Modeling and Diagnostics of Combustion in Spark-Ignition Engines

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ABSTRACT

Subjects are considered that have not been extensively covered in recent reviews. Information is not concluded. Simple ensemble averaging is not suited for engine flows. In an engine, the process that is turbulence and what is bulk (mean) flow is relative to what is influenced by the flow. Near TDC, turbulence is always insensitive to the details of the turbulence generated during intake. For a given engine, without strong squish and/or swirl, turbulence intensity and diffusivity near TDC increase with increasing initial turbulent diffusivity but run into upper limits imposed by turbulence damping due to the chamber walls. In spite of many uncertainties and limitations, multi-dimensional combustion models have been shown to be useful by industrial applications. Improved modeling of the flame structure is the subject of greatest current interest. Spatially and temporally resolved measurements are needed of: turbulence intensity with combustion; turbulence length scales without and with combustion; flame establishment and structure; interactions of flame and walls; and the onset of knock.

INTRODUCTION

Several reviews are available in which important aspects of engine flows and combustion are considered rather extensively. They deal with: the origin (1) and early developments (2-4) of multi-dimensional modeling; the question of the definition of engine turbulence (5); a framework for the identification of controlling processes in, and of suitable approximations for, confined reactive flows (6); multi-dimensional numerical methods for engine flows and combustion (7,8); some conclusions from the initial detailed comparisons of two-dimensional computations with measurements in premixed-charges (9); bifurcations of the combustion process in premixed-charges in engines (10); the structure of the flame in premixed-charge engines and zero-dimensional modeling of it (11); a broad view of engine combustion problems and approaches (12); critical examinations of classical engine measurement techniques (13,14); and the rapid growth of laser optical techniques (15,16). There are also recent detailed analyses of multi-dimensional modeling of intake and compression (17); of the structure of full-cone engine sprays (18); of the possible structure of premixed-charge engine flames (19); and of advanced optical techniques conveniently organized according to their suitability for different parts of the engine cycle (20). Thus I will consider subjects that have received less attention in (1-20). I will start from some background information and some definitions. Then some interesting aspects will be mentioned of the flows in the intake manifold; certain aspects have been clarified recently. Next some two-dimensional combustion computations will be examined with particular attention paid to studies published by industry research groups. Finally, some measurements will be identified that are feasible today and that are most needed for the next round of improvements in knowledge and modeling.

BACKGROUND

It is known that indicated efficiency and emissions of engines are influenced not only by the type of charge and the geometry of the combustion chamber but also by the design of the intake and exhaust manifolds. Thus a model that attempts to predict indicated efficiency and emissions should include the flows in the intake and exhaust manifolds, the details of the gas motion by the valves, and compression, combustion, and expansion of the burned charge. Moreover, the coupled computation of the cooling system should also be undertaken to evaluate precisely the local and instantaneous wall heat transfer.

The equations for such an approach are known but their numerical solution is outside the size and speed ranges of current computers. This situation is common in engineering where, in principle, all problems can be solved exactly, but in practice most problems must be dealt with approximately. In fact, engineering skill is not in including the possible, but in isolating the essential. Fortunately our problem can be broken down into a set of more manageable and still useful parts.

Only the wall temperature must be included in the calculation of the flows in the intake and exhaust manifolds. Since the thermal response time of the engine walls is long in comparison to that of the gas, during steady operation the walls may be assumed to be at a temperature that varies from point to point but
is constant in time. Then, by employing the local and instantaneous gas temperature and the vocal and time-averaged wall temperature, local and instantaneous heat transfer rates can be estimated as part of the computation of the gas flow.

Under certain conditions, the unsteady model for the flows in the intake and exhaust manifolds can be one-dimensional, but complex nonetheless, particularly for multi-cylinder engines. Programs of this type are already in use in most industries, often following the lead of Benson et al (21). However, the computation of the flow by the intake valve and into the cylinder presents several difficulties.

It would be convenient immediately to separate turbulence from bulk flow. However, turbulence as deviations from mean values is a clear concept only when time averages exist that are independent of the window over which the data are calculated, i.e., in flows that are steady in the mean. Since engine flows are unsteady, the distinction between turbulence and bulk flow is not unique. In fact, as we shall see, what is turbulence and what is bulk flow is relative to the process that is influenced by them.

Some (17) think that they are avoiding this difficulty by using ensemble (or phase) averages. In this approach, a quantity is measured within a small crankangle window around the same crankangle over many cycles. The average over many cycles is called the ensemble average and the difference between the value in one cycle and the ensemble average is the turbulence fluctuation of that quantity in that cycle. That this approach is wrong is clearly evidenced by a simple example. Consider a solid body rotating within the cylinder with a speed that is not constant and not synchronized with that of the engine so that, at the same crank angle, the velocity at a point within the cylinder is different in different engine cycles. The departure of the velocity in one cycle from the ensemble average would be called the turbulence in that cycle even though there is no motion at all within the solid body. It has been recognized for some time that:

1) the simple ensemble average definition of turbulence is not suited for engine flows.

Several researchers (22-24, 5, 25-27) have studied the issue and have proposed different ways of analyzing the signal. A consensus seems to be developing that in reciprocating engines it is necessary to obtain continuous records (or as close to continuous records as possible) in each cycle and to deduce from them both time and length scales of the motion. After that, our position is that the turbulence and bulk flow parts of the signal are relative to each application and generally different for different applications. For example, consider a laminar flamelet propagating within the engine charge near TOC. It is clear that the residence time within the laminar flame front and the thickness of the laminar flame impose the characteristic time and length scales with respect to which the flow immediately ahead of the flamelet must be analyzed. Since it is the flow immediately ahead of the flamelet that counts, conditional sampling may also be necessary (28, 29). If a spray is of interest, one must consider its length and time scales, which vary with distance from the injector. In order to decide which part of the local flowfield acts on the local part of the spray as turbulence and which as bulk flow. Ignition and wall boundary layers again have different characteristic time and length scales so that each perceives the same flowfield as having different turbulence and different bulk flows. Thus we conclude that:

2) In reciprocating engines the time and length scales of the flow must be resolved in each cycle and separation into turbulence and bulk motion is relative to the process that is influenced by the flow.

We will refer to "simple ensemble averaging" and "cycle-resolved" data even though there are many ways of analyzing cycle-resolved data.

The turbulence intensity deduced with cycle-resolved techniques is always smaller than that deduced from simple ensemble averaging and this difference is important in many applications and in assessing the accuracy of models.

In view of the above discussion, it would be necessary to measure the three components of the velocity, and pressure, density and concentrations, continuously in time and at several locations to determine the initial state of the charge within the cylinder and its compression and combustion. Numerically, it would require the three-dimensional computation of the flow by the valves and in the cylinder (with spatial and temporal discretizations capable of resolving molecular transport) coupled with the (at least one-dimensional) flows in the intake and exhaust manifolds and with wall heat transfer (at least to walls kept at time-averaged temperatures). But even this level of resolution is not yet practical.

Forced by current experimental and computational limitations, different groups have taken different short cuts, none of which is satisfactory but all of which have their practical usefulness. Moreover, the differences are likely to diminish with time.

At the Imperial College measurements continue to be made in low speed engine and turbulence and bulk flow continue to be defined using the simple ensemble average technique (4, 17). Numerically they have concentrated on three-dimensional computations of intake and compression but without considering the flows in the intake and exhaust manifolds. Using a k-ε submodel for turbulence, they have made extensive comparisons of bulk velocity and turbulence, mostly with the corresponding quantities measured at the Imperial College.

A rather general three-dimensional code has been developed at Los Alamos (30) for intake, compression, fuel injection, and combustion of premixed and fuel-injection charges, but without consideration of the flows in the intake and exhaust manifolds. It incorporates a turbulence model in which only the diffusive effects of the turbulent moton with scale smaller than the numerical grid size are modeled. For sufficiently small grid size this is a satisfying approach.
because small-scale turbulence tends to have
universal properties. But for the grid sizes that
are feasible today (of the order of some
millimeters), the computed results depend on the
numerical resolution, and this is not appealing.
And yet, for three-dimensional computations this
may be the least undesirable of the options
available today because it leaves minimum uncer-
tainty as to which part of the turbulence spectrum
is being submodeled. From this point of view, the
sensitivity of the computed results to the size of
the numerical grid becomes a useful indicator of
both the quality of the results and the adequacy
of the subgrid model. At this time it would be
desirable to make extensive and detailed com-
parisons of experimental data and three-
dimensional computations using subgrid turbulence
modeling to assess its capabilities.

When we started modeling engine flows and
combustion in the early 70's, we were struck not
by the complexity of the intake process but by the
apparent simplicity and reproducibility of the TDC
flowfield. After all, in a well designed produc-
tion engine, cyclic variations in peak pressure are
down to a few percents and this is a remarkably small variation for such a complex unsteady turbulent reactive field. Semenov, in
his outstanding paper of 1958 reporting his
measurements in a valve engine (22), concluded
that at TDC "with increasing distance from the
chamber center, v' does not change by more than
15% except near walls, i.e., TDC turbulence
intensity is rather homogeneous. He also stated
that "during combustion, v' at a given point of
the chamber does not vary by more than 10%".
Since the length scales are limited by the
clearance, Semenov deductions imply constant tur-
bulence diffusivity during combustion. (He was
also clearly aware of the difficulty in defining
turbulence in reciprocating engines and, although,
he used simple ensemble averaging, he also
employed filtering to separate and to study low
frequency motions.) Finally, for premixed-charges,
the combustion time and cyclic variations are not
very different for valved and ported engines
operated at the same scavenging efficiency) and
therefore the details of the intake system cannot
be of primary importance to TDC combustion.

Thus we interpreted chamber events as
follows. As Semenov had pointed out, the shear
layers of intake jets generate turbulence, i.e.,
motion with no net translational or rotational
resultants. However, the momentum of the intake
current always produces some net rotational motion
inside the cylinder at the end of intake. During
compression, turbulence tends to become spatially
and directionally uniform (except near walls),
and generally to decrease in intensity. The bulk
rotational motion, on the contrary, tends to per-
sist because only wall friction can reduce the net
angular momentum of the gas and even for very
strong bulk rotational motions, such as strong
swirl, the loss of angular momentum during
compression is only 30% to 50%. As Semenov
indicated, by TDC the velocity of the bulk motion
is of the same order as the turbulence intensity.
But it is the small scale motion an its main effect
is to displace and distort the flame front dif-
frently in different cycles. Such cyclic
variations in the velocity field alter the burning
rate little but perhaps enough to contribute to
the cyclic variations in peak pressure.

Accordingly, initially, we concentrated on
combustion around TDC and in our computations we
used simple turbulence diffusivities (9). However
at the time our interests were primarily in
direct-injection and divided-chamber stratified-
charge rotary and reciprocating engines in which
the spray or the prechamber jets produce local
shear layers for which the turbulent diffusivity is
not spatially uniform. Thus we converted to the
use of a k-e turbulence submodel that is par-
ticularly suited for shear flows. But for open-
chamber premixed-charged engines with small bulk
flows, a turbulent diffusivity that is propor-
tional to the engine speed still is a reasonable
approach and alternative approaches have yet to
demonstrate clear superiority. But we are jumping
ahead of ourselves. Since 1980 more has been
learned about the compression flow that is worth
summarizing before reconsidering combustion.

COMPRESSION

In 1980-81 comparisons were presented of
computed and measured turbulence near TDC, prior
to ignition, in two reciprocating engines. The
model was for two-dimensional axisymmetric
flowfields and employed a k-e submodel for
turbulent transport. It was called REC-A and was
derived from the Los Alamos code called CONCHAS
(31). The same k-e model constants were used in
all the Princeton computations mentioned in this
review. For a pancake-like combustion chamber and
in the absence of strong bulk flows, the computed
TDC turbulence intensity was compared with that
measured by Lancaster (24) versus engine speed,
load, and compression ratio. With swirl, computed
turbulence and tangential velocities were compared
with those measured by Witzie et al (32) at two
engine speeds. In good agreement with the exper-
imental data, the model reproduced proportionality
of TDC turbulence intensity to engine speed and
mildly increasing intensity with increasing load
and decreasing compression ratio.

At the same time, using the model in para-
metric and sensitivity studies, it was also found
that, in the absence of strong initial bulk flows
and of squish, intake turbulence tends to become
spatially uniform during compression. The relaxa-
tion crankangle is about 100° and is independent
of engine speed, load, and compression ratio.
Thus, in the absence of strong initial bulk flows
and squish, TDC turbulence is insensitive to the
details of the intake process. It was also found
that, for a given engine configuration and speed,
all TDC turbulence properties are functions only
of the initial turbulence diffusivity. For a given
initial diffusivity, large dissipation rates are
associated with large intensities, and small
dissipation rates with small intensities, so that
initial intensity differences tend to disappear
during compression. Hence strong initial bulk
flows tends to make the TDC flowfield even
less sensitive to the intake process, particularly
on the piston shoulder and near the edge of the
cup. The only bulkflow that was then studied was
solid body swirl. It was concluded that with or
without squish, swirl generates its own tur-
bulence, that in turn modifies the swirl, and that
the initial strength (angular momentum) of the
swirl is remembered at TDC, both in the mean flow
and in the turbulence, but initial nonuniformities in turbulence again disappear rapidly during compression.

The results of the above studies were published in (33,34) and were confirmed and extended by El Tahry (35) who used a similar k-ε submodel and a two-dimensional axisymmetric code, also derived from CONCHAS. He extended those studies by considering two-piston geometries (a flat-crown piston, giving a pancake-like combustion chamber without squish, and a reentrant bowl) and the effects of the initial swirl angular momentum, swirl velocity distribution, and turbulence kinetic energy level on the compression motion and the TDC flowfield. His plotted results show that in the absence of squish, i.e. with the flat-crown piston, different initial swirl profiles with the same angular momentum rapidly tend to solid body profiles (except near walls), lose about the same fraction of their initial angular momentum during compression, and practically give the same flowfield at TDC. However, near TDC, say at -40°, the swirl with initial flat-top profile gave a higher turbulence intensity than that with initial solid-body profile and it is necessary to consider the flowfield also prior to TDC since combustion does not start at TDC. El Tahry also confirmed the complex interplay between swirl, squish and piston cup geometry that leads to a variety of mean flow patterns in the cup near TDC. This important phenomenon had been identified by Gosman et al (36) who also had used a two-dimensional model and a k-ε submodel.

Thus the early experimental work and the two-dimensional computations made with k-ε turbulence submodels in 1978-82 indicated that:

3) Near TDC turbulence is always insensitive to the details of the turbulence generated during intake;

4) For a given engine and in the absence of strong squish and of strong initial bulk flows, turbulence intensity near TDC is rather homogeneous and isotropic (except near walls) and increases only with increasing initial turbulence diffusivity. The intake process sets the magnitude of the initial turbulent diffusivity;

5) In the presence of strong initial bulk flows and/or squish, both turbulence and bulk flows near TDC depend on the details of the initial bulk flows and of the chamber geometry. But the details of the initial turbulence field are insignificant.

Subsequent two-dimensional results (27,37) led to another important conclusion:

6) In the absence of strong initial bulk flows and/or squish, there is a limit to the maximum turbulence intensity that can be obtained at TDC.

In point 6 it is understood that the intensity of turbulence is defined as the intensity of the high frequency components of the velocity fluctuations in cycle-resolved measurements. The limit is due to the chamber walls (37). The greater is the initial diffusivity, the shorter is the time by which the turbulence-damping effect of the wall is felt throughout the chamber field. Thus, after a point, further increases in initial diffusivity produce smaller and smaller gains in TDC turbulence intensity. Since the TDC length scale is also limited by the chamber geometry, it follows that the TDC turbulent diffusivity is limited too. Therefore, without initial strong bulk flows and/or squish, it becomes more and more difficult to increase the flame speed by modifications of the intake system. To increase the flame speed, say in lean mixtures, one is forced to use swirl, or squish, or special additives, or higher compression ratios, or multiple spark plugs, or other devices, each of which has its own disadvantages.

In points 3-6, no equations are given that define sensitivity, details of initial turbulence, strong initial bulk flows, strong squish, extent of homogeneity and isotropy of TDC turbulence, and initial diffusivity. The main reasons for the lack of specificity are that: diffusive processes do not exhibit sharply defined regimes; the same flow is seen as having different characteristics in different applications; there is no commonly accepted definition for engine turbulence. The available computed and measured information is limited both in extent and in reliability. Three-dimensional computations should help clarify some of the points. But well-characterized and extensive measurements are needed the most.

The measurements reported in (27) were made at many locations within pancake-type combustion chambers and are unique in that they are cycle-resolved LDV measurements at practical engine speeds (600 to 2400 rpm) and include data from both direct and valved engines without and with swirl. Turbulence measurements in ported engines do not seem to have been previously reported. The drastic difference in intake design between valved and ported engines shed some light on the influence of the details of the intake system on the flowfield near TDC. Data were collected from between -45° and -30° to between +40° and +30°. The signal in each cycle was Fourier-analysed and frequencies above a cutoff frequency were called turbulence and those below were called bulk velocity. The turbulence intensity was the RMS of the ensemble average of the turbulence within 1° windows. The cyclic variation in the bulk velocity was the RMS of the ensemble average of the bulk velocity within the same window. The cut off frequency corresponded to the residence time of the reactants within the flame zone in premixed-charge engines. If the same data had been analyzed using simple ensemble averaging, the deduced turbulence intensity would have been as much as three times larger than the one obtained with the cycle-resolved analysis.

It was found that near TDC the turbulence intensity (Fig. 1) scaled with rpm, increased with swirl, and exhibited minimal cyclic variations in both engines, and was homogeneous and isotropic to within 20% in the ported engine. The cyclic variations in the bulk velocity (Fig. 2) also increased with engine speed, but decreased with swirl (consistently with cyclic variations in peak pressure and flame propagation), and were larger in the valved engine than in the ported engine. These trends are consistent with points 3-6 and
were found with dramatically different intake systems.

At the same engine speed, without swirl and near TDC, an additional finding of some interest is that the turbulence intensity in the ported engine was larger than in the valved engine (Fig. 1). But in the ported engine it was also decreasing rapidly with crankangle whereas in the valved engine it was not (as Semenov had indicated). Both trends were reproduced by the model (37). They are due primarily to the fact that in the ported engine the time between the mid-point of intake and TDC is shorter than in the valved engine; TDC turbulence is at an earlier stage of decay in the ported engine than in the valved one.

COMBUSTION

The overall conclusion from the previous two sections is that there are many uncertainties but there is also a remarkable continuity of agreement that in the absence of strong squish and of purposely induced strong bulk motions, around TDC, high frequency velocity fluctuations scale with engine speed and are rather reproducible, homogeneous and isotropic (except near walls), whereas low frequency velocity fluctuations, that are of similar magnitudes, are less reproducible but also less influential on the combustion rate (but seem to be closely connected with cyclic variations in peak pressure). Thus in the absence of strong squish and purposely induced strong bulk motions, it is preferable, but not essential, to make three-dimensional computations of intake, compression and combustion in homogeneous charges. Combustion computations around TDC are less expensive and justified. Probably the most reasonable approach is to perform extensive parametric studies around TDC and in two dimensions and then to check the main conclusions with three-dimensional computations. In three-dimensional computations of intake and compression, at least one-dimensional estimates of the flows in the intake and exhaust manifolds should be included since waves in those conduits are important in establishing the initial state of the charge at intake valve closing that the three-dimensional computations of in-cylinder flows are attempting to reproduce accurately. In both two- and three-dimensional flow calculations, the wall temperature will probably continue and be assumed to be varying in space but constant in time.

Two-dimensional computations of premixed-charge engine combustion near TDC first appeared around 1975 (see Ref. 2). They were started either at the closing of the intake valve or at
spark ignition from uniform values of k-c and from selected profiles of bulk motion or without it. (Only those efforts are considered in which detailed comparisons of model predictions with measured data were also presented). The early two-dimensional combustion assessment computations were reviewed in (9) and will not be reconsidered except to say that they included results using either a constant diffusivity for turbulent transport or a k-c turbulence submodel, and a one step irreversible Arrhenius kinetics for chemical conversion. Of those early computations, particularly rewarding was a study in which the origin was identified of the pressure waves that are often found in divided-chamber engines (38).

One study, not reviewed in (9), was performed in 1979 with a k-c submodel for turbulent transport and a mixing-controlled one-step irreversible conversion rate model (39). Its results were compared with pressure and flame data from a divided-chamber stratified-charge engine. The mixing-controlled approach does not include any Arrhenius term, directly or indirectly, and thus denies that laminar flames play any role in engine combustion. That went against the trend suggested by many of the curves of engine flames that explicitly rely on the laminar flame speed. But the mixing-controlled concept was being supported by studies, e.g. (40), that, however, did not include comparisons with engine measurements. Our computations and comparisons with pressure and engine flame data concluded that the mixing-controlled model was inherently inadequate to reproduce combustion near cold walls where kinetic rates eventually must become controlling. In engine combustion, mixing-controlled models can also be expected to be inadequate for self ignition (knock and Diesel), pollutant formation, and rich and lean misfire limits. Thus, ultimately they would have to be supplemented with chemical kinetics information. However, it was also indicated that a combination of mixing and Arrhenium kinetics controlled conversion rate may prove more appropriate. Such a model had originally been proposed by Spalding in a different context (41), and was explored a little further in (42).

Although two-dimensional combustion models had been in use in some industries for some time, industrial reports about their results started appearing around 1980. They are particularly interesting.

The first such report was from Volkswagenwerk AG (43) and its abstract reads: "The thermal efficiency of an engine can be improved by increasing its compression ratio. Further improvements - especially under part load conditions - are expected by optimizing the combustion chamber design: Thus, Crowfield and the flame propagation should be influenced in such a way that the combustion duration becomes reasonably short and that simultaneously heat losses are not too high. A two-dimensional mathematical model has been applied in order to study some configurations of high compression ratio. This part of the investigation has not been published: The parameters, which have been varied, are the squish area and the clearance gap. The model is able to simulate the effects on the combustion process for those arbitrary geometries. A single cylinder research engine was used to confirm the computations. The results indicate that the good thermal efficiency of the selected high compression ratio engine can be further improved by designing an optimum combustion chamber. The amount of additional efficiency in this particular engine is smaller than the improvement which has been achieved by changing the conventional compression ratio into a higher one".

The VW authors used REC-P, a Princeton code that was derived from the RICE code of Los Alamos (44) and was for two-dimensional chamber geometries that near TDC could be approximated by two-dimensional planar coordinates and time-varying local clearances. It employed a k-c submodel for turbulence and a one step irreversible Arrhenius rate. Two aspects of this application are particularly interesting: its methodology and its results.

The methodology consisted of obtaining pressure data over a range of operating conditions for the engine whose behavior was to be studied. A few model constants were then adjusted for an acceptable reproduction of the measured data. The model was then used to predict what effect possible changes in the original engine would have on indicated efficiency. The most promising changes were isolated and implemented. Hypothetical new configurations were then made and were found to agree with the predictions. The model-tuning procedure that was employed recognizes that models are only approximations and that many aspects of engine combustion are anything but quantitatively understood and therefore even the best of models cannot be expected to be complete and self sufficient, even in principle. The significance of the results is that a two-dimensional combustion model had guided the selection of engine combustion configurations in an industry for the first time.

Researchers at FIAT reported an even more systematic and extensive application of REC-P to the FIAT 138 production engine. They used again an iterative procedure and wrote in their abstract (45): "Measurements of pressure, flame arrival and wall temperature were taken in one cylinder of a four-cylinder production engine. Changed in the experiment were engine speed, load, spark advance, and air-to-fuel ratio for a total of 190 conditions. Then nine cases were selected differing in speed, load, spark advance, and air-to-fuel ratio and their combustion computed with a two-dimensional planar model based on a k-c turbulence sub-model, one overall irreversible reaction for the oxidation of the fuel and the law-of-the-wall and Reynolds analogy for wall heat transfer. The same model constants were used in all computations. Computed and measured pressures and flame arrivals were compared and the agreement was judged adequate even though the computed expansion-stroke pressure was somewhat above the measured one in some cases, probably due to an underestimate of wall heat losses. The tested model was then used to predict the effect of compression ratio and of a change in chamber geometry on indicated efficiency at 3500 rpm, full load, and stoichiometric mixture."

The engine head used in the study is shown in Figure 3 and one of their comparisons between the computed and the measured flame arrival is presented in Figure 4. Here isothermers indicate the computed flame position, open circles those
An important aspect related to indicated efficiency is engine knock. This subject was not addressed directly by the applications of (43, 45, 46) but the same VM group was also the first one to explore the extension of two-dimensional combustion models to consider knock (47). Independently, we reviewed proposed mechanisms and models for engine knock and selected the so-called "Shell" global submodel for the low-temperature ignition chemistry of hydrocarbon/air mixtures (48). The model was first applied to spatially uniform charges in a constant volume bomb and in a rapid compression machine. The computed trends were found to compare favorably with the measured ones. Next, cool flames in isocetane/air and n-heptane/air mixtures in a stirred reactor were computed and compared with experiments. Trends matched closely but magnitudes did not. Finally the charge in a spark-ignition engine was considered and a fully coupled two-dimensional model (with a finite-thickness flame) was used to study engine knock. It was found that the structure of the finite thickness flame determines whether it is accelerated by the preflame reactions or is not affected by them. The two limits were studied and the trends computed in the latter one were found to be in better agreement with the majority of the experiments. It was also found that, while single stage ignition is sufficient to model strongly knocking cycles, it is inadequate for those of marginal knock, which are the more important ones in practice, in which cool flames precede and, in fact, delay the onset of knock. Researchers at VM ultimately selected the same Shell global submodel for the low-temperature ignition of hydrocarbon/air mixtures and reported similar experiences with it (49). Applications of multi-dimensional modeling of engine knock are still very limited.

Thus it is not unreasonable to conclude that:

7) In spite of their limitations, when used in an iterative manner two-dimensional premixed-charge combustion models have been shown to predict the correct indicated-efficiency trends for complex chamber geometries with and without moderate squish and swirl.

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Fig. 3. Actual and Computational (REC-P) Geometry of the FIAT 138 Production Engine Head (45).

Fig. 4. Computed (REC-P) Isotherms, Velocity Vectors, and Flame Arrival at the Measured Ionization Probe Positions (Case 9 of Table 3 of (45)).
Fig. 5. Five Combustion Chamber Designs Studied with REC-P (46).

but they should prove useful if they are implemented iteratively as applications of combustion models have been.

In the course of the preceding studies a peculiarity surfaced of the usage of one step irreversible global conversion rates: for rich mixtures they can lead to the incorrect evaluation of the chemical energy released. Such peculiarity is totally unacceptable in engine computations. The main equilibrium products of lean hydrocarbon-air mixtures (actually, for $\phi < 0.9$) are $\text{CO}_2$, $\text{H}_2\text{O}$, and $\text{O}_2$ and conservation of the C, H, and O atoms invariably leads to the correct evaluation of their amounts and of the energy released. But for rich mixtures (actually, for $\phi > 0.9$) the main equilibrium products are $\text{CO}_2$, $\text{H}_2\text{O}$, $\text{CO}$, $\text{H}_2$ and conservation of atomic species is insufficient to determine their amounts. When conventional irreversible global rates are used, information about the actual equilibrium composition is not used in any place and therefore there is no guarantee that the computed composition will converge to the proper equilibrium and heat release. In general it does not, particularly when the composition ahead of the flame changes in space and time.

To eliminate this problem, a formulation was proposed (50) that expresses the global rate in terms of the difference between the local and instantaneous concentrations of the various species and their local and instantaneous equilibrium values. As the reaction rate goes to zero, this local equilibrium formulation forces all species to their equilibrium unconditionally and yields the equilibrium energy release. The local equilibrium formulation, or similar ones, are not necessary if $\phi < 0.9$, but they are essential if $\phi > 0.9$, even locally and temporarily, as in stratified-charge and Diesel engines.

The engine combustion studies of (38, 39, 42, 43, 45, 46) had varying degrees of success in matching experimental results. But all of them share two limitations: the use of a numerical spark time that differs from the experimental one; and a predicted energy release rate that is generally somewhat slower than the experimental one at the beginning of combustion and somewhat faster toward the end of combustion.

The use of the numerical spark time as a free parameter has been justified on account of the numerical grid being too large to resolve the details of the ignition process. For applications this has not been a serious limitation since one is often interested in the maximum indicated efficiency of a selected engine design at a given set of operating conditions. The maximum can be found by starting the computations at different crank angles from a flame kernel. Such procedure corresponds to the standard experimental selection of best spark timing. Even though the crank angle of the computational kernel does not correspond to the actual experimental spark timing, both procedures lead to the identifications of the best efficiency that can be obtained with the given chamber design and operating conditions. Yet it is obvious that it would be better if the model could use the experimental spark time to reproduce the experimental pressure curve. A first attempt in this direction was reported recently (51).

The discrepancy in the energy release rate has been small but disturbing nonetheless because
it points to a basic inaccuracy of the models. The model improvements presented in (51) seem to reduce this discrepancy and to provide an explanation for its origin. A k-ε model for turbulent transport and a combination of a mixing controlled and an Arrhenius controlled conversion rate were used. The constants of the k-ε model were those determined by comparisons with TOC turbulence intensity data in the absence of combustion (33) and the constants of the Arrhenius kinetics were determined in comparisons with laminar burning speed data using the local equilibrium formulation (50). The most important change with respect to earlier models was an explicit, if ad hoc, attempt to account for the dominance that laminar flame parameters seem to have in the initial propagation of the engine flame (52-54). The resulting computed turbulent engine flame speed increased at first and then leveled off, as indicated by the measurements; the computed pressure histories fitted better the measured ones; and computations were started at the actual engine spark time.

To complete our review of published multi-dimensional computations of combustion in premixed-charge engines, it is important to point to one factor that contributes both their strength and their weakness: the local and instantaneous flame speed, and not the local and instantaneous structure of the flame, is the main quantity that determines premixed-charge engine combustion.

It is true that the correct flame speed follows if the structure of the flame is properly understood and represented. But it is not true that one must represent the flame structure correctly in order to get the correct flame speed. In most zero-dimensional models, for example, a spherical discontinuity is assumed to separate reactants from products and the speed of the discontinuity is imposed using experimental curvature, i.e., the structure of the flame is not considered at all. Such an approach has given useful results for simple open combustion chambers without squish or swirl.

The reason for the predominance of the flame speed in premixed-charge engines is that, under certain conditions, the local and instantaneous values of all thermodynamic variables depend almost exclusively on flame position (that can be computed if the flame speed is known), on the chamber geometry and on elements of the initial and boundary conditions while the local and instantaneous gas velocity is nearly proportional to the flame speed. These properties hold for any number of species, any forms of the diffusivities, any flame structure, and any number of space dimensions. The conditions are: 1) the thickness of the flame zone and of wall boundary layers must be much smaller than the dimensions of the chamber; 2) the speed of the gas must be much smaller than that of the sound; 3) the charge initially must be uniform; 4) the geometry of the chamber must be compact and unobstructive; 5) the ratio of the rate of wall heat transfer to the rate of energy release must be nearly independent of flame speed; 6) the ratio of the wall velocity to the flame speed must also be independent of the flame speed. The conditions are verified, at least approximately, in premixed charge engines except for non-equilibrium emissions of NOx, CO, and unburned hydrocarbons and where flames and wall boundary layers interact directly. These scaling properties are the reason for the usefulness of zero-dimensional models in the absence of squish and swirl and away from walls. Intuitively they have been known for a long time (55). Mathematically they have been clarified recently (6).

In the multi-dimensional models discussed so far, the flame speed is allowed to vary along the front and with time. Moreover the front is not required to be spherical and can adjust itself to complex chamber geometries, squish, and swirl. The local and instantaneous wall heat transfer is also part of the output of such multi-dimensional computations. But the equations that indirectly determine the local and instantaneous flame speed have still been selected so as to reproduce pressure and flame shape data. This is equivalent to fitting the flame speed to the measured one locally and instantaneous. The reason for this procedure is that quantitative knowledge of the flame structure, and corresponding reliable equations were, and still are, not available. However, this situation may now be changing.

8) Even if a reliable and tested theory of the engine flame structure is still many years into the future, the time may be approaching when some elements of it may be accounted for explicitly in multi-dimensional models.

Such development would be particularly relevant to the computation of the interaction of the flame with the wall regions and, perhaps, to ignition, cyclic variations, flammability limits, and knock.

The measurement that J.R. Smith reported in 1982 (56) may be viewed as the first contribution to the new chapter. He passed a pulsed-laser (0.01 μs) beam (diameter <0.1 mm) through a premixed-charge engine parallel to the piston surface and collected the light scattered at 90° by the molecules within the flame zone whose thickness was of the order of 1 cm. The resolution along the axis of the beam was of the order of 0.1 mm. From the intensity of the scattered light he could deduce the local and instantaneous thickness by along the laser beam within the flame zone. He ran the engine up to 1800 rpm. He concluded that within the flame zone there were wrinkled laminar flames of varying thicknesses but of the order of 0.2 mm. That engine flames may be wrinkled laminar flames at practical engine speeds (as the speed tends to zero, the flame must tend to the laminar flame) had been argued by many, notably by the MIT group (11), but never satisfactorily substantiated experimentally. Very recently (57) a pulsed-laser sheet (0.01 μs, 0.1 mm thick, 10 mm wide) was passed through a premixed-charge engine parallel to the piston surface and the light scattered at 90° by seeding particles was collected with a two-dimensional array of diodes, thus obtaining the first two-dimensional cross sections of the flame zone. The engine was run up to 1800 rpm and Smith's laminar flame results were confirmed. But at the higher speeds the laminar flame was highly convoluted and, possibly, thicker than it would be in a laminar field. Convolution will continue to increase as the engine speed increases. Efforts are in progress to obtain two-dimensional cross sections at speeds up to 4000 rpm.
Finally a rather extensive review of theoretical considerations was undertaken (19) and lead again to the conclusion that the flame zone of premixed-charge engines should be made up of wrinkled laminar flames at least up to moderate engine speeds. The essence of the argument is that the turbulence time scale and the Kolmogorov length scale are estimated to be larger than the residence time within the laminar flame front and the laminar flame thickness so that the laminar flame should simply be distorted by the turbulence. This distortion increases with engine speed because the turbulence time and length scales decrease with it. But the argument is simplistic because in an engine turbulence exhibits ranges of integral time scales and Kolmogorov length scales and the disruption of the laminar flame can be so extensive at practical engine speeds that a broad spectrum of laminar flame processes may have to be accounted for.

MEASUREMENTS

Recent, extensive, detailed, and knowledgable reviews of conventional (13,14) and advanced optical (16,20) techniques are available so I will just mention some premixed-charge problems to which the application of advanced optical techniques is particularly timely.

In the absence of combustion, innumerable in-cylinder measurements of turbulence intensity have been made with hot wire anemometry and laser Doppler velocimetry in a variety of practical and impractical engines and operating conditions (see (27,20), for example, for references to them) but the length scale seems to have been measured only once and under limiting conditions (58). And yet even homogeneous isotropic turbulence requires two parameters for its characterization. Obviously turbulent length scales should be measured (20).

In the presence of combustion, turbulence intensity is being measured (28,29,59). Such information is necessary to determine to what extent measurements made in the absence of combustion are applicable when combustion is present. For theoretical developments it is also very useful to know the changes that turbulence parameters undergo across the flame zone.

Measurement of turbulent length scale are are also necessary in the presence of combustion.

Although a significant fraction of the fuel is burned toward the end of flame propagation, when the distance between the flame zone and the cylinder wall is of the order of the thickness of the flame zone, no measurements of turbulence length scales, or even intensity, seem to have been made near walls. Similarly, regions near the cylinder and engine-head walls have not been characterized. As previously indicated, the interactions between the flame zone and wall boundary regions are particularly difficult to understand and model.

Important questions about the structure of the flame zone at practical engine speeds remain unanswered even after obtaining (57) two-dimensional cross sections of it. They regard the thickness, tilt and continuity of the laminar flames within the flame zone and the presence or absence of isles of reactants and products. Such questions can be answered with three-dimensional measurements.

It would appear that the fully development turbulent flame is preceded by a first phase in which the flame kernel grows to the size of the turbulence integral length scale and a second phase in which the turbulent flame completes its development. It is also believed that the second phase is the one mostly responsible for cyclic variations in the pressure. It would be advisable to reexamine those processes with the higher-resolution technique now available (20).

The onset of knock is still a matter of some controversy (60). Cycle resolved measurements of species concentrations in regions in which rapid heat release first occurs would be of considerable help (20).

CONCLUSIONS

Points 1-8 and the suggestions about quantities that should be measured constitute the conclusions.

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