ignition combustion, computational fluid dynamics (CFD), participating radiation, discrete transfer method (DTM), weighted-sum-of-grey-gases (WSGG)

NOTATION

ATDC	after top dead centre
BDC	bottom dead centre
CFD	computational fluid dynamics
DOHC	double overhead cam
DTM	discrete transfer method
EDC	eddy dissipation concept
EGR	exhaust gas recirculation
EVC	exhaust valves close
EVO	exhaust valves open
SIMPLE	semi-implicit pressure linked equations
TDC	top dead centre
WSGG	weighted-sum-of-grey-gases

1 INTRODUCTION

The in-cylinder combustion dynamics of spark-ignition engines involves turbulence, mixing, ignition, chemical

reaction and heat transfer. For most of these phenomena the analyst may choose from a well-established selection of numerical models, with one important exception. Models to describe the participating thermal radiation within the combustion gases fall short of the state of the art in other areas. To date calculations have almost exclusively employed empirical relations [1], but these do not provide any description of the spatial or wavelength dependence of the radiative heat flux. Moreover, while the cycle-averaged radiative heat flux is small, instantaneous values during combustion may be appreciable. This may have an important effect on other combustion-related phenomena via localized changes to the flame or cylinder wall temperatures. Furthermore, the design of optical combustion control systems would stand to benefit significantly from numerical studies of how the detailed geometry and turbulent flow field influence the flame radiation.

In this vein a full-cycle firing simulation of a four-valve pent-roof engine is undertaken with particular attention given to the radiation transport. The modelling difficulties of this 'grand challenge' problem [2] are substantial, not least because of the complex engine geometry and computationally intensive nature of the transient solution. Therefore, to keep the calculation tractable several

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sources of error cannot be entirely eliminated, such as those due to limits on the spatial, angular and spectral discretization, those due to uncertainties in the boundary conditions and those associated with neglecting the effects of turbulence intermittency—the present combustion and radiation models use mean properties. However, the present level of resolution is sufficient for demonstrating the prediction of instantaneous radiation in realistic engine flows. Here the authors are guided by previous engine-combustion studies [3–5] and their own independent verification of the radiation models [6, 7]. A feel for the sensitivity of predictions to variations in model parameters has also been gained with two-dimensional engine-radiation studies documented within reference [8]. Finally, it is noteworthy that while a specific application is addressed here, the approach described lends itself to the treatment of other combustion systems involving complex, transient, participating radiative heat transfer.

2 ENGINE TEST CONDITIONS AND CYLINDER PRESSURE MEASUREMENT

This study is of a single-cylinder, four-stroke, naturally aspirated, double overhead cam (DOHC) research engine with a pent-roof combustion chamber, four canted valves and a flat-topped piston. Key parameters are shown in Table 1. The cylinder pressure variation is measured in house with an air-cooled piezoelectric transducer integrated with the centrally located spark plug. The pressure signal is sampled at 2° crank angle intervals, averaged over 50 consecutive engine cycles, and scaled such that at intake bottom dead centre (BDC) it equals the mean inlet manifold absolute pressure. The instrumentation and procedures used follow those of

Lancaster *et al.* [9]. The measured pressure variation is plotted in Fig. 1. It is noted that the pressure readings during the gas exchange strokes are subject to sizeable error owing to thermal effects on the transducer.

3 ANALYSIS OF FLOW, COMBUSTION AND RADIATIVE TRANSFER

3.1 Modelling methodology

The engine-specific computational fluid dynamics (CFD) code KIVA-II [10, 11] is used for the present calculation, but with several modifications to the solution scheme, new and enhanced physical models and the capability to simulate canted ports and valves. These changes are detailed by Henson [8]. Therefore, for brevity only salient features of the mathematical models and numerical scheme are summarized here.

3.2 Turbulent combustion model

A description of the multispecies reacting flow is obtained by solving the Favre-averaged conservation equations for species mass, total mass, momentum and internal energy, together with the two transport equations of a k - ϵ turbulence model for variable density flow. The fuel combustion is characterized by a simplified mechanism involving a single irreversible one-step reaction in which iso-octane and oxygen convert directly to combustion products carbon dioxide and water. The mean reaction rate is taken to be proportional to the harmonic average of the rates given by a kinetic Arrhenius-type model [12] and a mixing-controlled eddy dissipation concept (EDC) model [13]. It is of note that such rate expressions invariably require ‘tuning’ for a given set of solution parameters (e.g. turbulence constants, wall functions, etc.). The constant of proportionality is used for this purpose and set by comparison with engine pressure data. Reactions to describe nitrogen oxidation and the thermal dissociation of key species (i.e. CO₂, H₂, O₂, N₂, OH) are also incorporated into the overall combustion scheme. These provide for the future study of the radiative emission from products such as CO, NO, etc. The chemistry and flow are coupled via source terms in the species mass and internal energy equations.

3.3 Non-grey radiative heat transfer model

The simulation of the in-cylinder radiation transport employs three stages of delineation (a) to compute the spectral variation in absorption, (b) to rationalize this into a set of independent grey gases and (c) to solve for the transport in each gas. In the first stage a combined

Table 1 Engine design and operating parameters

Compression ratio	9.22
Bore	80.065 mm
Stroke	79.35 mm
Conrod length	132.0 mm
Speed	1500 r/min
Fuel	Propane (C ₃ H ₈)
Equivalence ratio	0.88
Ignition timing	−15° ATDC
Valve cant angle	All ±20° to axis
Charge mass	0.4 g (0% EGR)
Inlet valves	2 (poppet)
Diameter	25.5 mm
Maximum lift	8.53 mm
Open at	−372° ATDC
Close at	−124° ATDC
Exhaust valves	2 (poppet)
Diameter	22.5 mm
Maximum lift	9.79 mm
Open at	−596° ATDC
Close at	−348° ATDC

Fig. 1 Measured and calculated full-cycle (a) pressure–time and (b) pressure–volume curves for firing operation. An enlargement of the exhaust blowdown and displacement is also shown in (a)

narrow- and wide-band model [14] is used to compute the variation in spectral absorption coefficient as a function of wavelength, temperature, pressure and composition. The model correlates experimental absorptance data, averaging out its path length dependence. Band correlation parameters for CO_2 , CO , H_2O , CH_4 , C_2H_2 and NO are tabulated [14]. However, the present analysis is limited to the principal participating species, namely CO_2 and H_2O in the infrared spectrum from 1 to $10\ \mu\text{m}$ [15]. The continuous radiation from soot particles is

expected to be very small, and hence it is also neglected. A novel weighted-sum-of-grey-gases (WSGG) method [16, 17] is then applied to discretize logarithmically the modelled CO_2 – H_2O absorption domain into N discrete levels of uniform absorption, κ_k , where $k = 1, 2, \dots, N$. The coefficients κ_k must depend on the local gas properties in order to describe the non-uniform absorption of the in-cylinder gases (see reference [17]). This approach offers greater generality than classical WSGG correlations and affords excellent economy compared with

other techniques giving similar levels of accuracy. In the final stage the radiation transport for each level is solved for independently, and in a manner analogous to a grey gas, with the discrete transfer method (DTM) [18] using a relatively fine angular discretization of 400 rays per surface element. These N solutions are then summed to obtain the total radiative heat flux at the cylinder walls and radiative heat source of the internal energy equation—through which the flow and radiation solvers are coupled. In the present calculation six levels (grey gases) are employed, i.e. $N = 6$. This was found to be the minimum number required in order to ensure a total heat flux solution within a few per cent of that with an extremely fine spectral discretization equivalent to $N > 80$, i.e. see benchmark studies in reference [8].

3.4 Mesh description and boundary conditions

The transport equations are cast into curvilinear form and transformed to a moving, body-fitted coordinate system of hexahedral elements. This flexibility enables the computational mesh to be aligned with the physical boundaries of the cylinder walls, contracting and expanding with the piston motion. Elliptic smoothing [19] is used to ensure a well-conditioned mesh without large aspect ratios or excessive skew. However, the elliptic solver is over-constrained if one tries to include both the valve/port detail and the surface curvature of the pent-roof cylinder head. Consequently, the surface shape is somewhat simplified during the valve open period and restored to its exact profile during the closed period (Fig. 2). Computational limitations restrict the mesh size to $34 \times 34 \times 16$ (x, y, z) cells. This resolution is quite coarse but adequate to ensure that spatial discretization errors are small and of a similar order to the uncertainties in boundary conditions. Two-dimensional sensitivity studies [8] indicate that, with further refinement of the mesh, mean quantities vary by less than 10 per cent.

3.5 Solution procedure and boundary conditions

With the exception of radiation transport, all other conservation equations are discretized with a finite volume scheme that approaches second-order accuracy. Temporal differencing is first-order accurate and performed with respect to a sequence of discrete times t^n , such that the solution is marched forwards in time through a series of finite time steps $\Delta t^n = t^{n+1} - t^n$. Several convergence trouble spots arise owing to sudden changes in the flow acceleration and strain rate, for example at exhaust blowdown. Therefore, to ensure unconditional numerical stability, differencing of the diffusion and acoustic mode terms is arranged to be fully implicit. These implicit equations are solved in

a coupled, iterative SIMPLE-like procedure. Subsequently, convection terms are solved in a fully explicit, quasi-second-order upwind (QSOU) scheme, subcycled within the time step Δt^n . During the combustion phase the routines to calculate the mass sources and heat fluxes due to chemical reaction and radiation are also called.

Pressure boundaries are specified at both the inlet port and exhaust ports. The specified exhaust pressure is dynamically adjusted such that the instantaneous port mass flow matches that computed in a one-dimensional wave action analysis of the exhaust system. At the inlet boundary the pressure is fixed at a level for which the total inducted mass is equal to that measured (i.e. 0.4 g), and the densities of incoming species propane, oxygen and nitrogen are set for the 0.88 equivalence ratio. The turbulent kinetic energy is assigned as 10 per cent of the mean inflow velocity squared, and its dissipation rate is found for a length scale equal to half the maximum lift of the inlet valve. Mean temperatures on the combustion chamber surfaces are estimated on the basis of thermal maps for a similar sized engine and compression ratio [20]. The cylinder walls are coolest at 450 K, the piston face is somewhat hotter at 490 K and the highest temperatures are on the cylinder head. Here the temperature varies smoothly between 450 K at the cylinder wall boundary 480 K near the central spark plug and local maxima of 505 K and 585 K specified on surface elements coincident with the inlet and exhaust valve faces respectively. For the radiation transport calculation all surfaces are taken to be grey with an emissivity of 0.8. The simulation is started with assumed distributions of the flow variables in the combustion chamber and run until there is a 1 per cent difference in global values between consecutive cycles.

4 RESULTS

4.1 Flow characteristics

The calculated and measured mean cylinder pressures are plotted in Fig. 1. Here, the mean reaction rate is tuned to reproduce the measured peak cylinder pressure of 47 bar, but the close agreement observed elsewhere on the pressure curves can be attributed solely to the predictive ability of the combustion model. Activating the radiation model results in enhanced heat losses to the combustion chamber walls leading to lower gas temperatures, slower combustion and, ultimately, a slight underprediction of the peak pressure. The constant of proportionality in the reaction rate expression is increased by 7 per cent to compensate for this. Hence, in studies where the radiation transport is neglected, the effect on the heat release rate is being implicitly accounted for via the combustion model parameters. The agreement in Fig. 1 is poorest in the later stages of

Fig. 2 Computational meshes for (a) the valve open period (-597 to -123° ATDC) and (b) the closed period (-123 to 123° ATDC). Also shown are the locations of i and j planes on which vector field data are plotted in Figs 3 to 5

the expansion stroke where computed pressures are 1 bar (i.e. 20 per cent) higher than measurements just prior to exhaust blowdown. This in turn results in some over-prediction in the amplitude of the pressure oscillations during the exhaust stroke; nevertheless, the blowdown/displacement simulation is remarkably good, despite severe velocity gradients and numerous uncertainties in the exhaust boundary conditions.

Figures 3 to 5 plot velocity vectors on mesh planes $i=12$ and $j=12$ (see Fig. 2) for the gas exchange strokes from -540° to -90° after top dead centre (ATDC). These planes lie on the port centres and show the largest flow gradients. Figure 6 plots the subsequent flow motion on the centre-line planes $i=18$ and $j=18$ during compression and combustion from -45° to 67.5° ATDC.

Fig. 3 Computed velocities—exhaust blowdown and displacement

Fig. 4 Computed velocities—exhaust, valve overlap and intake

Fig. 5 Computed velocities—intake and compression

Fig. 6 Computed velocities—compression, firing and expansion

The three plots in Fig. 3 highlight the abrupt flow reversal during a backflow wave into the cylinder near the tail end of the exhaust blowdown. At this stage in the cycle the flow is characterized by an ordered upwards movement with very little streamline curvature, apart from around the valve heads. At -372° ATDC the inlet valves open and there then follows a brief period of valve overlap until the exhaust valves close at -348° ATDC. The slant of the pent-roof results in the upper edges of the ports being in close proximity such that there is a significant amount of short-circuiting of the inflow directly into the exhaust, e.g. see the j plane plot in Fig. 4 at TDC (-360° ATDC). Elsewhere the inflow first deflects off the cylinder walls before circulating beneath the valve heads into the exhaust. This structure efficiently scavenges the remaining burnt gas as the calculated residual gas fraction is only 5.6 per cent.

Complex flow patterns are established during the induction stroke. Gas issues through each inlet port into the cylinder as a conical jet at about 40 m/s, i.e. 10 times the mean piston speed. Separation of the jet from the valve seat and lip produces strong shear layers around the inlet valve periphery. These deflect off the cylinder walls and moving piston face to set up several tumbling regions of recirculation. Consider the j plane at -315° ATDC (Fig. 4). Two centres of rotation may be discerned, immediately below, to the left and right of the inlet valve. What is seen is in fact the cross-section of an inclined torus-like vortex extending completely around the valve head. A second vortex extends around the other intake valve such that four centres of rotation are visible in the i plane passing through both intake valves. As the piston descends the vortex structure closest to the cylinder wall is extruded into a large tumble motion. Moreover, velocity vectors in selected k planes at BDC (Fig. 7) also reveal the superposition of strong swirling rotations, particularly close to the piston face. A three-dimensional interpretation of this tumbling-swirling motion is sketched alongside.

At -124° ATDC the intake valves close, removing the energy source driving the vortex field. Shearing forces quickly deplete the vortex energy and the global flow structure breaks down into an ordered upwards movement during compression. As the piston approaches TDC it tends to 'roll up' the boundary layer and new regions of recirculation form. After ignition at -15° ATDC the burnt gases expand rapidly away from the central spark plug. Unburnt gas ahead of the flame front is squeezed into the squish regions. It then swirls around the cylinder wall to join fluid recirculating back towards the centre along the pent-roof ridge. Eventually, an ordered downwards movement prevails some way into the expansion stroke.

4.2 Flame propagation

The flame front is characterized by a rapid transition in

local temperature from about 800 K at the leading edge to in excess of 2200 K at the trailing edge. Thus, its development may be visualized as a series of iso-surfaces plotted through points at some intermediate temperature. Figure 8 shows a sequence of iso-surfaces at 2000 K from -5° to 20° ATDC. Initially, the enflamed region is quite spherical about the central spark plug. However, its outwards growth is influenced markedly by flow motion.

Immediately beneath the cylinder head the flame is rapidly convected down the inclined surfaces of the pent-roof (parallel to the x axis), but its propagation in a perpendicular direction is impeded by fluid recirculating radially inwards along the ridge of the pent-roof. Consequently, the flame front intersects the cylinder head with an hourglass-shaped profile. Close to the piston face the situation is quite different. Here, the enflamed region is initially able to expand uniformly in all radial directions. However, an opposing pressure gradient develops as unburnt gas ahead of the flame is compressed into the squish regions. This gradually shapes the flame front to the inner profile of the squish regions as it sweeps towards the cylinder wall. An extremely contorted flame geometry results from these quite different profiles on the cylinder head and piston face. The squish and the corner regions at either end of the pent-roof ridge are the last volumes of gas to be engulfed by the flame. The calculated cylinder pressure peaks just prior to this at 18.5° ATDC. Thereafter, all combustion is of unburnt gas pockets within the flame. The overall burning angle (i.e. 0–90 per cent burnt) is 37° crank angle.

4.3 Instantaneous radiative heat flux

Figures 9 and 10 plot the spatial and temporal variation in net radiative surface heat flux over the cylinder head and walls from -5° to 115° ATDC (shortly after which the exhaust valves open). The flux is negligible until there is sufficient volume of hot products, at a time after ignition when the fuel mass fraction burned is 1–2 per cent. The flux then rises rapidly to peak at 21° ATDC, some 2.5° after the peak mean pressure and 7.5° after the peak in the chemical heat release rate. A local maximum of 210 kW/m^2 is predicted on the cylinder head, closest to the central spark plug, but on the squish surfaces where there is no direct line of sight to the enflamed region the flux is only 40 kW/m^2 . The fuel mass fraction burned is about 88 per cent. Further into the expansion stroke the flux falls away as the burnt gases expand and cool, and it is once again negligible after the combustion products are exhausted. The peak radiative flux is estimated to be about 5 per cent of the peak convective flux.

The observations from several optical studies of spark-ignition combustion strongly support the present calculation. Notably, Baker and Laserson [21] measured

Fig. 7 (a) Computed velocities and (b) their interpretation, showing the three-dimensional flow structure at intake BDC (-180° ATDC)

Fig. 8 Flame front propagation visualized as a sequence of iso-surfaces at 2000 K. This is the temperature of gas in the trailing edge of the flame front. Note that mfb = (fuel) mass fraction burned

a peak radiative flux of similar order (i.e. 260 kW/m^2), Remboski *et al.* [22] corroborate the relative timing of the flux with pressure and heat release and Nutton and Pinnock [23] observed that the peak flux correlates with a burned mass fraction of about 90 per cent.

However, the calculation also affords further insight into the spatial variation in radiative flux over the surface, not easily measured experimentally. Comparison of Figs 8 and 9 shows that the flux contours follow the

flame front, effectively registering both its shape and its passage in time. Consider the plot at 15° ATDC when much of the gas volume is enflamed. The hottest contour traces an early profile of the flame front and each cooler contour corresponds to a progressively more recent position of the front. During the expansion stroke mixing in the post-flame gases gradually evens out thermal and species concentration gradients such that a more uniform flux distribution results on the surface.

Fig. 9 Computed contours of radiative surface heat flux (kW/m^2)

Fig. 10 Computed contours of radiative surface heat flux (kW/m^2)

5 CONCLUDING REMARKS

1. The full-cycle firing numerical simulation of a modern spark-ignition engine configuration with consideration of the detailed geometry, gas exchange, flow field, chemical reaction and combined modes of heat transfer is demonstrated.
2. Key difficulties are (a) avoiding numerical instabilities during exhaust blowdown, (b) the tuning of the combustion model and (c) the explicit modelling of radiation transport.
3. Key achievements are the insights gained into (a) how the pent-roof geometry and flow field interact with the turbulent flame front to influence its propagation characteristics and (b) how this in turn affects the spatial and temporal variation in radiative heat flux on the cylinder walls.
4. Engine flow visualizations need to be combined with detailed in-cylinder measurements of pressure, temperature, velocity and radiation intensity at multiple sites and over a wide range of operating conditions to enable a more complete validation of the present models and their improvement.

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