LA-SUB--95-104

FINAL REPORT ON SUBCONTRACT #3027—

~~N0014-9C~~ (U OF MN #530-6215)

FROM LOS ALAMOS NATIONAL LABORATORY

MAR 11 1993

OSTI

Title:

OPTIMIZING THE TURBO-ROTO-COMPOUND
(TRC) ENGINE

Subcontract Period:

November 1, 1993 to September 30, 1994

Submitted to:

Dr. Norman L. Johnson
Mail Stop B-216
Group T-3
Theoretical Fluid Dynamics
Los Alamos National Laboratory
Los Alamos, NM 87545

Principal Investigator:

Dr. John Abraham, Assistant Professor
Department of Mechanical Engineering
University of Minnesota
111 Church Street S.E.
Minneapolis, MN 55455
Tel.: (612) 625-3864
FAX: (612) 624-1398

Date of Submission:

August 15, 1994

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

over

OPTIMIZING THE TURBO-ROTO-COMPOUND (TRC) ENGINE

Summary

Results of multidimensional computations of sprays in a very high pressure constant volume chamber are presented in two parts.

Part I:

Comparisons of computed and measured penetrations of non-vaporizing and vaporizing sprays are presented. A broad range of density ratios (0.005 to 0.243) is covered. It is shown that, provided sufficient numerical resolution is used, the model can adequately reproduce the measurements. Scaling laws for time and distance derived in a previous publication are found to apply also to the sprays over the broad range of density ratios considered.

Part II:

A combustion sub-model that has been used in spark-ignition engines, stratified-charge engines and Diesel engines is included in the model. The combustion sub-model represents low-temperature autoignition and high temperature heat release. Comparisons of computed and measured penetrations of combusting sprays and computed and measured chamber pressures are being made. In this report, only preliminary indicative comparisons of computed and measured chamber pressures for three cases are presented. Agreement of pressures within 5% is shown. The work is ongoing and a detailed report will be presented later.

Part I:

Title: Three-Dimensional Computations of Diesel Sprays in a Very High Pressure Chamber

ABSTRACT

Results of three-dimensional computations of non-vaporizing and vaporizing Diesel sprays in a very high pressure (up to 18.4 MPa without combustion) environment are presented. These pressures and corresponding density ratios of ambient gas to injected liquid are about a factor of two greater than those in current Diesel engines. The spray model incorporates a line source for drops, heat, mass and momentum exchange between the gas and liquid phases, turbulent dispersion of drops, collisions and coalescences, and drop breakup. The accuracy of the model is assessed by making comparisons of computed and measured spray penetrations. Reasonable agreement is obtained for a broad range of conditions. A scaling for time and axial distance clarifies these results.

CURRENT DIESEL ENGINES operate at a peak cylinder pressure of about 15 MPa during combustion. Several Diesel engine manufacturers have plans to raise this to about 20 MPa by 1998 through a combination of supercharging and use of higher injection pressures. In practice, the upper limit on pressures is imposed by structural considerations and the fuel injection system. From the point of view of combustion and emissions, it would appear that if sustained higher pressures could be achieved, there would be at least the following benefits: (1) the power density of the engine would be higher; (2) it would appear that the mixing of the fuel and air should improve [1,2] as the combustion chamber pressure (i.e. the ratio of ambient density to injected liquid density) increases, which will, in turn, lead to improved combustion and higher efficiency; and, (3) the improved mixing and combustion would also lead to reduced emissions. These are definitely sufficient motivations for striving to achieve higher pressures in the combustion chamber.

Since the penetration of the spray and its mixing characteristics are altered by the increase in density ratios

[1,3], combustion chambers will have to be redesigned to maximize engine performance. In fact, the entire system, including the chamber, injector and intake and exhaust, will have to be optimized. During the past decade, this optimization has been accelerated by the use of multidimensional models for the physical processes in the engine [4,5]. Since the processes in the engine occur on a multitude of spatial and temporal scales, not all of which can be resolved with available computational resources, submodels have to be used for several of these processes. These submodels incorporate our understanding of the processes, but their accuracy has to be assessed in comparisons with measurements. Such assessments of the accuracy of submodels that are in use in engine models today have been done in comparisons with experimental data under pressure and temperature conditions that exist in current Diesel engines. These submodels have several shortcomings [6,7], but have been useful [4,5,8] in making predictions of practical interest. However, the pressures, and hence ratios of ambient gas density to injected liquid density, that are being contemplated for Diesel engines of the next generation are about a factor of two greater than those currently used. Under these conditions, additional physical processes may have to be considered. For example, at such high chamber pressures, supercritical droplet vaporization and combustion will become important and this in turn will affect combustion and emissions. It may even become necessary to use a virial equation of state [9]. There are also likely to be influences on the atomization process itself and the drop dynamics. Even the linear theory of Taylor [10,3] implies a dependence of intact core length, drop size and spray angle on the density ratios. Hence it becomes necessary to consider all these processes at higher pressures. This is a challenging task. The objective of this work is to initiate this task by assessing the accuracy of computed and measured penetrations in a very high pressure environment, using a model that has been found adequate at lower pressures [3].

The ability to predict the penetration is only one condition for adequate accuracy of the model [11]. Penetration is controlled by the rate of momentum transfer to the ambient gas, i.e. the growth of the boundary layer between the injected medium and the ambient. An agreement between computed and measured penetrations do not imply, for example, that drop sizes, vaporization rates or drop distribution within the spray are also adequately reproduced. Nevertheless, our study is an important first step since this is the first time that such work has been carried out at such extreme conditions where the ratio of ambient gas density to injected density vary from 0.005 to 0.25.

In the next section, we describe the experimental setup and conditions. A brief description of the model follows. Next the results are presented and discussed. We close with summary and conclusions.

THE EXPERIMENTAL DATA

The experimental data used in this work were obtained in a constant volume, pancake-shaped chamber at Sandia National Laboratories. The chamber had a diameter of 114.3 mm and a depth of 28.56 mm. Fuel was injected into the chamber from an injector with a single hole of 0.32 mm diameter. The injector was located in the side wall at mid-height. The spray from the single hole was aimed through the center of the chamber. Fig. 1 shows a schematic of the arrangement.

The fuel was injected into the chamber that is filled with nitrogen. Non-vaporizing spray data were obtained by injection into N_2 at 300 K and vaporizing data by

Fig. 1. A schematic showing cross sections of the constant volume chamber

Table 1. Experimental conditions for non-vaporizing sprays

Case	ρ_a/ρ_l	T_a (K)	P_{inj} (MPa)
A	0.005	300	142
B	0.019	300	145
C	0.033	300	142
D	0.047	300	139
E	0.061	300	142
F	0.075	300	143
G	0.089	300	143
H	0.103	300	139
I	0.149	300	142
J	0.243	300	138

Table 2. Experimental conditions for vaporizing sprays

Case	ρ_a/ρ_l	T_a (K)	P_{inj} (MPa)
A	0.019	900	138
B	0.032	899	131
C	0.046	908	140
D	0.061	896	142
E	0.075	895	145

injection into inert gases at higher temperatures. Very high chamber pressures and temperatures were achieved in the vaporizing cases by a premixed burn taking place prior to fuel injection [12]. The premixed burn phase was arranged such that, by the beginning of fuel injection, the premixed combustion would be completed and all oxygen in the chamber depleted. The chamber wall temperatures were about 450°K in all cases. The fuel used was Diesel fuel No. 2. The durations of fuel injection were about 2.6 ms in the non-vaporizing cases and about 2.9 ms in the vaporizing cases. The injected fuel amount was about 75 mg in the non-vaporizing cases, and about 81 mg in the vaporizing cases. Tables 1 and 2 show other experimental conditions for non-vaporizing and vaporizing sprays respectively. The density ratios of ambient gas to injected fuel, ρ_a/ρ_l , range from 0.005 to 0.243 with the corresponding ambient pressure ranging from 0.37 MPa to 18.36 MPa for non-vaporizing sprays, and from 0.019 to 0.075 with the corresponding ambient pressure ranging from 4.2 MPa to 16.9 MPa at about 900 K for vaporizing sprays. The combinations of injected fuel quantities and density ratios would correspond to an overall equivalence ratio range of 0.93 to 0.017 for the non-vaporizing cases, and 0.27 to 0.064 for vaporizing cases, if the am-

Fig. 2. Measured penetrations of non-vaporizing sprays vs. time

Fig. 3. Measured penetrations of vaporizing sprays vs. time

bient were air. The higher density ratios achieved in this study are well beyond the current Diesel range and thus are of great interest to designers of the next generation of Diesel engines.

The chamber had optical access for visualization of the spray. The penetration of the spray was derived from high speed photography. Figs. 2 and 3 show the measured tip penetrations as a function of time for the non-vaporizing and vaporizing sprays respectively.

THE 3-D MODEL

The KIVA-3 code [13,14] is used in this study with modified physics. The submodels for computing momen-

tum and energy transfer through the walls and spray atomization are different from those in the standard KIVA-3 code. While the modification of the submodel for computing momentum and energy transfer through the walls would have minimal influence on the results of this work, the atomization submodel would affect the results. In the solution procedure, the general conservation equations for mass, momentum and energy are solved with a number of submodels. Turbulence is represented by a $k-\epsilon$ model with terms that account for spray/turbulence interactions, and the effects of compressibility [15]. The fluxes of momentum and energy at the walls are calculated by use of wall functions as described in reference [15].

The spray model incorporates a line source for drops [16]. The length of the line source, X_1 , is proportional to $(\rho_l/\rho_a)^{1/2}$, which implies a shorter intact core length when the ambient density becomes higher. In addition, the spray model solves equations for the exchange of heat, mass and momentum between the gas and liquid phases [3]. Turbulent dispersion of the drops are accounted for by adding to the mean gas velocity u a fluctuating velocity u' [11]. Droplet collisions and coalescences are modeled by a statistical sampling procedure [11]. Breakup of the droplets is calculated by the TAB model [17].

The initial drop sizes and spray angles are determined based on Taylor's theory [10,3]. The following formulas are used:

$$\frac{X_1}{d_0} = C_c \left(\frac{\rho_l}{\rho_a} \right)^{1/2} f_m^{*-1} \quad (1)$$

$$d_{d,0} = B_d \frac{2\pi\sigma}{\rho_a V_T^2} \lambda_m^* \quad (2)$$

$$\tan \frac{\theta}{2} = \frac{1}{A_\theta} 4\pi \left(\frac{\rho_a}{\rho_l} \right)^{1/2} f_m^* \quad (3)$$

where, X_1 is the intact core length, d_0 is the diameter of the nozzle hole, ρ_l is the injected liquid density, ρ_a is the ambient gas density, $d_{d,0}$ is the initial Sauter mean diameter of the droplets, σ is the surface tension of the injected liquid, V_T is the relative liquid-gas velocity, θ is the spray full angle, $f_m^* = \lambda_m^* \omega_m^*$; λ_m^* is the dimensionless wave length of fastest growing surface wave, ω_m^* is the dimensionless growth rate of fastest growing surface wave (f_m^* , λ_m^* , and ω_m^* are functions of the Taylor number, T_a , where $T_a = \rho_l \sigma^2 / \rho_a \mu_l^2 V_T^2$; μ_l is the liquid viscosity), C_c , B_d and A_θ are constants. All constants are those used in references [3,16]. The accuracy of this model has been assessed in a wide range of studies [7,18,19] and it has been applied to a range of different problems [1,20-22].

For the fuel injection velocity profile, we consider a constant injection velocity though we also examine the effect of having an initial ramp.

RESULTS AND DISCUSSIONS

2-D Computations

Since our initial investigations led us to believe that the penetration of the spray is not influenced significantly by the geometry of the chamber in the experiments, we made 2-D computations of the spray injected into an axisymmetric chamber. These computations gave us greater flexibility over grid resolution and arrangement. We were able to use non-uniform grid with higher grid resolution close to the injector and lower grid resolution away from the injector. The conditions in the axisymmetric chamber correspond to the conditions listed in Tables 1 and 2 for non-vaporizing and vaporizing sprays respectively. Fig. 4 shows the grid used. The computational domain has dimensions of 50 mm(radius) $\times$ 120 mm(axial distance).

To obtain the spray penetration from the computations, we examine the liquid fuel mass distribution in non-vaporizing cases and the vapor fuel mass distribution in vaporizing cases along the axis of the spray. Figs. 5 and 6 show typical examples of such distributions for the non-vaporizing and vaporizing cases respectively. Fig. 5 shows the computed liquid mass as a function of distance along the axis of the spray, for a non-vaporizing spray case, at different times after start of injection. At any time, the graph is obtained as follows: The liquid mass in sections which are perpendicular to the axis of the spray and of thickness of about 1.2 mm, which corre-

Fig. 4. The 2-D axisymmetric grid

sponds to the width of a computational cell, are obtained along the axis of the spray. Close to the injector orifice there is less liquid. More liquid concentrates in the head vortex. Fig. 6 shows the fuel vapor mass for a vaporizing case, obtained in the same manner, as a function of axial distance in the spray at different times after injection. For the non-vaporizing spray, the penetration is defined as the distance from the orifice to the point where the liquid mass is 5 percent of its peak value. For the vaporizing spray, the penetration is defined as the distance from the orifice to the point where the fuel vapor mass is 5 percent of its peak value.

Fig. 5. Liquid fuel mass vs. spray axial distance plot used to determine the penetrations of non-vaporizing sprays

Fig. 6. Vapor fuel mass vs. spray axial distance plot used to determine the penetrations of vaporizing sprays

Fig. 7. Comparisons between computed and measured penetrations for the non-vaporizing sprays (Cases A-C, F, and G)

Fig. 8. Comparisons between computed and measured penetrations for the non-vaporizing sprays (Cases E, H, and J)

Fig. 9. Comparisons between computed and measured penetrations for the non-vaporizing sprays (Cases D and I)

Fig. 10. Comparisons between computed and measured penetrations for the vaporizing sprays (Cases A, B, and D)

Fig. 11. Comparisons between computed and measured penetrations for the vaporizing sprays (Cases C and E)

Figs. 7-9 show the computed penetrations versus time for Cases A-J of the non-vaporizing cases, and Figs. 10 and 11 show the computed penetrations versus time for Cases A-E of the vaporizing cases. It may be seen that there is adequate agreement of the computed and measured results.

In an early work [1], it had been shown that for an incompressible, fully developed gas jet the following scales for distance and time may be derived:

$$\text{distance} : \left(\frac{\rho_i}{\rho_a} \right)^{1/2} d_0$$

$$\text{time} : \left(\frac{\rho_i}{\rho_a} \right)^{1/2} \frac{d_0}{u_i}$$

where, u_i is the injection velocity, and ρ_i is the injected gas density.

Indeed, it was shown that even for transient gas jets these scaling laws appeared to hold.

In order to assess whether these scaling laws also hold for sprays under the conditions of this study, we plot in Figs. 12 and 13 the non-dimensional penetration (measured) as a function of the non-dimensional time for Cases A-J of the non-vaporizing ones and Cases A-E of the vaporizing ones. In applying the scaling laws, we put $\rho_i = \rho_l$. It may be seen that the results collapse approximately to a single curve when the scales above are used to normalize distance and time. This collapse may in part be due to the fact that the initial drop sizes that are computed have very small Stokes numbers, i.e. < 0.1 . Hence, they transfer their momentum to the ambient gas relatively quickly and subsequently the ambient gas transports most of the injected momentum. In the

Fig. 12. Non-dimensional penetration vs. non-dimensional time plot for non-vaporizing sprays

Fig. 13. Non-dimensional penetration vs. non-dimensional time plot for vaporizing sprays

vaporizing cases, the vaporization is very rapid and the mixture of ambient gas and vaporized fuel transports the momentum. In these cases, provided the initial equilibration times are not too different from each other or that they are short relative to the overall penetration length, the scaling that has been shown earlier for gas jets may be expected to apply. This scaling has important implications for distribution of the vapor fuel and mixing characteristics in Diesel engines. This will be discussed in a forthcoming paper [23].

3-D Computations

The 2-D computations above predict the spray penetrations adequately, showing that the spray model is adequate in this respect. Since the influence of the walls and the flow field are likely to be different in the experimental configuration when compared to the 2-D geometry, computations were carried out in the fixed volume chamber. These computations were three-dimensional. Fig. 14 shows a typical computational grid used in these 3-D computations.

First, we assessed the influence of numerical resolutions on the 3-D results, since making computations with grid resolution comparable to the 2-D cases would require over a hundred hours per computation on a CRAY-2. We increased the temporal resolution by a factor of two and found no effect. We then varied the spatial resolution. Fig. 15 shows the computed spray penetrations for the non-vaporizing Case J for two different grid resolutions: in one case the mesh size is 1.2 mm which corresponds to a mesh number of $91 \times 91 \times 25$ (NX x NY x NZ),

Fig. 14. A top view of a 3-D computational grid of the actual chamber (NX x NY x NZ = $91 \times 91 \times 25$)

Fig. 15. Spray penetrations with two different grid resolutions for non-vaporizing Case J

and in the other case 0.8 mm which corresponds to $141 \times 141 \times 37 (NX \times NY \times NZ)$. The results are sensitive to the grid resolution. Adequate agreement is obtained for a mesh size of 0.8 mm. Additional refinement is found to bring about a smaller change. We find that a higher grid resolution is necessary when there is vaporization and the gradients close to the injector are very sharp due to rapid vaporization of the injected fuel droplets. Similarly, we find that higher resolution is required at higher ambient gas to injected liquid density ratios. This may be because as the density ratio is increased, the injected momentum is transferred to the ambient gas over a shorter physical length. Hence the gradients in physical space are greater near the orifice and thus higher resolution is needed near the injector. So, in principle, each case has to be independently assessed for numerical accuracy. Such computations require prohibitively large

Fig. 16. Computed fuel droplet distributions and velocity vector field of a non-vaporizing spray (Case E)

computer resources. For example, a $91 \times 91 \times 25$ grid computation of non-vaporizing spray takes about 35 hours on the CRAY-2. This need for higher resolution to obtain grid-independent solutions is also found in the 2-D axisymmetric computations where mesh sizes close to the injector are of the order of the orifice diameter.

Shown in Figs. 16 and 17 are examples of computed drop positions and flow field of a non-vaporizing spray, and a contour of vapor fuel mass fraction and flow field of a vaporizing spray. It may be seen from Fig. 16 that the flow field is only affected in a region close to the axis of the spray for this case. This is because the overall equivalence ratio for this case is 0.073 and the entrainment process affects only a small fraction of the ambient gas. The vapor distribution in Fig. 17 shows that a significant fraction of the vapor fuel (> 20 percent) is in

regions where the equivalence ratio is greater than 2.0, i.e. vapor fraction of 0.12. This rich region is close to the axis of the spray. It may also be seen that close to the injector, i.e. within $25 d_0$, there is less vapor fuel. This is because of the high convective velocities near the injector which convect the liquid fuel and vapor fuel further downstream.

Fig. 18 shows computed and measured spray penetrations for some typical density ratios in the non-vaporizing cases (Cases A, B, E, F, and J). Here a grid size of 1.2 mm is used. This corresponds to a mesh number of $91 \times 91 \times 25$. It is shown that, over a very wide range of ρ_a/ρ_l (0.005 to 0.243), the computed spray penetrations show the correct trends and the agreement is within 20 percent past 2 ms. Similar agreement in trends are obtained for vaporizing cases as well, as shown in Fig. 19.

Fig. 17. Computed vapor fuel mass fraction contour and velocity vector field of a vaporizing spray (Case B)

Fig. 18. Comparisons between computed and measured penetrations for the non-vaporizing sprays (Cases A, B, E, F, and J) from 3-D computations

Fig. 20. Spray penetrations with two different initial drop sizes for non-vaporizing Case E

Fig. 19. Comparisons between computed and measured penetrations for the vaporizing sprays (Cases A, B, and D) from 3-D computations

Fig. 21. Injection velocity profiles without and with an initial ramp

Effect of Initial Drop Size - The drop sizes used in all computations above are those obtained from Taylor's theory [3]. However the initial drop size has been of some contention [17,24], and the rate of momentum transfer from the injected liquid may depend on the initial drop size [1]. Drop sizes computed above are of $O(0.1\mu\text{m})$ in radius for the conditions of the experiment. We investigated the effect of this initial drop size on penetration by changing it drastically. Fig. 20 shows the computed penetrations of the non-vaporizing Case E for initial drop sizes, i.e. the Sauter mean radius (SMR), of $0.12\mu\text{m}$ and $10\mu\text{m}$. It may be seen that in spite of two orders of magnitude difference in initial drop sizes, the penetration is only slightly affected.

Effect of Initial Injection Velocity - In the previous computations, we assume a constant injection velocity. However, in practice, there would be an initial velocity ramp during the nozzle opening, as schematically indicated in Fig. 21. During this period, the injection velocity is lower than its peak value, and the droplet size calculated is larger. To assess the effect of a ramp in the injection velocity, a computation was made in which the duration of the ramp was taken to be 5 percent of the total injection duration. Fig. 22 shows the results. The difference between the two cases is negligible, showing that the effect of this ramp on the penetration is negligible. However the actual injection rate has to be determined from experiment to evaluate this aspect of the model.

In general, while it may be prudent to consider the effects of individual parameters one by one, as above, in order to isolate their individual effects, we find in our computations that the parameters are seldom independent of one another. The inter-relationship between different parameters can result in very complex and unanticipated behaviors. For example, using relatively smaller initial

Fig. 22. Computed spray penetrations without and with an initial ramp in the injection velocity for non-vaporizing Case E

drop Sauter mean radius, say of the order of $0.1\mu\text{m}$ or less, may result in a rapid transfer of injected momentum from the drops to the ambient gas. This results in the formation of a head vortex close to the injector which, in turn, convects the smaller drops towards the axis of the spray. Near the axis the drops collide, coalesce and form larger drops. These larger drops travel relatively close to the axis, unaffected by the ambient gas motion, and may then lead to increased computed penetration. The computed penetration is sensitive to these inter-relationships between the injection parameters and the flow field in ways which may be counter-intuitive. This points to the need for more experimental data to assess the accuracy of these spray models over a broad range of parameters.

Prohibitive numerical resolution is required to obtain grid-independent results in the 3-D computations. This points to the need to use non-uniform grids with very high resolution, at least, near the tip of the injector. The 2-D computations provide guidance in this direction. In the 2-D computations the grid resolution used near the tip of the injector is comparable to the orifice diameter.

In spite of these limitations, our work appears to show that the spray models that have been found to be adequate for operating conditions of current Diesel engines are also adequate to predict spray penetration at much higher chamber pressures, i.e. higher ratio of ambient gas density to injected liquid density. However many other computed parameters of the spray have to be compared with experimental data before the model can be used for design of advanced Diesel engines. These parameters include drop sizes and drop size distributions, drop velocities, distributions of vapor and/or liquid fuel, and drop turbulence.

In the case of vaporizing sprays, we also used a modified drag coefficient proposed in Ref. [25] and also experimentally verified in Ref. [26] but found that this had negligible effect in our cases as the drop sizes are relatively small (Stokes number < 0.1) and vaporization times (ratio of vaporization time / mixing time $\ll 1$) are also relatively short.

SUMMARY AND CONCLUSIONS

2-D and 3-D computations of non-vaporizing and vaporizing sprays over a broad range of density ratios of ambient gas to injected liquid (ρ_a/ρ_l) were carried out to assess the accuracy of the model in computing spray penetrations. The 2-D computations which use non-uniform grids with very high grid resolution close to the injector are able to reproduce the penetration within 15 percent. The 3-D computations reproduce the measured spray penetrations within about 20 percent in accuracy; however, it requires a significant amount of computer resources to get grid-independent results when the density ratio becomes very high, and when there is rapid vaporization. Scaling laws for time and distance derived in a previous paper for gas jets are found to apply also to the sprays over the broad range of density ratios presented in this paper.

The results appear to indicate that the model can predict spray penetrations at much higher ambient density than the current Diesel range. While the spray model is able to adequately predict the spray penetrations, the accuracies of the model in predicting many other spray parameters, for example, drop size distribution, drop velocities, and vapor distribution, have to be assessed before the model can be used for the design of engines.

ACKNOWLEDGEMENTS

Support for this work was provided by the Los Alamos National Laboratory under contract No. 3027N0014-9C. The authors are grateful to Drs. T. Butler, N. Johnson and A. Amsden for helpful discussions.

The authors thank the Minnesota Supercomputer Institute, University of Minnesota, for providing computing resources and access to its facilities. Part of the computing support was provided by CRAY Research through a grant to the University of Minnesota.

J.A. also thanks Prof. F. V. Bracco, Princeton University, for his interest and suggestions during this work. He is grateful to Prof. J. M. MacInnes, University of Sheffield, for his input during the early part of this work.

Some of the results were presented at the 11th Engine Workshop sponsored by the Army Research Office, Princeton University, Princeton, March 14-15, 1994.

REFERENCES

1. Abraham, J., Magi, V., MacInnes, J. and Bracco, F. V., "Gas Versus Spray Injection: Which Mixes Faster?," SAE Paper 940895, also in SAE Publications No. SP-1028, Diesel Combustion Processes and Emission Control, 1994.
2. Abraham, J., "Computations of Sprays in a Very High Pressure, Constant Volume Chamber," paper presented at the 11th ARO Engine Workshop, Princeton University, March 14-15, 1994.
3. Bracco, F. V., "Modeling of Engine Sprays," SAE Paper 850394, also in SAE Trans., Vol. 94, and in SAE Publication No. P-156, Engine Combustion Analysis: New Approaches, 1985.
4. Abraham, J. and Bracco, F. V., "Fuel-Air Mixing and Distribution in a Direct-Injection Stratified-Charge Rotary Engine," SAE Paper 890329, also in SAE Trans., Vol. 98, 1989.
5. Abraham, J. and Bracco, F. V., "Combustion Optimization Computations - Part I: Swirl and Squish Effects in Air-Assist Injection Engines," SAE Paper 922240, also in SAE Trans., Vol. 101, 1992.
6. MacInnes, J. M. and Bracco, F. V., "Stochastic Particle Dispersion Modeling and the Tracer-Particle Limit," to appear in Physics of Fluids A, 1994.
7. MacInnes, J. M. and Bracco, F. V., "Radial Distribution of Drop Size in Full-Cone Sprays," submitted to Atomization and Sprays, 1993.
8. Patterson, M. A., Kong, S.-C., Hampson, G. J. and Reitz, R. D., "Modeling the Effects of Fuel Injection Characteristics on Diesel Engine Soot and NOx Emissions," SAE Paper 940523, 1994.
9. Sonntag, R. E. and Van Wylen, G. J., Fundamentals of Statistical Thermodynamics, Robert Krieger Publishing Co., 1966.
10. Batchelor, G. K. (Editor), Collected Works of G. I. Taylor, Cambridge University Press, 1958.
11. O'Rourke, P. J. and Bracco, F. V., "Modeling of Drop Interactions in Thick Sprays and a Comparison with Experiments," Institute of Mechanical Engineers, Publication 1980-9, 101-116, 1980.
12. Siebers, D. L., "Ignition Delay Characteristics of Alternative Diesel Fuels: Implications on Cetane Number," SAE Paper 852102, 1985.
13. Amsden, A. A., "KIVA-3: A KIVA Program with Block-Structured Mesh for Complex Geometries," Los Alamos National Laboratory report, LA-12503-MS, 1993.
14. Amsden, A. A., O'Rourke, P. J. and Butler, T. D., "KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays," Los Alamos National Laboratory report, LA-11560-MS, 1989.
15. Grasso, F., Wey, M.-J., Bracco, F. V. and Abraham, J., "Three-Dimensional Computations of Flows in a Stratified-Charge Rotary Engine," SAE Paper 870409, also in SAE Trans., Vol. 96, 1987.
16. Chatwani, A. U. and Bracco, F. V., "Computation of Dense Spray Jets," ICLASS-85, London, U. K., 1985.
17. O'Rourke, P. J. and Amsden, A. A., "The TAB Method for Numerical Calculation of Spray Droplet Breakup," SAE Paper 872089, 1987.
18. Andrews, M. J. and Bracco, F. V., "On the Structure of Turbulent Dense Spray Jets," Encyclopedia of Fluid Mechanics, Vol. 8, N. P. Chermisinoff, ed., Gulf Publishing Co., 1989.
19. Tomboulides, A., Andrews, M. J. and Bracco, F. V., "On the Anisotropy of Drop and Particle Velocity Fluctuations in Two-Phase Round Gas Jets," Modern Research Topics in Aerospace Propulsion, G. Angelino, L. Deluca and W. A. Sirignano, eds., Springer-Verlag, N. Y., 1991.
20. Abraham, J., Wey, M.-J. and Bracco, F. V., "Pressure Non-Uniformity and Mixing Characteristics in Stratified-Charge Rotary Engine Combustion," SAE Paper 880624, SAE Trans., Vol. 97, 1988.
21. Abraham, J., Epstein, P. and Bracco, F. V., "3-D computations to Improve Combustion in a Stratified-Charge Rotary Engine - part IV: Modified Geometries," SAE Paper 930679, SAE Trans., Vol. 102, 1993.
22. Abraham, J. and Bracco, F. V., "Simple Modeling of Autoignition in Diesel Engines for 3-D Computations," SAE Paper 932656, SAE Trans., Vol. 102, 1993.
23. Abraham, J., "Some Scaling Characteristics of Gas Jets and Vaporizing Sprays and Implications for Combustion Chamber Designs," paper in preparation, 1994.
24. Reitz, R. D., "Modeling Atomization Processes in High-Pressure Vaporizing Sprays," Atomization and Spray Technology, 3, 309-337, 1987.
25. Chiang, C. H., Raju, M. S. and Sirignano, W. A., "Numerical Analysis of Convecting and Interacting Vaporizing Fuel Droplets with Variable Properties," Intl. J. Heat Mass Transfer, Vol. 35, pp. 1307-1314, 1992.
26. Song, Y.-H. and Santavica, D. A., "An Experimental Study of Drag and Lift Acting on Evaporating Droplets Following Curvilinear Trajectories in a Laminar Flow," paper submitted to Combust. Sci. Tech., May 1994.

Part II:

Title: Preliminary Computations of Combusting Sprays in a Very High Pressure Chamber

The objective of this part of the work is to assess the accuracy of the model in the presence of combustion. A combustion model [1,2] whose accuracy has been assessed in several studies in the past [for example, 1-6] is included in the model.

The Combustion Submodel

Our basic model [1] follows the evolution of seven species (fuel, O₂, N₂, CO₂, H₂O, CO) by solving the following species conservation equations ($i = 1, 2, \dots, 7$) together with all other flow and spray equations

$$\frac{\partial Y_i}{\partial t} + v_j \frac{\partial Y_i}{\partial x_j} = - (1/\rho) \frac{\partial(\rho_i V_{ij})}{\partial x_j} + \dot{\omega}_i \quad (1)$$

In the above equation, Y_i is the mass fraction of species i , v_j is the velocity in the direction j , x_j is the distance in the direction j , ρ is the gas density, V_{ij} is the diffusion velocity of species i in the direction j , and $\dot{\omega}_i$ is the rate of formation of species i .

Now we add to the seven species a new species that represent the evolution of the radicals that lead to self-ignition. The evolution of this eighth species is controlled again by convection, diffusion and chemical formation. Thus equation (1) is used also for it, together with the following ones:

$$V_{8j} = - (D_e \frac{\partial Y_8}{\partial x_j}) / Y_8 \quad (2)$$

$$\dot{\omega}_8 = \frac{1}{\tau_8} \quad (3)$$

$$\tau_8 = A \left(\frac{P}{P_0} \right)^B e^{D(1+C\Pi-\phi)/T} \quad (4)$$

where D_e is the effective diffusivity, i.e., the sum of the laminar and turbulent diffusivities, P is the pressure in atm, T the temperature in K, ϕ is the equivalence ratio and A, B, C, D are constants that are determined by comparisons with measured ignition delay times.

Since the eighth species represents radicals, its mass is negligible and its value at ignition is an additional parameter. Actually, for any selected value of Y_8 at ignition, a value of A in equation (4) can be found that keeps τ_8 constant. Thus we say that ignition occurs when $Y_8 = 1$ and keep A, B, C, D as the only constants to be determined by comparisons with ignition delay measurements. When Y_8 reaches 1.0 in any numerical cell at any time the smaller of the stoichiometric oxygen or the stoichiometric fuel of that cell is converted to products totally and instantly (for numerical reasons, the conversion is actually carried out in 5 μ s). In all other cells in which $Y_8 \neq 1$, our high temperature and/or mixing-controlled conversion model [1] determines the conversion of fuel to products. While, in principle, this high temperature model converts reactants to products at all temperatures, in practice, it is inactive at the low temperatures at which the formation of Y_8 is in progress. Also, in practice, after the initial premixed charge has burned, the conversion of reactants to products occurs mostly through mixing controlled combustion.

We model high temperature chemical conversion as follows:

In the species and energy conservation equations the time rate of change of the partial density of species i , ρ_i , or $\rho \dot{\omega}_i$ due to conversion from one chemical species to another is written

$$\dot{\rho}_i = (\rho_i - \rho_i^*) / \tau_c, \quad (5)$$

where p_i^* is the local and instantaneous thermodynamic equilibrium value of the partial density of species i and τ_c is the characteristic time for the achievement of such equilibrium and is assumed to be the same for the seven species considered: $C_3H_8, O_2, N_2, H_2O, CO_2, CO$, and H_2 . The

formulation of Eq. (5) assures that the proper thermodynamic equilibrium and heat release is approached for all equivalence ratios and chamber conditions.

The characteristic conversion time τ_c in turn is assumed to be longer of the laminar conversion time τ_1 and the turbulent mixing time τ_1 :

$$\tau_c = \max(\tau_1, \tau_c) \quad (6)$$

The laminar conversion time was obtained by applying Eq. (5) with $\tau_c = \tau_1$ to laminar flames and matching the measured laminar burning speed for hydrocarbon-air mixtures at various equivalence ratios.

The turbulent conversion time is given below.

$$\tau_1 = C_{m2} \frac{k}{\epsilon} \quad (7)$$

$$\text{if } \frac{C_{m3}(Y_P - Y_{ps})}{C_{m2}(1+s)(Y_F - Y_F^*)} \geq 1,$$

$$\tau_t = C_{m3} \frac{k}{\epsilon} (1+s) \left(\frac{Y_F - Y_F^*}{Y_P - Y_{ps}} \right)$$

$$\text{if } \frac{C_{m3}(Y_P - Y_{ps})}{C_{m2}(1+s)(Y_F - Y_F^*)} < 1, \quad (8)$$

where $s = (Y_{O_2} - Y_{O_2^*}) / (Y_F - Y_F^*)$. Y_P , Y_F , Y_{O_2} are the product, fuel and oxygen mass fraction respectively, and Y_{ps} is the residual product mass fraction.

Table 1: Experimental Conditions for Combustion Sprays

Case	ρ_a/ρ_e	T_a (°K)	p_{inj} (MPa)	p_a (MPa)
A	0.0135	1194	1523	4.07
B	0.0180	903	137	4.09
C	0.0312	906	127	7.11
D	0.0446	909	118	10.2
E	0.0448	905	152	10.2
F	0.0578	907	88.4	13.2
G	0.0580	904	149	13.2
H	0.717	903	141	16.3

The experimental data used in this part of the work were obtained in the same constant volume, pancake-shaped chamber described in Part I. A premixed charge was burned in the chamber to obtain high pressure and temperature prior to fuel injection. The premixed charge was rich in oxygen so that after the premixed charge burned the products had the approximate mass fraction of oxygen corresponding to that of air. The balance of the charge prior to injection was nitrogen, carbon dioxide and water vapor. The conditions in the chamber at the time of fuel injection are shown in Table 1. The density ratios of ambient gas to injected fuel, ρ_a/ρ_l , range from 0.0135 to 0.0717 with the corresponding ambient pressures, P_a , ranging from 4.07 MPa to 16.3 MPa and ambient temperatures from 1194 K to 903 K. Injection pressures, p_{inj} , range from 88.4 MPa to 152 MPa. The overall equivalence ratios range from 0.5 to 0.08.

In this work comparisons of computed and measured spray penetrations are being made as well as that of computed and measured chamber pressures. In this preliminary report, only comparisons of computed and measured chamber pressures are presented. Figs. 1 to 3 show computed and measured pressures for Case B (low density ratio), C (medium density ratio) and F (high density ratio). These computations are made with a constant injection rate and with relatively coarse resolutions. These results are representative of those of the other cases. At the higher density ratios, the agreement is within 5 percent. These computations are in progress.

References

1. Abraham, J., Reitz, R.D., and Bracco, F.V., "Comparisons of Computed and Measured Premixed Charge Engine Combustion," *Combust. & Flame*, Vol. 60, pp. 309-322, 1985.
2. Abraham, J. and Bracco, F.V., "Simple Modeling of Autoignition in Diesel Engines for 3-D Computations," SAE Paper No. 932656, SAE Trans., Vol. 102, 1993.
3. Abraham, J. and Bracco, F.V., "Fuel-Air Mixing and Distribution in a Direct-Injection Stratified-Charge Rotary Engine," SAE Paper No. 890329, SAE Trans., Vol. 98, 198.
4. Abraham, J. and Magi, V., "Effects of Ignition Cavity Flows on the Performance of a Stratified-Charge Rotary Engine: Initial 3-D Predictions," SAE Paper No. 941027, 1994.
5. Hou, Z.-X. and Abraham, J., "Modeling Soot and NO_x Emissions in a Direct-Injection Diesel Engine," paper under preparation.
6. Patterson, M.A., Kong, S.-C., Hampson, G.J., and Reitz, R.D., "Modeling the Effects of Fuel Injection Characteristics on Diesel Engine Soot and NO_x Emissions," SAE Paper No. 940523, 1994.

CASE B

Fig. 1 - Computed and measured pressure in the chamber (CASE B)

CASE C

Fig. 2 - Computed and measured pressure in the chamber (CASE C)

CASE F

Fig. 3 - Computed and measured pressure in the chamber (CASE F)