LA-UR-96-1982

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: **NUMERICAL MODELING OF HYDROGEN-FUELED INTERNAL COMBUSTION ENGINES**

AUTHOR(S): Norman L. Johnson, T-3
Anthony A. Amsden, T-3
T. Daniel Butler, T-3

SUBMITTED TO: *1996 Annual Hydrogen Peer Review for DOE, Miami, Florida, May 1–3, 1996*

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

NUMERICAL MODELING OF HYDROGEN-FUELED INTERNAL COMBUSTION ENGINES

(LA-UR-96-1982)

Norman L. Johnson, Anthony A. Amsden, and T. Daniel Butler
Los Alamos National Laboratory
Theoretical Division, Group T-3
Los Alamos, NM 87545
(NLJ@LANL.GOV)

Abstract

Major progress was achieved in the last year in advancing the modeling capabilities of hydrogen-fueled engines, both in support of the multi-laboratory project with SNL and LLNL to develop a high-efficiency, low emission powerplant and to provide the engine design tools to industry and research laboratories for hydrogen-fueled engines and stationary power generators. The culmination of efforts on many fronts was the excellent comparison of the experimental data from the Onan engine, operated by SNL. These efforts include the following. An extensive study of the intake flow culminated in a major understanding of the interdependence of the details of the intake port design and the engine operating condition on the emissions and efficiency. This study also resulted in design suggestions for future engines and general scaling laws for turbulence that enables the KIVA results to be applied to a wide variety of operating conditions. The research on the turbulent combustion of hydrogen brought into perspective the effect of the unique aspects of hydrogen combustion and their influence on possible models of turbulent combustion. The effort culminated in a proposed model for turbulent hydrogen combustion that is in agreement with available literature. Future work will continue the development in order to provide a generally predictive model for hydrogen combustion. The application of the combustion model to the Onan experiments elucidated the observed improvement of the efficiency of the engine with the addition of a shroud on the intake valve. This understanding will give guidance to future engine design for optimal efficiency. Finally, a brief summary is given of the extensions and refinements of the KIVA-3 code, in support of future designers of hydrogen-fueled engines.

turbulence intensity (u') at the beginning of the simulation was specified to be one-tenth of the maximum piston velocity. The CLR engine, in the experiments and simulations, showed large reductions in NO_X levels at lean fuel mixtures, sufficient to satisfy the "zero-emission" standard without a catalytic converter. In the KIVA simulations, we found that modifications to the standard hydrogen kinetics were required for the CLR simulations, as were required for the injection simulations. Because the experimental results suggested that the bulk flow from the intake process was influencing the performance of the engine and that the combustion rate in SI engines, and subsequently the emissions and engine efficiency, is dependent on the turbulence levels at the time of combustion, it was concluded that a predictive simulation capability was needed to include the intake flow. A valve model for KIVA was begun in late 1994 and mostly completed in FY95. The addition of the valve model into KIVA is one of the more important improvements in KIVA over the last decade and has attracted significant attention in industry and academia. A pre-released version of KIVA with the valve model is currently being tested at two major diesel manufacturing companies, two universities, and a government engine design laboratory. A national release of the version with documentation is expected within this fiscal year.

Preliminary results of the modeling of the Onan engine, the second experimental engine at SNL, were reported in last year's annual review (Johnson, Amsden et al. 1995). The intake flow and valve configuration of the experimental Onan engine were designed by LLNL to result in a quiescent flow at the time of combustion in order to maximize the efficiency by minimizing heat transfer to the walls. An additional spark plug was added to offset the slower ignition duration. In the absence of experimental data on the Onan engine at the time, a computational investigation was undertaken to evaluate the importance of modeling the intake flow on the combustion and NO_X emissions. A simulation that began with the compression of a quiescent hydrogen-air mixture was compared to a simulation of the air induction process with resolved opening and closing of the intake valve. Although moderate differences were observed in the cylinder-averaged pressure, temperature, bulk-flow kinetic energy and turbulent kinetic energy, large differences were observed in the hydrogen combustion rate and NO_X emissions. We conclude that (1) the Onan engine is not a typical quiescent engine, (2) the flow state at combustion is heterogeneous and sensitive to the details of the bulk and turbulent flow, and consequently an accurate simulation of the Onan engine must include the modeling of the air-fuel induction and (3) the single-equation hydrogen combustion model is deficient for modeling the Onan engine due to unrealistic precombustion. Results from this study suggested that minor changes to the engine geometry by the addition of a shroud on the inlet valve would have the desirable effect of switching the dominant tumble flow to a more swirling flow, thereby producing less heat transfer and a higher efficiency. This modification was implemented in the Onan engine in the following months and did result in an increase in the efficiency of the engine (details of these experiments can be found in the annual review paper by Van Blarigan). The success of this collaboration between the experimental and computation program illustrates the importance of the simulations in understanding in the details of the engine dynamics, which are not experimentally available. More details of these results are provided in the section below on the intake flow and shrouded-valve simulations.

Hydrogen Combustion

Introduction

The combustion characteristics of hydrogen are the unique aspects of hydrogen that differentiate the modeling of hydrogen-fueled engines from all other fuels, including hydrocarbon gases, such as methane, and liquid hydrocarbon fuels. In the absence of these differences, the existing techniques for non-hydrogen fuel could be directly applied to hydrogen engines. Because of the unique combustion properties of hydrogen, we address this aspect of the project first, even though it is the most recent area of study and is not yet completed.

Our goal is to provide a combustion model that accurately describes the dependencies of turbulence, fuel-oxygen ratio, fuel mixtures, temperature and pressure, but that is also applicable to repetitive, full-engine simulations, required by industry. An accurate combustion model, that is too complex and computationally intensive, has limited application, both in the current project and by engine

designers in industry. While we are now focusing on hydrogen-air mixtures, later work will include mixtures of hydrogen with hydrocarbon gases.

The main questions to be answered in this section are: How does turbulent combustion of hydrogen differ from that of hydrocarbon gases? Can the models for hydrocarbon turbulent combustion be used accurately for hydrogen combustion? Fortunately, the answer appears to be that turbulent hydrogen combustion does differ from hydrocarbon combustion, but not in a way that invalidates the use of the hydrocarbon combustion models.

The Unique Behavior of Hydrogen Laminar Combustion

Most researchers of combustion of gases are familiar with the low flammability limit of hydrogen and very high flame speeds or burning velocities of hydrogen, about 3.5 m/s in air at STP (Al-Khishali and Bradley 1983, Koroll et al., 1993), about ten times the flame speed as found in low molecular weight hydrocarbon gases (Liu and MacFarlane 1983; Tseng, Ismail et al. 1993). What is not broadly known is the origin of these differences, and this section focuses on the results of a thorough literature search on laminar and turbulent combustion, both as the basis of the current research, and as a resource for other researchers concerned with hydrogen combustion. Unfortunately the needed information in the literature is not complete, but the existing literature was generally found to be consistent. As an aid to other researchers, relationships are given between the various measures of hydrogen concentration used in the literature in an attached Appendix and will aid in comparisons of experimental data.

The extremely high molecular diffusivity of hydrogen produces many of the unique properties of hydrogen, such as the desirable traits of flammability and robust combustion at lean mixtures for both hydrogen-air and hydrogen-hydrocarbon gas-air mixtures. The high mobility of the hydrogen also contributes to an instability in a laminar flame front at lower values of φ, the fuel equivalence ratio (here, an unstable flame front means that a protuberance in the flame front will speed up and a trough will slow down - making a wrinkle grow in size). The instability occurs because the hydrogen is depleted in the troughs and collects in the tips, coupled with the fact that the flame speed increases with increasing hydrogen concentration in this regime. Although an instability in a planar flame front occurs for all combustion gases at some concentration, due primarily to the difference in molecular weight of oxygen and any gaseous fuel, what is unusual for hydrogen is that this instability in air occurs at values of φ in the normal operating conditions of engines, at a φ less than 1.5 at standard temperatures and pressures (STP). This is in contrast to the region that is unstable for methane *($\varphi < 0.74$)*, propane *($\varphi > 1.44$)*, ethane *(>1.68)* and ethylene *($\varphi > 1.95$)* (Wu, Kwon et al. 1991; Kwon, Tseng et al. 1992; Tseng, Ismail et al. 1993). The existence of the laminar flame instability has been generally neglected in theories of laminar flame propagation for hydrogen and generally brings into question the validity of a thin, resolved flame front assumed in most treatments of turbulent combustion. This will be discussed again in the later section on turbulent combustion.

Another unique aspect of hydrogen combustion, which is not currently understood, is the separation of the value of φ where the maximum temperature (1.0) and the maximum flame speed (1.8) occurs (Kwon, Tseng et al. 1992); for all hydrocarbon fuels, the φ for these maximums coincide and occur in the range of values for φ between 1.0–1.2. Detailed information that is comparable for hydrogen-hydrocarbon mixtures is not available, but the combustion properties of a hydrocarbon gas have been found to change greatly with a small addition of the highly mobile hydrogen (Apostolescu and Chiriac 1996).

The kinetics of hydrogen combustion have been extensively studied, although comparisons between theory and experiments have been complicated by the diffusive instabilities described above. A successful effort in producing a limited reaction set of eighteen equations (Warnatz 1981) concluded the following on the concentration, temperature, and pressure dependence of hydrogen-air mixtures. 1) The existence of two competing mechanisms for hydrogen oxidation significantly complicates the laminar kinetics and is the source of unexpected sensitivity to initial temperature, pressure and equivalence ratio. The addition of a third species (N_2 to H_2 and O_2) reduces these dependencies. As a consequence, the laminar flame speed has a strong dependence on initial temperature, rising from 3.5 m/s for stoichiometric conditions *($\varphi = 1$)* in air at STP to about 23 m/s at 1000K, typical of

temperatures at ignition in the high compression Onan engine. The higher pressure at the time of combustion also increases the laminar flame speed, but to a weaker power ($p^{0.2}$). 2) The Zel'dovich model for NO_X production is better suited to hydrogen combustion than hydrocarbon combustion due to the absence of HC radicals which encourage the formation of "prompt" NO_X. About half of the NO_X is produced in the flame region and the rest in the post-flame region. This was also observed in the KIVA simulations, as noted below.

Overview of Modeling Turbulent Combustion

All spark-ignited engines have flame fronts that propagate in the presence of turbulence, and hence it is essential that an accurate combustion model include the effects of turbulence. For hydrocarbon fuels, the typical approach in large scale SI engine simulations is to neglect the laminar kinetics entirely and use models that include just the effect of turbulence on the flame front, e.g., the Magnussen or eddy-dissipation model (Magnussen and Hjertager 1978). For diesel engines the occurrence of the ignition delay requires a detailed kinetics model for its prediction, but once ignited, the kinetics model is typically replaced with a simplified turbulence combustion model.

In recent years, some progress has been made in understanding some of the details of the turbulent combustion by the introduction of flamelet or coherent flame models (Dillies, Marx et al. 1993) which solve, in addition to the turbulence transport equations, evolution equations for the generation and destruction of flame surface. Tables of laminar flame speed as a function of pressure, temperature, and composition are then used to determine the reaction rate at any time. The key assumption of the flamelet approach is that the flame thickness is thin compared to the dimensions of the turbulent eddies. The complication of the unstable nature of the laminar flame front for hydrogen has not been examined for the flamelet model and may violate the thin flame assumption.

Another alternative to understanding turbulent flame fronts, but one that is not practical for large engine simulations, is the technique of Direct Numerical Simulation (DNS) of both the turbulence and combustion (Rutland, Ferziger et al. 1990). In the DNS approach, all scales are resolved on the continuum level and no stochastic averaging is made. The systems that can be examined are limited in size and complexity, but full fidelity information is obtainable to test assumptions in stochastic theories, as required for simulations of more complex geometries.

Given this background in the current state of modeling turbulent combustion, the occurrence of the unstable laminar flame front in the regime of interest would seem to question the validity of applying models developed for hydrocarbon turbulent combustion to hydrogen. Furthermore, one would expect that the sensitivity to turbulence would be greater for hydrogen combustion because turbulence wrinkles the flame front, and once wrinkled, the flame front would become unstable and more wrinkled, hence increasing the flame speed and temperature, and the consumption of fuel.

In the following sub-sections, the existing experimental information, performance of the standard turbulent combustion models, and development of a simplified model for turbulent combustion for hydrogen are presented.

Experimental Data for Turbulent Combustion of Hydrogen

Little experimental information is available on the turbulent combustion of hydrogen, and what is available is at conditions different than typical engine regimes. The most complete set of data was found in (Koroll, Kumar et al. 1993) as needed to support the nuclear reactor safety studies, with less complete data in (Al-Khishali and Bradley 1983; Kwon, Driscoll et al. 1990; Wu, Kwon et al. 1991; Kwon, Wu et al. 1992; Meier, Köhler et al. 1994; Apostolescu and Chiriac 1996; Collier, Hoekstra et al. 1996). Some relevant data on lean methane turbulent combustion can also be found in (Ting, Checkel et al. 1995).

In an effort to develop correlations for hydrogen turbulent combustion, many of these researchers present the experimental information for hydrogen combustion using use correlations developed for hydrocarbon combustion, but the fits tend to be poor at lower hydrogen concentrations, presumably

due to the unstable nature of the laminar flame front extending the lean burn limit. A major conclusion by Koroll et al. (1993) is that the effect of turbulence is large for slow burning mixtures, and small for fast burning mixtures. For the Onan and future hybrid engines, the planned operating conditions (φ around 0.4) are in the unstable regime ($\varphi < 1.5$). Consequently, the laminar flame speed is in an intermediate regime and is observed to have moderate sensitivity to turbulence, with increases from 0 to 10 times for a range of turbulence intensity of 0–2.4 m/s. For very lean mixtures, the laminar flame speed can be 0–23 times for the same range of turbulence. At the maximum laminar flame speed, the increase is only 7 times at 2.4 m/s. Note that the typical turbulence intensities for the Onan engine during ignition as found from the KIVA simulations is in the range of 1–3 m/s. The second major conclusion made by Koroll et al. is that some additional mechanism, either the flame generated turbulence or preferential diffusion effects, must be included for accurate correlations for the flame speed; the increase of flame surface by pre-existing turbulence, which is generally argued to increase as $k^{0.5}$, is not sufficient. At fuel concentrations around $\varphi = 0.4$, the turbulent flame velocity in air is found to scale according to $k^{0.5}$, with a smaller exponent for lower concentrations and a larger exponent for higher concentration up to $\varphi = 1.5$, and then declining again for higher concentrations. Because the Onan engine is expected to operate in the range around $\varphi = 0.4$, this gives us some guidance as to how the turbulent flame speed should vary with turbulence intensity in the regime of interest.

One-Dimensional KIVA Runs of Turbulent Combustion and NO_X Production

To better understand and verify the standard turbulence combustion model on initial turbulence intensity, pressure, temperature, and fuel equivalence ratio, we have done a series of one-dimensional KIVA-3 runs at parametric values of pressures (1–5x10^7 dynes/cm^2), turbulence intensity (10^2–10^6 cm^2/s^2), and fuel equivalence ratios (0.4–0.8) and evaluated the flame speed, time to steady ignition, final combustion temperature, peak temperature, temperature at ignition, and NO_X production. The initial gas temperature was taken to be 900K, the typical gas temperature at the time of ignition in the Onan engine. The one-dimensional configuration was chosen to have approximately constant pressure combustion conditions (unlike an actual engine that has significant increased in pressure), and the simulation was forced to have a constant turbulence intensity (k) and dissipation rate (ε). The enforcement of constant turbulence levels prohibits the occurrence of flame generated turbulence, which can increase the flame speed (Koroll, Kumar et al. 1993). Although we will examine this effect later for generality, it is expected to be small for lean fuel mixtures of current interest. The KIVA simulations use a variation of the eddy-dissipation model (Magnussen and Hjertager 1978) that has successfully been applied to turbulent combustion of hydrocarbon fuels for large simulations, for both pre-mixed and injected fuels. Although we expect the unmodified model to underestimate the flame speed, our primary interest is to determine functional dependence on the independent variables.

A least-squares fit to the steady-state turbulent flame speed, s_t, gave a good fit and provides a compact summary of the simulations results:

$$s_t = 1.70\ k^{0.487}\ \varphi^{0.366}\ p^{-0.027} \quad \text{in cm/s}$$

in which k is the turbulent kinetic energy (cm^2/s^2), φ is the fuel equivalence ratio, and p is the pressure (dynes/cm^2). The adjusted correlation coefficient, r^2, for the fit is 0.9997, indicating an excellent fit of the data.

The expected exponent of k is 0.5, based on an analysis of the model, and more importantly approximately duplicates the observed coefficient for hydrogen combustion (Koroll, Kumar et al. 1993) for $\varphi = 0.4$, as described in the previous section. The pressure dependence is observed to be almost zero ($p^{-0.027}$) as expected from an analysis of the model. No experimental information on the pressure dependence of the turbulent flame speed could be found, but one might expect that the dominant effect of pressure is on the laminar flame speed in the turbulent eddies, and, consequently, the pressure dependence would be the same as the laminar flame speed, or approximately

proportional to $p^{0.2}$ (Warnatz 1981). The steady-state temperature was observed to depend only on the fuel equivalence ratio, as expected, since this determines the net heat released. Finally, no dependency was observed on the eddy dissipation rate, ε, as expected from the formulation of the model.

In the original development of the eddy-dissipation model (Magnussen and Hjertager 1978), the turbulent combustion rate is proportional to a constant A, that is held constant during a simulation, but is typically adjusted to match experimental data for operating conditions of the engine. Because it appears as a premultiplier of the turbulent combustion rate, A is expected to have a similar dependence on fuel equivalence ratio, initial pressure and temperature as the laminar flame speed. For the one-dimensional simulations, A is taken to equal 18, a value typically used for diesel engine combustion. Ideally, the parameter A should be a function of the fuel equivalence ratio, initial pressure and temperature and not require modification for different operating conditions.

The above correlation gives a flame speed of 160.0 cm/s for (k,φ,p) = ($5.0\text{x}10^4$ cm^2/s^2,0.4, $1.0\text{x}10^6$ dynes/cm^2), in comparison to the experimentally observed value for hydrogen in air of 230 cm/s (Koroll, Kumar et al. 1993) (note that the experimental laminar flame speed is 60 cm/s). This difference was expected, because the flame speeds for hydrogen are larger than for diesel fuels. This suggests that the parameter A in the eddy-dissipation model should be increased to 25 from 18 for constant pressure ignition at 900K. In an actual engine simulation where temperatures continue to increase during combustion, the flame speed would increase, and A would be correspondingly larger. This was observed in the full engine KIVA simulations, as noted below.

We also examined the dependence of the NO_X formation in the parametric study using the standard Zel'dovich model. NO_X was produced in the flame front. Behind the flame front, the NO_X production was constant with time under these constant pressure and temperature conditions. Because of the time for significant NO_X to be produced was much longer than the simulation time, no useful conclusions could be made in these simulations about the NO_X formation of in the presence of turbulence.

Direct Numerical Simulation of Turbulent Combustion of Hydrogen

The final source of information on turbulent combustion of hydrogen can be obtained from detailed computer experiments of the turbulent combustion in a continuum fluid, in which no stochastic models for turbulence are used. The direct numerical simulations (DNS) provide information that is unavailable from experiments that can be used to better understand the details of turbulent combustion and thereby to improve stochastic turbulence models. One preliminary study (Rutland and Trouve 1993) has been done on the effect of the preferential diffusion instability, as occurs in lean hydrogen combustion, on turbulent combustion. The conclusions of the study are very significant to the present research. A strong, almost linear, correlation was found between the local flame speed and the curvature of the flame front, supporting the observation that the local flame front is unstable. In contrast, no correlation was found between the flame speed and local strain rate. Most significantly, the enhanced curvature effects, observed at the local level, were found to cancel on the average or global level. Hence, the front instability affects the local flame front, but not the overall propagation of the turbulent flame. It was also observed that the preferential diffusion causes hot spots to form and persist in the flame front, which would likely affect the kinetics of the NO_X production. From this study, we can tentatively conclude that the global turbulence reaction rates may not be affected by the preferential diffusion instability, but quantities that depend on the details of the local flame front may be sensitive to this effect. This gives us some hope that a global turbulence combustion model, such as the eddy-dissipation model, that has been applied to stable laminar flames, may also be applicable to lean turbulent hydrogen combustion.

Conclusions and Future Work on Turbulence Combustion Modeling

The above review of the literature and of the one-dimensional KIVA simulations suggest that a straightforward modification of the model used for hydrocarbon-based fuels may be appropriate for turbulent, hydrogen combustion in the regime of operation of the Onan engine. In the following

section on the three-dimensional simulations of the Onan engine, the eddy-dissipation model is applied directly to the hydrogen turbulent combustion in KIVA-3, with understanding that the parameter *A* must be increased to account of the increased flame speed. Because *A* is taken to be a constant and not dependent on the changing conditions during ignition, we expect there to be some deficiencies in the details of the model. Comparable difficulties arise in the application of the same model for hydrocarbon fuels. Preliminary results with the modified parameter look promising, as is reported in the next section.

Future work will include the addition of the dependence on the fuel equivalence ratio, pressure and temperature on the parameter *A*, through the known dependence of the laminar flame speed on these variables. We believe that this should significantly improve the predictability of the model. Although not necessary for the simulation of the spark-ignited engines, a simplified model for the laminar hydrogen kinetics is still needed to complete the model for both compression ignited and spark-ignited engines. This work will be done in collaboration with LLNL.

Intake Flow, Turbulence, and Scaling Studies of the Onan Engine

Introduction

The majority of the effort in the last year has focused on the importance of accurate modeling the intake flow in a spark-ignited engine and the effect of various design choices on the performance of the engine. Because of the sensitivity of the combustion rate and pollutant formation on the intake port design and turbulence level (Khalighi, El Tahry et al. 1995; Kühn, Abthoff et al. 1996; Neußer and Geiger 1996), little progress could be made on the turbulent combustion modeling for the Onan engine until we were confident about the turbulence levels at the time of combustion. The modeling issues of concern were the accuracy of the newly implemented valve model and the best model for the intake port to duplicate the experimental driving conditions. The following subsections describe the KIVA-3 simulations that model the intake flow and the turbulence generation. These naturally divide into three topics: the study of the scaling of the turbulence intensity, the effects of the intake port changes and the simulations with and without shrouded valves. The discussion of the simulations with combustion are described separately in the following section.

Description of the Onan Engine, the KIVA Mesh and Motored Simulations

Details of the SNL Onan engine can be found in (Van Blarigan 1995; Hoekstra, Van Blarigan et al. 1996). The Onan engine is a converted diesel engine with a modified head containing two valves and two spark plugs. Table 1 summarizes the engine specifications. Note that the compression ratio has changed from the last annual report, reflecting a better measurement of the combustion volume.

Table 1. Modified Onan Engine Specifications

Bore	82.55 mm
Stroke	92.08 mm
Displacement	493.0 cm^3
Geometric compression ratio	14.04:1

Details of the KIVA mesh and initial conditions for the Onan engine are given in the last year's annual report (Johnson, Amsden et al. 1995) and are summarized here. The mesh and one time of the simulation are shown in Fig. 1. The mesh was generated with 41 pseudo-blocks, resulting in 5 logically hexahedral blocks of mesh with about 75,000 cells in the full 360° mesh or half this number

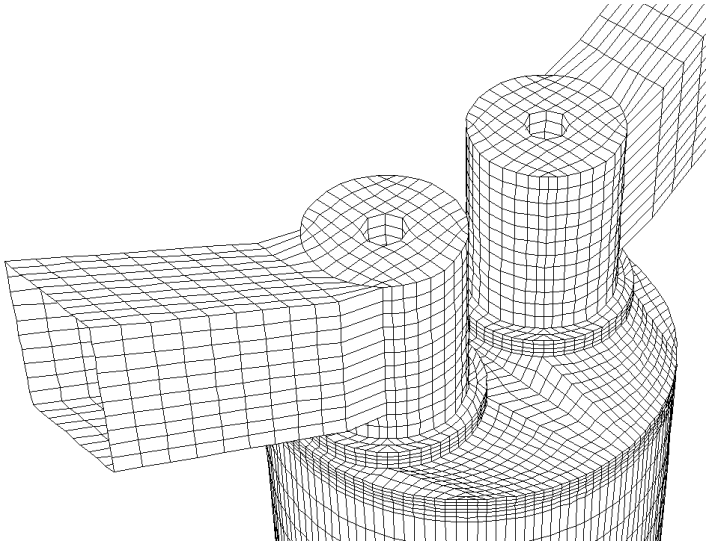

Fig. 1a. A detail of the exterior of the mesh for the Onan engine.

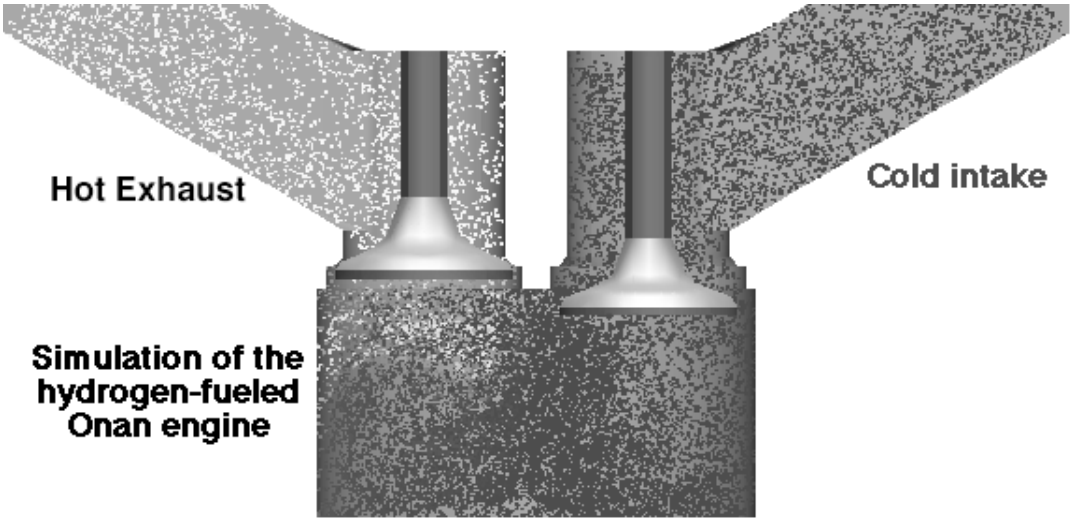

Fig. 1b. The intake flow at one time during the KIVA simulation. The cold air represented by the dark dots is compressing the hot residual gases, represented by the white dots. Note the exact rendering of the valve shapes and pockets.

for the simulations that model only half of the engine. The full mesh of the Onan engine includes a slight azimuthal twist of 27° in the intake port as occurs in the Onan engine. Without this twist in the intake port, the flow and combustion is symmetric through a plane passing through the two valves. Because the effect of this twist was found to be negligible (see the section on the intake flow modeling, below), for simulations that do not use a shroud to induce swirling flow, the half mesh was used, thereby reducing computational times by half.

The only major simplifications made in the computational mesh were the square cross-section of the intake and exhaust manifolds (See Fig. 1a). To reduce the effect of the simplification, the flow area of the simulated and actual manifolds are identical. Other simplifications are the omission of the

volume associated with the spark plugs (3.5% of the minimum cylinder volume) and the volume above the piston rings (0.7% of the minimum volume). The valve shapes and seating were modeled accurately to within the resolution of the mesh (See Fig. 1b). Two types of boundary conditions were used to model the intake flow of the Onan engine: a constant pressure boundary condition and a time-varying boundary condition as taken from the experimental pressure measurements in the intake port. For studies of the comparison between different simulation runs, the former was used. The latter boundary condition was used for comparison to the Onan experiments and is discussed in more detail in the section on intake flow modeling. Other boundary conditions for the engine simulation with combustion are specified as in the prior annual report (Johnson, Amsden et al. 1995).

As a test of the proper compression volume, simulations were done of the motored Onan engine (operation without combustion) and the pressure shape and maximum pressure agree well with the experimental data, as in Fig. 2. For these simulations the temperature of all surfaces in the engine were taken to be room temperature since the engine was operated cold. The cold surfaces tend to cool the hot, compressed air, thereby reducing the maximum pressure expected from purely adiabatic compression. The slight difference in the maximum pressure between the experiment and simulation is due likely due to the temperature of the cylinder walls and piston being lower than in the experimental engine, which are slightly heated by the compressed gas.

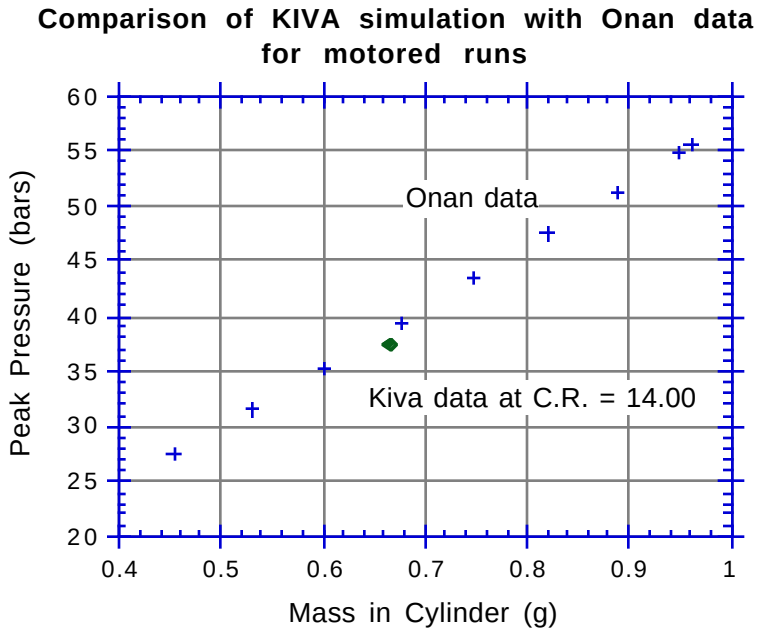

Fig. 2. Comparison of the KIVA simulations with motored Onan experiments of the peak cylinder pressure versus the air mass in the cylinder.

Scaling of Turbulence Levels in the Onan Engine Simulations

Prior to the availability of experimental results for the Onan engine, simulations were done to examine the dependence of the turbulence levels on many design parameters, such as the engine RPM and intake geometries and the twist in the intake port, as mentioned above. It was observed that for a given engine geometry and intake conditions (e.g., a given intake port length, or for shrouded or unshrouded valves), the turbulence levels of the cylinder gas simulated over the operating cycle of the engine can be superimposed if they are scaled by the maximum piston velocity (or engine RPM) and mass of cylinder air/fuel charge. This superposition applies for a wide range of volumetric efficiencies, engine speeds or operating temperatures. The scaling applies if the bulk flow does not

differ too greatly, as illustrated in Fig. 3 with the good comparison, with and without an angled port and with a cold and hot engine. Furthermore, during combustion, only a 20% increase in the scaled turbulence levels is observed over the motored simulations, although the bulk flow kinetic energy is significantly increased (detail in Fig. 3). (The increase in the bulk flow kinetic energy is due to the compression of the unreacted gases by the higher pressure combusting gases, thereby, causing a bulk flow.) This suggests that the turbulent levels in the unburned fuel during combustion do not change significantly for the Onan geometry for these lean operating conditions. The scaling does not apply if the bulk flow is drastically changed between simulations, as occurs with the addition of a shroud on the intake valve. This scaling law enables a single KIVA turbulence history to be applied to a variety of other operating conditions, as needed in the zero-dimensional, thermodynamic simulation codes. This has been done by Salvador and Smith at LLNL in support of the project, and they have found that the burning duration correlates well with average turbulence intensity during combustion (see their contribution to the annual review).

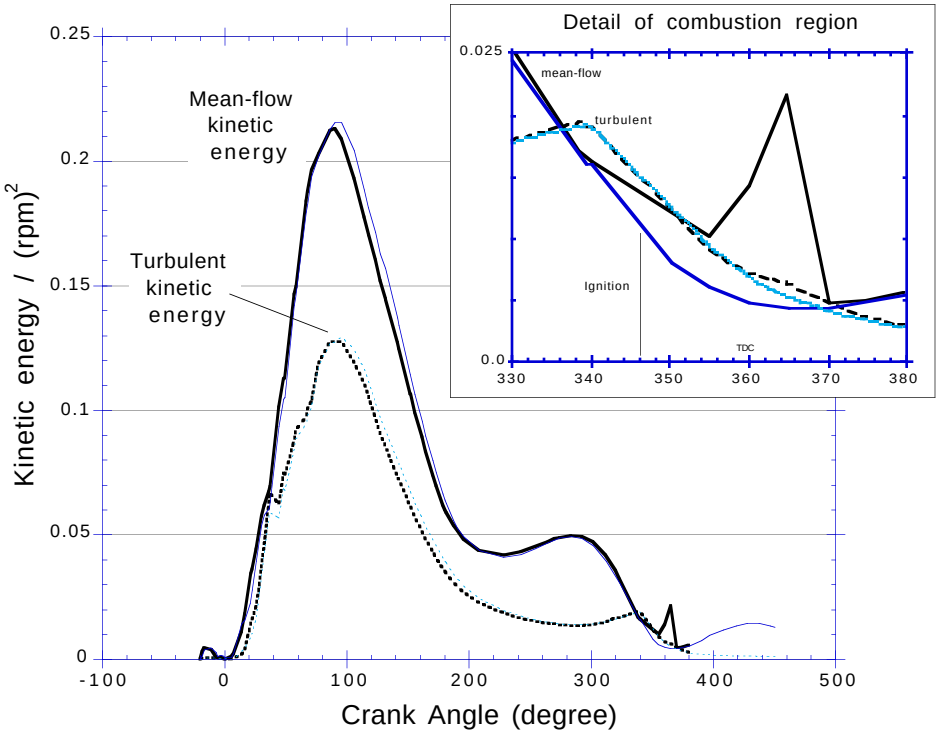

Fig. 3. Illustration of the scaling of kinetic energy in KIVA simulations for different operation conditions. The heavy lines are for a run with combustion in a hot engine and an angled port with minor swirl at 1206 RPM. The thin lines are for a run with no combustion and no swirl in a cold engine at 1500 RPM.

Modeling of the Intake Ports and Cylinder Pressure Oscillations

Intake Port Modifications

One of the challenges of any engine simulation is the approach used to duplicate the experimental conditions for the air delivery. The complication is that the computational mesh for the simulation must be terminated at some point and an appropriate boundary condition applied. This is

additionally complicated by the fact that the experimental information available is pressure histories at various points in the experimental setup, but momentum flux and thermodynamic state, as is needed to fully determine the inlet conditions in the simulation (i.e., the pressure at a point gives no information about the momentum flux through a point, nor the temperature or density of the gases). The use of the experimentally available information to duplicate the conditions and amount of the air/fuel charge in the cylinder is an outstanding problem in engine modeling (Stephenson and Rutland 1995). Because of the sensitivity and complexity of the cylinder pressure on details of the intake port geometry and driving history (Kühn, Abthoff et al. 1996; Neußer and Geiger 1996), the trend in engine modeling is to forgo direct comparisons and use simulations generically to design engines (Stephenson and Rutland 1995; Bauritaud 1996).

A study of the intake flow in the Onan engine was undertaken and moderate success in comparing with the experimental data was achieved. An unexpected result of this study was the discovery that tuning the intake port on a naturally aspirated engine can significantly increase the charge density; in one simulation, with no attempt to optimize the charge density, a 7% increase above ambient density was observed in a particular combination of port length and experimentally-derived, pressure-history boundary condition. This indicates that significant supercharging can be obtained for the hybrid engine, because the intake port design can be optimized for just one engine speed. This is in contrast to multiple-speed engines that compromise performance at one RPM in order to operate at many engine speeds.

In order to aid in the computer modeling of the Onan engine, SNL added additional pressure diagnostics in the intake port and a more sensitive cylinder pressure transducer. This data significantly clarifies the operation of the air/fuel delivery system of the Onan engine and illustrated dynamics that were not previously observed: the cylinder pressure during the early intake flow (0–100 CA) oscillates with a frequency of 180–260 Hz and a large amplitude of 1–3 psi (data 101895AB). To understand the origin and effect of these oscillations, a KIVA simulation was done with a much longer intake port (from 7.4 cm to 37 cm). This simulation clearly exhibits the same amplitude oscillations, but with an even lower frequency (90–130 Hz). The simulation with the longer port also resulted in 4.5 percent lower mass in the cylinder and a 16 percent increase in the turbulent kinetic energy per unit mass at the time of combustion. Additional simulations showed that the dynamics of the intake flow are more sensitive to small changes in the initial state and geometry than expected, with large variations possible in magnitude and frequency and significantly different cylinder mass charges and turbulent levels. For example, a 20°C temperature increase of the gas in the port (a 7% decrease in density) results in a 20% increase in the amplitude of the first oscillation of the cylinder pressure.

These observations highlight the difficulty of matching the experimental data and the need for accurate experimental operating conditions. The source of the oscillations was found to occur in the simulations with the long, narrow intake port, and could likely be eliminated by larger diameter ports. The sensitivity and the difficulty of matching just one set of Onan data has led us to suggest that the intake manifold for future experimental engines needs be modified to eliminate or reduce this phenomenon. The experimental operation that is ideal for the KIVA simulations is a steady or slowly varying driving pressure and temperature, measured in a mostly stagnant volume near the intake valve. But, as mentioned in the opening of this section, these intake port simulations also suggest that the port dynamics can be exploited to provide supercharging in a naturally aspirated engine.

In addition to modifying the dimensions of the inlet port and the initial density, KIVA simulations were also done that duplicated the slight twist (27° from the plane through the two valves) in the intake port. These simulations did not change the prior conclusions concerning the dominant flow at time of combustion, a tumble flow, which is many times the intensity of the swirling flow. Steady-state swirl intensity was measured for the Onan engine (Swain 1995) for various valve lifts and flow rates. The KIVA simulations produced similar swirl characteristics: low swirl at small and large valve openings, larger swirl at moderate valve openings. More details are given on these simulations in the following section on the effect of the addition of a shroud on the intake valve.

Shrouded-Valve Simulations

As discussed in the introduction of this section, earlier KIVA simulations of the Onan engine lead to the conclusion that by inducing a swirling flow in the cylinder, in the place of the dominant tumble flow that was observed in the KIVA simulations (Johnson, Amsden et al. 1995), the efficiency of the engine might be improved. The experimental technique of inducing the swirl that was suggested by LANL was the addition of a shroud on the intake valve. Various shroud heights and extents on the edge of the valve were tried experimentally, and it was found that the apparent introduction of a moderate amount of swirl increased the efficiency of the engine (Hoekstra, Van Blarigan et al. 1996). The reason for this increased efficiency, as elucidated by the KIVA simulations, is the focus of this section. But first the technique for implementing a shroud in KIVA is presented.

A simple scheme was used to model a shroud on a valve in KIVA-3: a zero-thickness wall at an element boundary was added at the perimeter of the valve to duplicate the blocking of the flow by the shroud. For a full-height shroud, this wall extended up into the valve pocket, thereby preventing all flow through the valve gap at that azimuthal angle. For a lower-height shroud that allows flow past the shroud at large valve openings, a constant number of element sides above the edge of the valve were similarly blocked. The number of element sides that were blocked where chosen such that the average height of the numerical shroud was similar to the experimental height of the shroud. For example, for the 1.5 mm high shroud, the sides of two elements were blocked. This approach allowed for full blockage of the flow for small valve openings and allowed the flow over the shroud at large valve openings.

During the past year many KIVA simulations were done comparing the effects of different shroud heights and orientations, and it was found that the shroud caused significant changes in the turbulence level, combustion time, and NO_X emissions. Experimentally it was observed that the engine had its peak efficiency with the 1.5 mm shroud and had lower efficiency for either higher shroud heights or no shroud. It was thought that the shroud introduced more swirl into the engine, which resulted in a more ideal turbulence intensity history, since it is known that tumble, as predicted to be the dominant flow in the Onan engine by KIVA, tends to create high turbulence intensity at maximum compression, where swirl tends to produce turbulence uniformly during combustion (Khalighi, El Tahry et al. 1995). Because additional turbulence can increase the heat transfer to the wall, it was thought that the efficiency increased with the shroud because of the more favorable turbulence intensity history.

To resolve the question as to the cause of the increased efficiency, four simulations were compared: with and without the 1.5 mm shroud and for two ignition timings of 20° and 12.5° BTDC. Fig. 4 illustrates that the addition of the shroud does indeed increase the swirl, although these values are low for engines designed to have swirl (Floch, Frank et al. 1995; Swain 1995). The indicated thermal efficiencies were calculated for all of the simulations by integrating over the compression, combustion and expansion cycle the work done by the cylinder pressure due to the change of cylinder volume and then dividing by the total energy produced by the hydrogen fuel. An identical method was used to calculate the thermal efficiencies of the Onan experiments (Hoekstra, Van Blarigan et al. 1996). The resulting efficiencies are plotted in Fig. 5. Although experimental data does not exist for the same operating conditions, preliminary Onan data with and without the 1.5 mm shroud tended to exhibit a 3% increase in the thermal efficiency, when it was observed to have an effect. What is of primary concern here is to understand the improved efficiency at the ignition timing of 12.5° BTDC in the simulation with the shroud.

In Fig. 6 the turbulence intensity is plotted for all of the simulations during the time of combustion and expansion. It is immediately apparent that the turbulence intensity, and hence the turbulent flame speed, would be similar for these four simulations. In fact, a more careful examination of the turbulence intensity shows that the different timing of ignition has a larger effect on the turbulence intensity than the presence or absence of the shroud. An examination of the heat transfer to the wall in Fig. 7 yields a similar conclusion that the dominant effect is the ignition timing. Note that even

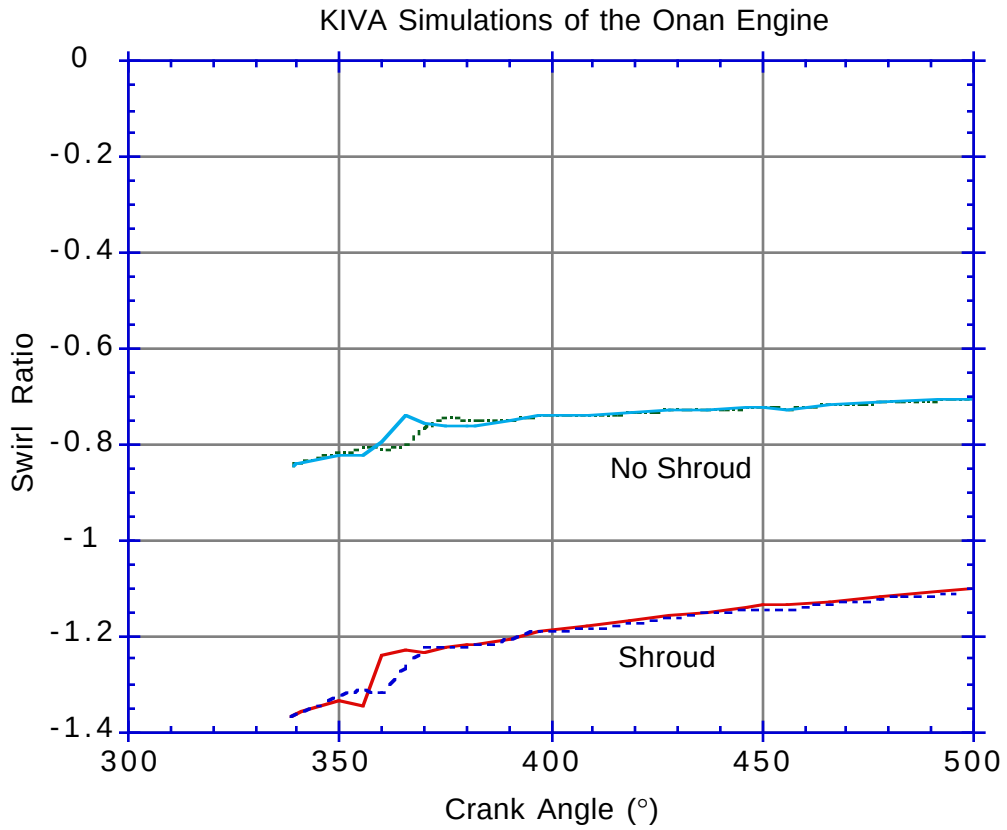

Fig. 4. The swirl ratio for KIVA-3 simulations with and without a 1.5 mm shroud and for two ignitions timings (20° (solid lines) and 12.5° (dashed lines) BTDC). The swirl ratio is the angular momentum in the cylinder divided by the product of the total mass in the cylinder and the angular velocity of the piston.

though the simulations with the shroud have a higher heat loss to the wall, the more optimal pressure histories of the runs with the shroud compensate of the additional heat loses, thereby either improving the efficiency at 12.5° case or keeping the efficiency constant in 20° case.

The plot of the hydrogen mass in Fig. 8 as a function of crank angle illustrates that even though all the simulations have similar turbulence intensities, the consumption of hydrogen is faster for the simulations with the shroud than without, even though the turbulence levels and hence the local combustion rates are comparable. The source of the different combustion rates is the stretching of the flame front by the slow swirling flow. The increased efficiency with the shrouded valve, as explained by the KIVA simulations, is due to the faster combustion rate from the bulk flow from the gentle swirl, thereby producing more work near TDC, but with not too large a swirl that causes a loss of efficiency due to increased heat loss. With this understanding of the delicate balance between competing effects, an optimal design can be made of the intake port in the final prototype engine.

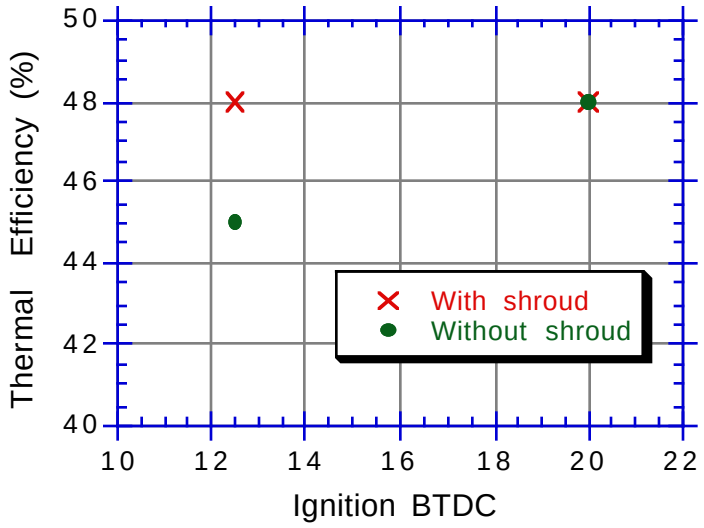

Fig. 5. The indicated efficiencies for the KIVA simulations.

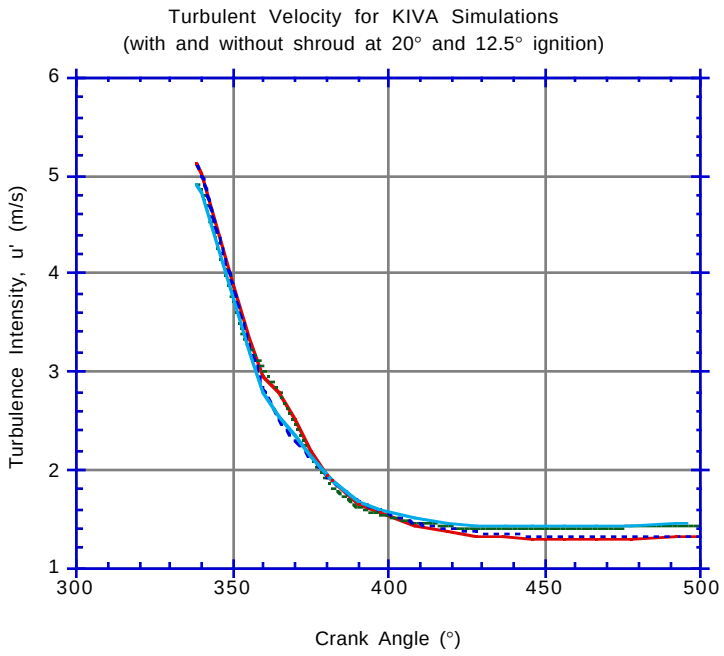

Fig. 6. The turbulence intensity for four simulations are shown, illustrating that the turbulent intensities are almost the same for all the simulations.

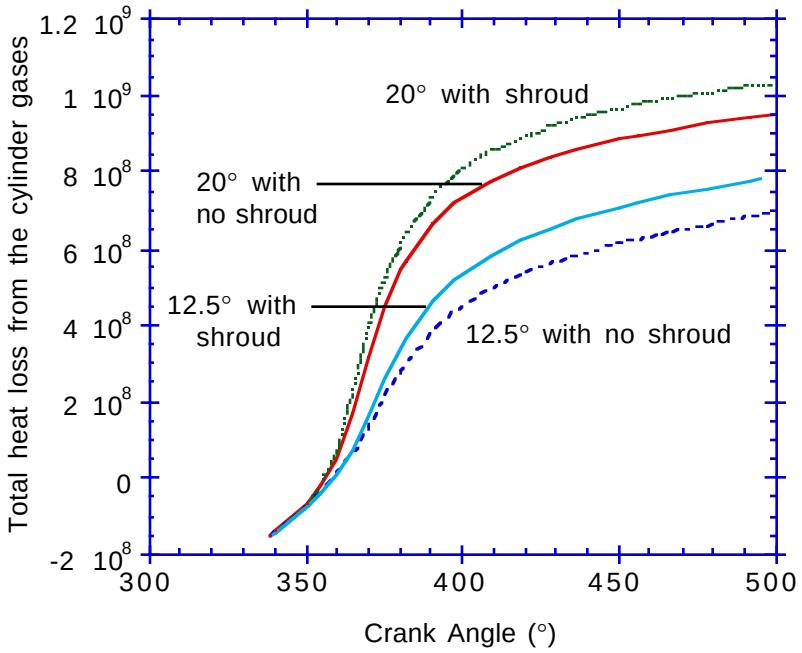

Fig. 7. The accumulated heat transferred to the wall from the cylinder gases in ergs.

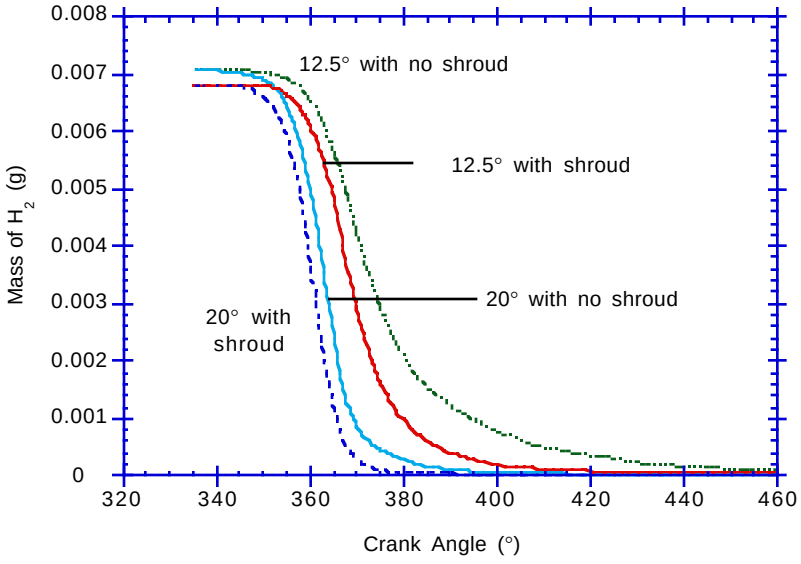

Fig. 8. The mass of hydrogen for the four KIVA simulations.

Comparison to the NO_X and Efficiency of the Onan Engine

The ability to compare the KIVA simulations with the Onan engine data is a culmination of all the successes in modeling the intake flow with a short shroud and the development of a turbulent combustion model for hydrogen. The experimental comparison was also made possible by the large parametric set of data for the Onan engine made available by SNL. The large data set circumvented the problem of matching the intake flow history in order to achieve the same cylinder charge. Instead, an experimental data set could be chosen that most closely matched the volumetric efficiency in the KIVA simulations. The KIVA simulations were done at both 1200 and 1800 RPM and at a variety of ignition timings (from 20° to 7.5° BTDC) at an equivalence ratio of 0.4. The results presented here are for the 1800 RPM simulations.

As discussed in the section on modeling turbulence combustion, the eddy-dissipation model in its current undeveloped form has one free parameter that must be determined from a comparison to the experiments, and is comparable to determining the laminar flame speed for a specific hydrogen-air mixture at a certain temperature and pressure. This was accomplished by picking a value for *A* that best matched the pressure history of one Onan simulation (Run 111495fa). The parameter *A* was then held constant for all other simulations with different ignition times, but at the same equivalence ratio and volumetric efficiency. By then applying the model to a variety of ignition times, a fairly severe test of the model is achieved because by changing the ignition times, the conditions during combustion - the turbulence, pressure and temperature - also change significantly.

The resulting NO_X values from the simulations compare excellently with the experimental values, without any adjustment of the NO_X model for hydrogen (Fig. 9 below). Because NO_X is very sensitive to the burn rate and flame temperature, this is a sensitive test for the accuracy of the turbulent combustion model. This comparison is better than is generally found for hydrocarbon simulations and supports the conclusion in the literature (Warnatz 1981) that the slow NO_X kinetics are more accurate for hydrogen combustion. The difference in the slope between the simulations and experiments is likely due to keeping *A* constant when it should be varying with the changing conditions at ignition and during combustion. Inclusion of these effects would increase the flame speed and the combustion temperature at later spark timing, and hence the NO_X levels, resulting in even better agreement at other spark timings.

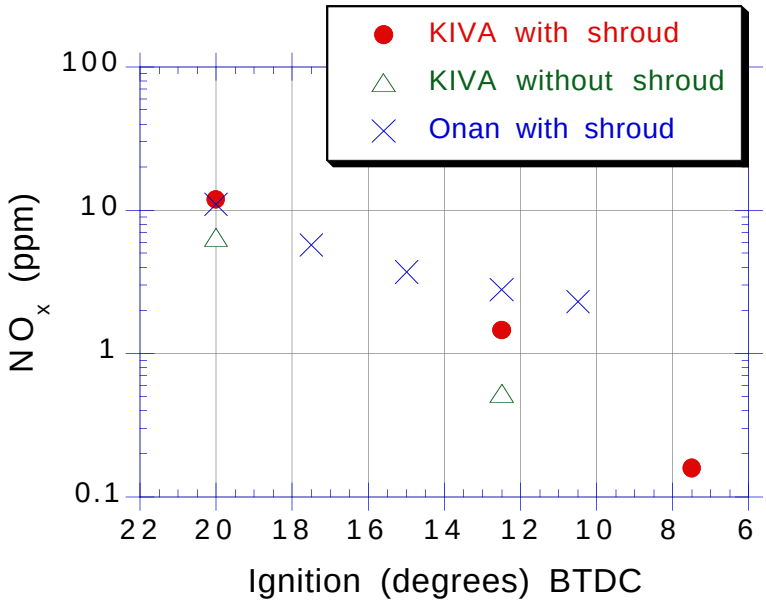

Fig. 9. Comparison of the NO_X for the KIVA simulations and Onan experiments.

Comparisons of the efficiencies and pressure histories between experiments were also made (Fig. 10 below). The trend in the indicated thermal efficiencies duplicates the Onan data, but the values in the KIVA simulations are about 4% higher than in the experimental data. Because of the uncertainty in the wall temperatures in the engine and the difficulty in experimental determination of efficiencies, the offset is not unexpected. The duplication of the trends is an important validation of the turbulence and combustion model in KIVA. The rapid drop in the efficiency of the data at small ignition advance is generally seen to occur in other experimental data and is an expected trend in the simulation results.

All the results for the five simulations in Fig. 9 were obtained with about 15 hours of Cray YMP time. A large reduction in the required computing time was achieved by running the simulation to just before the earliest ignition time and then restarting the simulation from this time for the different ignition times.

In summary, KIVA simulations of the Onan engine agreed very well with the experimental results and largely validates the chosen approach for the intake flow modeling and the turbulence combustion modeling. Indeed, fewer "adjustments" of the models in KIVA were required than is typically necessary for modeling hydrocarbon-fuel engines. As additional comparisons with the Onan data are made and as data from the larger experimental engine are made available, the performance of KIVA will be reassessed and improvements in the models will be made.

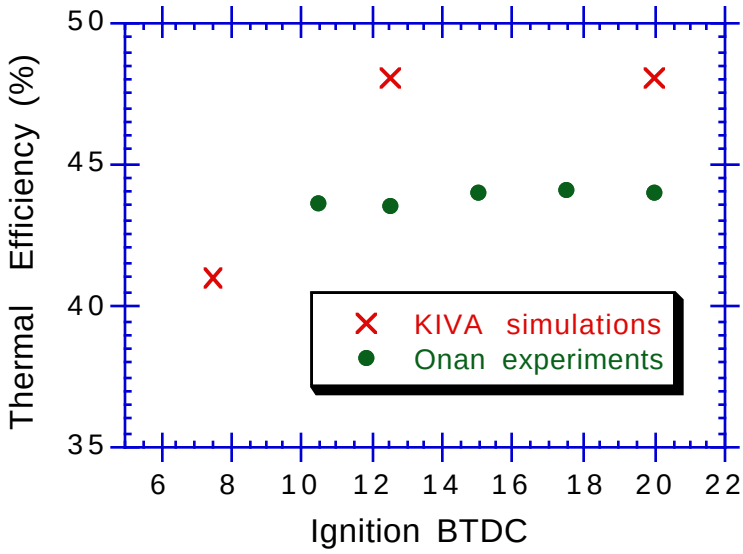

Fig. 10. Comparison of the indicated thermal efficiency for the KIVA simulations and Onan experiments.

Improvements in the KIVA-3 Code

Extensions to the Valve model

The implementation and testing of the valve model was covered in the prior annual report (Johnson, Amsden et al. 1995). Prior KIVA-3 simulations were limited to vertical intake and exhaust valves. Given that the turbulence and bulk flow patterns significantly affect the combustion in homogeneous-charged hydrogen engines, as demonstrated in the current Onan engine simulations, the capability to model valves at any inclined angle is essential for future hydrogen engine modeling. With some modification of the prior vertical-valve model, this capability has been added to the current setup and simulation codes and an angled-valve version of the Onan engine is shown in Fig. 11. This is a significant extension of the KIVA capability, because inclined values are used in almost all gasoline-fueled engines and likely will be used in many future hydrogen-fueled engines.

Improvement of Ease-of-Use of the KIVA-3 Code

Two additional features have been added to the KIVA-3 code that reduce the time needed to simulate a new engine. One is the addition of a "no-hydro" option that quickly runs through the opening and closing of the valves and the movement of the piston, in the exact manner as a full simulation, except no hydrodynamics are calculated. Thus, the integrity of the mesh can be checked in a few minutes, instead of hours. This is particularly useful for complex meshes in order to avoid the common difficulty of running a problem many hours, only to discover a difficulty with the mesh connectivity or entanglement late in the simulation and then have to redo the entire simulation. The second user-friendly feature is the simplification of different initial conditions within the computational mesh by specification in the input file. Prior versions required that the source code be modified to, for example, have a different state in the intake port than in the cylinder volume. Included in this feature is the direct specification of the air composition and temperature, along with the fuel equivalence ratio, thereby making the input variables similar to those typically specified in the experimental setup.

Fig. 11. An outside view of an angled-valve variation of the Onan engine. (Compare with Fig. 1.)

Improved Wall Heat-Transfer Model

Research done for future versions of the KIVA family of codes has improved the wall heat transfer model and has been implemented in the current version of KIVA-3. Analysis shows that the improved treatment gives better agreement with the experimentally observed wall heat flux.

Improved State Conservation During Mesh Remapping

An accuracy problem with KIVA during valve and piston movement was characterized and corrected. During the simulation of the Onan engine, mesh is added or removed from the calculation during the movement of the piston and valves. At these times, information (mass, momentum, energy, turbulence, etc.) must be remapped from the old mesh to the new mesh. Ideally all quantities are conserved during the remapping, but in practice the complexity of the process (multiple dimensions and multiple, but interrelated, variables) allows for only approximate conservation. It was observed that the prior method for remapping resulted in unexpected jumps in the state of the gas, in particular the velocity, during remapping. Because of the additional remeshing required by the new valve treatment in KIVA, this difficulty became more obvious than in prior simulations.

A better remapping scheme was formulated and tested. The worst case of momentum nonconservation was reduced to a tenth of prior change, and the new formulation usually resulted in no changes during remapping. Past Onan simulations were redone to assess the errors made previously. The turbulent energy levels in a typical Onan simulation differed by at most 10 percent between the old and new versions, although at the time of combustion the turbulent levels were negligibly different. The problem of nonconservation was a concern, because combustion flame velocities are proportional to the square of the turbulent kinetic energy. With this improvement in KIVA, we are more confident in the turbulence levels, and hence the hydrogen combustion rates, in the simulations.

Conclusions

Technical Presentations of the Project and Outreach to Industry

During the last year, many technical presentations of the project were made at conferences, universities and industry — to many attendees which had not previously heard of the Hydrogen Program. These are now summarized. A paper on the hydrogen injection modeling was presented at the '95 *High Performance Computing Conference* at Phoenix. A similar talk on "Three-dimensional modeling of hydrogen injection and combustion" was given at *The 8th International Symposium on Transport Phenomena and Combustion* at San Francisco. A technical paper, "Progress toward an Optimized Hydrogen Serial-Hybrid Engine," was presented in the Alternative Fuels Session at the ASME Internal Combustion Engine Conference in Milwaukee. The presentation covered the contributions of LLNL, LANL and SNL. Many of the attendees represented management and technical personnel from the major engine manufacturers. Requests for the research papers and video of a simulation of the Onan engine were made from industry and universities. A similar presentation was made at the *Engine Research Center* at the University of Wisconsin, Madison, briefing their modeling group on the unique challenges and opportunities in the hydrogen program.

In the last six months, the version of KIVA-3 that has been modified for the hydrogen project has been distributed to selected industrial and university collaborators for final testing and evaluation. The version will be more broadly released to our collaborators in the current fiscal year, followed by an official release to all the current users of KIVA-3, estimated to be more than two hundred users, as based on the KIVA email mailing list. The KIVA email list was developed to facilitate communication among KIVA users and to quickly disseminate information about the code. Currently over 220 subscribers have registered and represent industry, universities and national laboratories in the US and around the world.

Progress in the Project

During the past year, three milestones were achieved:

- The prediction of the NO_X and efficiency of the Onan experiments.
- The implementation and successful testing of a simplified chemistry model for hydrogen combustion.
- The transfer of the modified KIVA-3 code to industry and academia.

Future Work

The planned work over the next two years falls in three broad areas: the development of the KIVA simulation code for powerplant design, the support of the design and interpretation of the optimized, low-emission powerplant and industrial outreach and collaboration. These activities are concurrent and mutually supportive.

The extension of the KIVA code focuses on two areas: the continued development of the advanced chemistry and combustion modeling for hydrogen and hydrogen-hydrocarbon mixtures and the additions to the code for broader application and more user-friendly features. While the latter is straightforward and largely completed, the former is a significant challenge and is at the forefront of current research. The goal is to provide a combustion model that not only accurately describes the dependencies of turbulence, fuel-oxygen ratio, temperature and pressure, but that is applicable to repetitive, full-engine simulations, required by industry.

The engine modeling capability will be validated by comparisons with the data from the prior and current SNL engines. The current SNL engine has a similar combustion chamber geometry as the Onan engine, but with about double the total volume. The two data sets will enable a test, both experimentally and computationally, of the expected scaling of efficiency with engine volume. Furthermore, the different intake port geometry, and the subsequent different turbulence levels during combustion, will provide further understanding on the optimum intake port design for maximum engine efficiency. The simulation capability is an essential component for understanding the performance in experimental engines, because the simulations provide details and causal effects that are not experimentally measurable. A unique design opportunity is presented because the operating conditions of the powerplant is at constant RPM: the engine geometry, in particular the intake port and valves, can be optimized for maximum efficiency, in contrast to all existing engines which are a compromise of performance over a wide RPM range. The KIVA simulation capability can economically examine many possible geometries and is an essential component to the success of the final engine design.

Concurrent with the above tasks, the transfer of the technology to industry and universities and the collaboration with industrial partners will be undertaken. Outside participation on the development of the hydrogen simulation capability in KIVA is ongoing and will easily continue, due to the active interest of our collaborators.

Appendix A - Useful Relationships between Different Measures of Concentration

Hydrogen concentration can be given as:

φ = fuel equivalence ratio, the moles of fuel divided by the moles of fuel that would exactly be consumed by the available oxygen,

V_{H2} = the volume fraction of hydrogen,

f_{H2} = the mole fraction of hydrogen,

n_{H2}/n_{O2} = the number of moles of hydrogen divided by the moles of oxygen

% (molar) hydrogen concentration = 100 x f_{H2}

The assumption is made in the following that hydrogen mixtures can be assumed to be an ideal mixture of gases, i.e., the gases are non-interacting and hence the volume fraction is equal to the mole fraction ($V_{H2}/V_{O2} = n_{H2}/n_{O2} = f_{H2}/f_{O2}$). This is a good assumption at typical pressures and temperatures encountered in combustion engines. For hydrogen the fuel equivalence ratio is given by:

$\varphi = (1/2)\ f_{H2} / f_{O2}$

independent of the presence of a diluent, such as nitrogen.

For hydrogen-oxygen mixtures, the above concentration measures are related by:

$$\frac{n_{H2}}{n_{O2}} = \frac{f_{H2}}{f_{O2}} = \frac{f_{H2}}{1 - f_{H2}} = 2\varphi$$

$$\varphi = \frac{1}{2}\frac{f_{H2}}{1 - f_{H2}} \quad or \quad f_{H2} = \frac{2\varphi}{1 + 2\varphi}$$

The following table gives representative values between these measures:

φ	f_{H2}	n_{H2}/n_{O2}
0.4	0.44	0.8
1.0	0.66	2.0
1.8	0.78	3.6

For hydrogen-air mixtures, with an composition of air assumed to be 77% N_2, 22% O_2 by mass or 79% N_2, 20% O_2 by volume or moles, with the average molecular weight of air taken to be 28.90. The above concentration measures are related by:

$$\varphi = \frac{1}{0.44}\frac{f_{H2}}{f_{air}} \quad or \quad \frac{f_{H2}}{f_{air}} = 0.44\varphi$$

$$f_{H2} = \frac{0.44\varphi}{1 + 0.44\varphi} \quad or \quad \varphi = \frac{2.\overline{27} f_{H2}}{1 - f_{H2}}$$

The following table gives representative values between these measures:

φ	f_{H2}	n_{H2}/n_{O2}
0.4	0.15	0.176
1.0	0.306	0.44
1.8	0.442	0.792

References

Al-Khishali, K.J. and D. Bradley. 1983. "Turbulent Combustion of Near-Limit Hydrogen-Air Mixtures." *Comb. and Flame,* **54**: 61-70.

Amsden, D.C. and A.A. Amsden. 1993. "The KIVA Story: A Paradigm of Technology Transfer." *IEEE Transactions on Professional Communication,* **36**(4): 190-195.

Apostolescu, N. and R. Chiriac. 1996. "A Study of Combustion of Hydrogen-Enriched Gasoline in a Spark Ignition Engine." *SAE Technical Paper Series* (960603).

Bauritaud, T. 1996. Personal communication on Intake Flow Modeling at IFP.

Collier, K., R.L. Hoekstra, N. Mulligan, C. Jones and D. Hahn. 1996. "Untreated Exhaust Emissions of a Hydrogen-Enriched CNG Production Engine Conversion." *SAE Technical Paper Series* (960858).

Dillies, B., K. Marx, J. Dec and C. Espey. 1993. "Diesel Engine Combustion Modeling Using the Coherent Flame Model in Kiva-II." *SAE Technical Paper Series* (930074).

Floch, A., J.V. Frank and A. Ahmed. 1995. "Comparison of the Effects of Intake-Generated Swirl and Tumble on Turbulence Characteristics in a 4-Valve Engine." *SAE Technical Paper Series* (952457).

Hoekstra, R.L., P. Van Blarigan and N. Mulligan. 1996. "NO_X Emissions and Efficiency of Hydrogen, Natural Gas and Hydrogen/Natural Gas Blended Fuels." *SAE Technical Paper Series* (961103).

Johnson, N.L., A.A. Amsden and T.D. Butler. 1995. "Hydrogen program combustion research: three dimensional computational modeling." In *The 1995 DOE/NREL Hydrogen Program Review, Vol. II,* 285–304. Coral Gables, Florida: National Renewable Energy Laboratory.

Johnson, N.L., A.A. Amsden, J.D. Naber and D.S. Siebers. 1995. "Three-Dimensional Computer Modeling of Hydrogen Injection and Combustion." In *High Performance Computing '95 Conference,* Phoenix, Arizona: Society for Computer Simulation.

Khalighi, B., S.H. El Tahry, D.C. Haworth and M.S. Huebler. 1995. "Computation and Measurement of Flow and Combustion in a Four-Valve Engine with Intake Variations." *SAE Technical Paper Series* (950287).

Koroll, G.W., R.K. Kumar and E.M. Bowles. 1993. “Burning Velocities of Hydrogen-Air Mixtures.” *Comb. and Flame,* **94**: 330-340.

Kühn, M., J. Abthoff, R. Kemmler and T. Kaiser. 1996. Influence of the Inlet Port and Combustion Chamber Configuration on the Lean-Burn Behavior of a Spark-Ignited Gasoline Engine. *SAE Technical Paper Series* (960608).

Kwon, M.S., J.F. Driscoll and G.M. Faeth. 1990. “Turbulent Premixed Hydrogen/Air Flames at High Reynolds Numbers.” *Comb. Sci. and Tech.,* **73**: 327-350.

Kwon, S., L.K. Tseng and G.M. Faeth. 1992. “Laminar Burning Velocities and Transition to Unstable Flames in H2/O2/N2 and C3H8/O2/N2 Mixtures.” *Comb. and Flame,* **90**: 230-246.

Kwon, S., M.S. Wu, J.F. Driscoll and G.M. Faeth. 1992. “Flame Surface Properties of Premixed Flames in Isotropic Turbulence: Measurements and Numerical Simulations.” *Comb. and Flame,* **88**: 221-238.

Liu, D.D.S. and R. MacFarlane. 1983. “Laminar Burning Velocities of Hydrogen-Air and Hydrogen-Air-Steam Flames.” *Comb. and Flame,* **49**: 59-71.

Magnussen, B.F. and B.H. Hjertager. 1978. “On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion.” In *16th Symposium on Combustion*, The Combustion Institute.

Meier, F., J. Köhler, W. Stolz, W.H. Bloss and M. Al-Garni. 1994. “Cycle-Resolved Hydrogen Flame Speed Measurements with High Speed Schlieren Technique in a Hydrogen Direct Injection SI Engine.” *SAE Technical Paper Series* (942036).

Neußer, H.-J. and J. Geiger. 1996. Continuous Variable Tumble - A New Concept for Future Lean Burn Engines. *SAE Technical Paper Series* (960607).

Rutland, C.J., J.H. Ferziger and S.H. El Tahry. 1990. “Full Numerical Simulations and Modeling of Turbulent Premixed Flames.” *Comb. Inst.,* : 621-627.

Rutland, C.J. and A. Trouve. 1993. “Direct Simulations of Premixed Turbulent Flames with Nonunity Lewis Numbers.” *Comb. and Flame,* **94**: 41-57.

Stephenson, P.W. and C.J. Rutland. 1995. “Modeling the Effects of Intake Flow Characteristics on Diesel Engine Combustion.” *SAE Technical Paper Series* (950282).

Swain, M. 1995. Personal communication on The Measurements of Swirl in the Onan Engine.

Ting, D.S.-K., M.D. Checkel and B. Johansson. 1995. “The Importance of High-Frequency, Small-Eddy Turbulence in Spark Ignited, Premixed Engine Combustion.” *SAE Technical Paper Series* (952409).

Tseng, L.K., M.A. Ismail and G.M. Faeth. 1993. “Laminar Burning Velocities and Markstein Numbers of Hydrocarbon/Air Flames.” *Comb. and Flame,* **95**: 410-426.

Van Blarigan, P. 1995. “Experimental Program for the Development of the Hybrid Engine.” In *The 1995 DOE/NREL Hydrogen Program Review, Vol. II,* Coral Gables, Florida: National Renewable Energy Laboratory.

Warnatz, J. 1981. “Concentration-, Pressure-, and Temperature-Dependence of the Flame Velocity in Hydrogen-Oxygen-Nitrogen Mixtures.” *Comb. Sci. Tech.,* **26**: 203-213.

Wu, M.S., S. Kwon, J.F. Driscoll and G.M. Faeth. 1991. “Preferential Diffusion Effects on the Surface Structure of Turbulent Premixed Hydrogen/Air Flames.” *Comb. Sci. Tech.*, **78**: 69-96.