LA-UR-95-210

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: **THREE-DIMENSIONAL COMPUTER MODELING OF HYDROGEN INJECTION AND COMBUSTION**

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SUBMITTED TO: *'95 SMC Simulation Multiconference, Phoenix, Arizona, April 9–13, 1995*



Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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

# THREE-DIMENSIONAL COMPUTER MODELING OF HYDROGEN INJECTION AND COMBUSTION

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*Key words:* KIVA code, computational fluid dynamics, hydrogen combustion, gas injection, reaction modeling.

## ABSTRACT

The hydrodynamics of hydrogen gas injection into a fixed-volume combustion chamber is analyzed and simulated using KIVA-3, a three-dimensional, reactive flow computer code. Comparisons of the simulation results are made to data obtained at the Combustion Research Facility at Sandia National Laboratory–California (SNL-CA). Simulation of the gas injection problem is found to be of comparable difficulty as the liquid fuel injection in diesel engines. The primary challenge is the large change of length scale from the flow of gas in the orifice to the penetration in the combustion chamber. In the current experiments, the change of length scale is about 4000. A reduction of the full problem is developed that reduces the change in length scale in the simulation to about 400, with a comparable improvement in computational times. Comparisons of the simulation to the experimental data shows good agreement in the penetration history and pressure rise in the combustion chamber. At late times the comparison is sensitive to the method of determination of the penetration in the simulations. In a comparison of the combustion modeling of methane and hydrogen, hydrogen combustion is more difficult to model, and currently available kinetic models fail to predict the observed autoignition delay at these conditions.

## INTRODUCTION

Hydrogen has long been considered to be the ideal fuel for power generation and the eventual replacement of hydrocarbon-based fuels, due to the absence of carbon-based pollutants, the abundance of hydrogen in nature, and the ability to generate hydrogen from sustainable energy sources (solar, hydro, wind, and biomass). Until fuel cell technology matures, an internal combustion engine using hydrogen fuel is the likely interim solution to a zero or low emission power plant, either for vehicles or stationary power plants.

Our objective is to develop a computational capability for the design of hydrogen-fueled engines by industry, and in the present work, focus on the development of tools for the simulation of hydrogen injection, as required for hydrogen-fueled diesel engines and for the formation of hydrogen mixtures for homogeneous-charged spark-ignited engines. The hydrogen simulation capability is benchmarked by comparisons with experiments in a combustion bomb (Fig. 1) at the Combustion Research Facility at Sandia National Laboratory - California. The work contributes to two areas by developing the knowledge (1) to enable industry to build a stationary hydrogen-fueled internal combustion engine to power an electric generator system, and (2) to build an advanced, high-power-density internal combustion engine fueled by hydrogen to meet zero emission requirements.

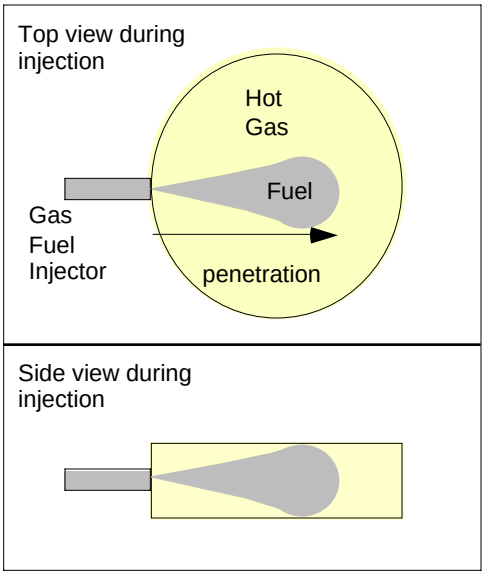


Figure 1. Schematic of the combustion bomb for fuel injection experiments.

Los Alamos National Laboratory has developed computer models, the KIVA family of codes, that have gained wide acceptance in the automotive industry, as well as the gas turbine, stationary combustion and aerospace industries, primarily for hydrocarbon fuels. The approach to developing a modeling capability for hydrogen fueled systems is to modify the latest of the publicly released codes, KIVA-3, and one soon to be released, KIVA-F90, to facilitate the analysis of hydrogen combustion with both pure hydrogen as a fuel and mixtures of hydrogen and natural gas.

KIVA-3 has been successfully applied to scavenging studies (Amsden, et al., 1992, Zhu, et al., 1994) and to liquid diesel fuel injection into the same combustion bomb (Hou, Abraham and Siebers, 1994, 1995). In the scavenging studies the gas flow was found to be accurately described on moderately refined meshes, but an accurate simulation of the liquid fuel injection experiments required a highly refined mesh. These studies give us confidence that, to within the unique aspects of gas injection and hydrogen combustion, KIVA can be successfully applied to hydrogen injection and combustion systems. Our approach to the gaseous injection problem is to divide the flow into tractable problems that can be analyzed separately and then sequentially coupled. For hydrogen combustion, in the absence of reaction kinetics for hydrogen in the regime of interest, two existing kinetic descriptions of hydrogen combustion are examined.

## DESCRIPTION OF BOMB EXPERIMENTS

The combustion vessel in the SNL-CA experiments is a pancake-shaped, cylindrical combustion chamber with a 114.3-mm diameter and a 28.6-mm axial width as in Fig. 1. The apparatus using natural gas injection is described in Naber et al., 1994a and 1994b; the hydrogen injector is essentially the same fuel injector, with different seals to accommodate the higher pressure of hydrogen. The two circular walls of the chamber are sapphire windows that permit full field-of-sight optical access to the chamber. Characteristics and operating conditions of the chamber and injector are summarized in Table 1. The gas is introduced through a single orifice as in Fig. 1. The injection profile is a square pulse with a 100-μs rise time to 0.9 of its steady state value.

Table 1 Details of Combustion Bomb.

| | |
|---|---|
| Chamber volume ($cm^3$) | 293.2 |
| Chamber wall temperature (°K) | 450 |
| Orifice diameter (μm) | 250.0 |
| Orifice length (μm) | 1000 |
| Injection pressure (MPa) | 20.7 |
| Injection duration (s) | 0.011 |
| Mass of $H_2$ injected (gm) | 0.00490 |

The initial conditions of the air mixture in the chamber before injection are achieved by the premixed combustion of a small amount of combustible gas ($H_2$ and $C_2H_4$), such that the resulting composition is similar to air (Table 2). After combustion, the heated mixture is allowed to cool until the desired chamber pressure is achieved, and the gas fuel injection is initiated. Because of the transparency of hydrogen in the air mixture, the penetration of the gas jet cannot be observed with the Schlieren system until the hydrogen autocombusts, and the flame front propagates to the edge of the jet.

Table 2 Initial Species Gas Density ($g\text{-}cm^{-3}$) before Injection.

| | |
|---|---|
| Oxygen | 0.00398 |
| Nitrogen | 0.01312 |
| Carbon dioxide | 0.00115 |
| Water | 0.00067 |
| Average molecular weight: | 29.47 |

## COMPUTATIONAL MODELING

### Description of the KIVA Reactive Flow Code

The KIVA family of codes, developed at Los Alamos National Laboratory (LANL), is a mature, three-dimensional, computational fluid dynamics software for chemically reactive, transient flows with fuel sprays (Amsden et al., 1989). The numerics of KIVA include a combination of explicit and implicit solutions on a staggered mesh. The code features sophisticated sub-models, which simulate the complex flow, thermodynamic and chemical processes accompanying injection and combustion. These models include for applications to combustion engines: turbulence, spray atomization, fuel penetration and vaporization, auto-ignition and combustion. The chemical combustion model can describe complex equilibrium and kinetic reactions, giving it the capability of modeling soot in the presence of carbon and $NO_x$ production. The KIVA-3 version (Amsden, 1993) enables complex geometries, through the use of interconnected blocks of logical hexahedral mesh, to be modeled. These meshes are typical of combustion engines with moving pistons and inlet and exhaust ports. The connectivity of the mesh can change to allow for piston movement and opening and closing of ports. KIVA-3 runs on generic workstations and on supercomputers and can be obtained through the Energy Science and Technology Software Center (ESTSC@OSTI.GOV). The current, unreleased version of KIVA-3 includes the capability to simulate engines with valves. A new version of KIVA, KIVA-F90, is written in FORTRAN-90 and will execute on massively parallel machines. For the current application, KIVA-3 is used to model the SNL-CA experiments.

## Computational Approach

The physical processes that are important in the SNL-CA experiments are the flow of the gaseous fuel in the injector nozzle, the transitional flow of the fuel from the tip of the injector into the chamber, the interaction of the gas jet with the gas in the chamber and the consequent generation of turbulence and the heat exchange, mixing and eventual combustion of the fuel and air. The production of $NO_x$ emissions and timing of the autocombustion are sensitive to the extent of turbulence mixing.

Computational modeling of the SNL-CA hydrogen combustion experiments requires specification of the initial conditions in the combustion chamber and an approach to the modeling of the gas injection process. Despite the apparent simplicity of the injection of a gas in comparison to the injection of liquid fuel with phase changes, the disparate length scales in the gas flow present a formidable challenge to the computational modeling. The ratio of the largest length scale, the penetration of the gas jet, to the smallest length scale, the flow variations within the orifice (taken to be 1/10th the orifice diameter), is about 4000. This large ratio precludes the straightforward approach of treating the entire process in a single computational mesh that resolves all length scales, which would lead to impractical computational times.

Because the final goal of the computational modeling is to provide tools for designers of hydrogen fueled engines, a computational approach is ultimately required that will give accurate results on the comparatively coarse meshes that are necessary for full or partial engine simulations. Throughout the modeling of the SNL-CA experiments, the modeling choices were made with this goal in mind and are outlined in the following sections. The approach is to divide the flow problem into tractable portions that can be analyzed separately and then sequentially coupled. These are (1) the flow in the nozzle, which determines the nozzle exit conditions, (2) the expansion and cooling of the flow from the nozzle in the region just next to the nozzle, and (3) all processes that follow. The advantage of this approach is that the smallest length scales, a fraction of the orifice diameter, can be eliminated from the simulation of the jet penetration and combustion, thereby, significantly improving the simulation times.

## CHOKED FLOW NOZZLE DYNAMICS

The known experimental conditions for the gas injector are the pressure and temperature of the hydrogen reservoir behind the orifice and the measured mass injection rate. The exit conditions from the nozzle can be estimated by assuming, and later verifying, that the flow is limited by the sound speed of the gas, i.e., the flow is *choked*. If we further assume that under these flow conditions the hydrogen is nearly a perfect gas and flows isentropically through the short nozzle, the pressure, density, sound speed and temperature at the exit are given by:

$$P^* = P_0\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} = 10.9 \text{ MPa}$$

$$\rho^* = \rho_0\left(\frac{2}{\gamma+1}\right)^{\frac{1}{\gamma-1}} = 0.00707 \text{ g cm}^{-3}$$

$$c = \left(\frac{\gamma P^*}{\rho^*}\right)^{\frac{1}{2}} = 147{,}000 \text{ cm s}^{-1}$$

$$T^* = 375 \text{ K}$$

where $\gamma$ is 1.39 at these conditions, the pressure and temperature have values as in Table 1, and the density and temperature in the reservoir are found from the equation of state for hydrogen. Because of viscous losses on entry to the nozzle, the flow rate is typically lower than as determined from the soundspeed by some factor, taken to be 0.85 for a short nozzle with sharp corners. This gives an actual value for the exit velocity of $v_{act}$ = 0.85 c = 125,000 cm $s^{-1}$ and the mass flow rate, assuming a uniform velocity profile for fully developed turbulent flow, of 0.444 g $s^{-1}$. This value is in agreement with the experimentally-observed mass flow rate of 0.445 g/s, resulting in a discharge coefficient of 0.87, which is close to the assumed value of 0.85. This gives confidence in the calculated exit values for the pressure, density and temperature that are used in the next section.

## HIGHLY RESOLVED MODELING OF NEAR-NOZZLE DYNAMICS

Upon exiting the orifice, the hydrogen undergoes expansion and cooling, due to the drop in pressure, and rearrangement of the velocity field across the jet. To better understand this process and to provide inflow conditions for the less resolved simulations discussed in the following section, a detailed simulation of the fluid dynamics in the neighborhood of the nozzle was performed. The flow in the region of the nozzle is assumed to be axisymmetric, because the curvature of the wall is small and other bounding surfaces are far removed. Therefore, a highly-resolved, two-dimensional, axisymmetric mesh was used of 25 elements radially and 35 elements axially. Five elements of uniform spacing were used across the radius of the nozzle outlet (Fig. 2). Away from the nozzle, radially and axially, the mesh spacing was increased to reduce the total number of elements in the simulation. The inflow conditions of hydrogen gas are the values determined in the previous section, assuming the velocity profile at exit from the nozzle is flat. The turbulence is described by a k-$\varepsilon$ model. The turbulence intensity of the inflowing gas jet is

taken to be 1/100th of the kinetic energy of the jet. A solid wall boundary of constant temperature as in Table 1 is used on the side of the mesh where the jet exits. The other two sides of the mesh are specified to be outflow boundaries of constant pressure, taken to be the initial pressure of the gas in the chamber. The initial conditions and composition of the gas mixture are initialized with the values specified in Tables 1 and 2.

After about 60 μs, the mass of hydrogen within the mesh is constant and the system has reached a steady-state flow. The velocity vector field, Mach number and $H_2$ mass fraction at steady state are found in Figs. 2 and 3. The angle of expansion of the jet is observed to be about 7 degrees. In Figure 4, the normalized velocity, pressure, density and temperature along the axis are plotted. Significant expansion, subsequent cooling and acceleration occurs shortly after the hydrogen leaves the nozzle at about 0.04 cm from the exit and then quickly stabilizes and remains constant. This is typical behavior for a choked nozzle flow at these conditions. Also shown in Figure 4 are the spatially averaged values over the diameter of the nozzle just after the exit gas has stabilized. The averaged values differ from the centerline values because of the drag, heat transfer, and mixing of the gas in the chamber with the hydrogen. Comparisons of the averaged values with the axial values show that the major effect of the surrounding gas is to diffuse momentum away from the axis, as can be observed in the velocity field in Figure 2. The averaged values plotted in Figure 4 are given in Table 3. Simulations were redone with both a finer mesh and with a larger spatial domain, and no differences were observed in the results.

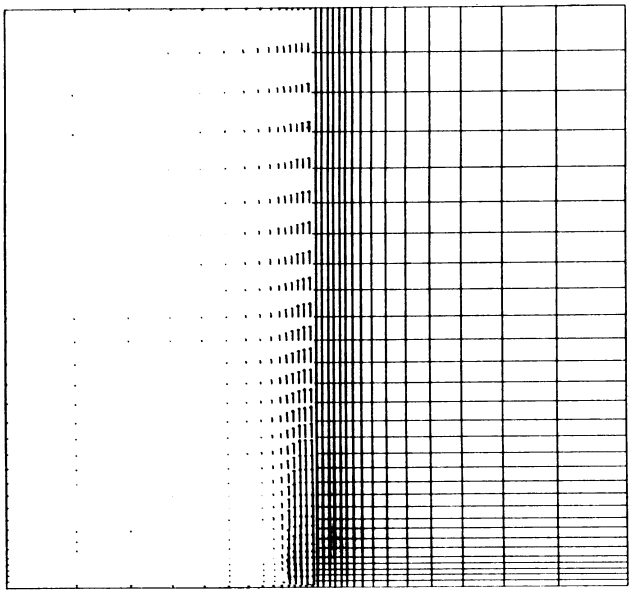

Figure 2. Velocity vector field and mesh for the 2D injection simulation near the orifice.

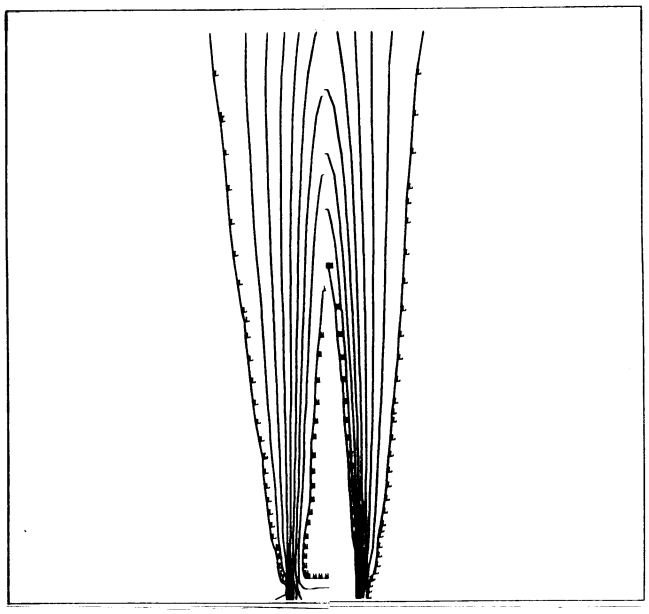

Figure 3. Mach number (left) and hydrogen mass fraction (right) contour plot for the 2D injection simulation near the orifice. The contour range for the Mach number is from 0.12 (marked L) to 1.1 (marked H) with intervals of 0.123. The contour range for the mass fraction is from 0.10 to 0.90 with intervals of 0.01.

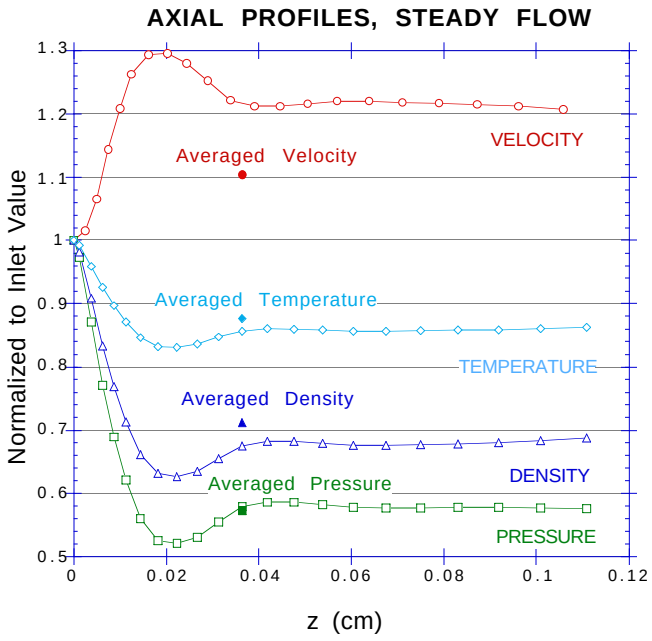


Figure 4. Plot of the axial profiles at steady state for the 2D injection simulation near the orifice.

Table 3. Steady State and Spatially Averaged Values of the Expanded Jet at an Axial Position of 0.037 cm.

| | |
|---|---|
| Axial velocity (cm $s^{-1}$) | 141,000 |
| Temperature (K) | 329 |
| Pressure (MPa) | 6.26 |
| Density (g $cm^{-3}$) | 0.0050 |

The results of this detailed simulation show that the effect of the expansion of the jet is significant and must be taken into consideration. The decrease in hydrogen temperature by 12 percent, or 45° K, will influence the delay in ignition. Furthermore the expansion occurs at a length scale that cannot be resolved on a typical mesh size required for practical engine simulations. Hence, if the nozzle exit conditions from the previous section had been used on a coarse mesh, the expansion of the jet would not be simulated correctly, and the simulation would be suspect.

## THREE-DIMENSIONAL MODELING OF COMBUSTION BOMB

The averaged values determined from the fine-scale simulation in the last section were used in a simulation of the injection into the full SNL-CA combustion chamber. In Figure 5, the 3D mesh that was used is shown. The mesh dimensions are 36 by 12 by 10. Also drawn on Figure 5 is the size of the 2D mesh used in the previous section in a blowup of the corner of the 3D mesh. This illustrates the drastic change of length scales that occur in this flow problem. For the 3D injection problem, the size of the orifice is the smallest dimension of the element in the corner of the mesh within the described 2D box. To minimize the computational times, only one fourth of the full system is modeled by taking advantage of the two planes of symmetry in the experiment. The orifice was resolved with a single element of square cross-section with one fourth the area of the orifice and one fourth the mass flow into the mesh. The boundary conditions are chosen appropriately: the chamber walls are modeled as solid walls of constant temperature, the internal fluid boundaries are reflective symmetry planes. The initial conditions of the gas in the mesh are specified as in the last section.

Many three-dimensional simulations were made to determine the sensitivity to the meshing and the numerical and physical models in KIVA-3. It was found that the penetration was most sensitive to the mesh size near the orifice and the treatment of turbulence. With either a poorly resolved mesh or the standard k-ε turbulence model, the fuel jet severely underpenetrated, even at early times. We concluded that to obtain the penetration necessary to describe the experimental data, a standard modeling approach would require a much finer mesh than would be practical for repetitive 3D simulations. Hence we examined

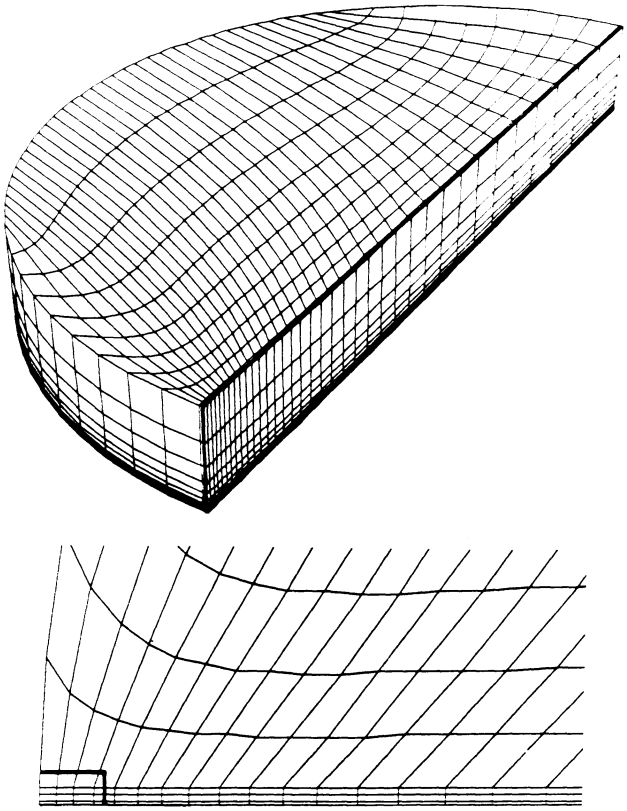

Figure 5. The three-dimensional mesh of one quarter of the SNL-CA combustion chamber. A blow up of the corner where the injection occurs is show in the lower figure. The box in the corner of this figure is the size of the mesh used in the simulations shown in Figs. 2-4.

modifications to the turbulence model that would allow an accurate computation on a coarser mesh. An alternative approach was used by Hou, Abraham and Siebers (1994) by using a highly resolved two-dimensional mesh and using standard models. The most successful modification of the k-ε model was based on the observation that on a coarse mesh unrealistic turbulent length scales, and consequently large diffusion, were generated. Hence, modifications were made to the KIVA models to limit the largest length scales in the region of the hydrogen jet. The approach used is to limit the length scale in the KIVA simulation to a length equal to the distance away from the orifice within a 7 degree cone along the axis. Although this scheme is somewhat arbitrary, it was found to universally apply to different conditions in the chamber for hydrogen injection and to the injection of methane. The major advantage of this scheme over the alternative approach used by Hou et al. (1994) is that it can be applied to full-scale engine simulations with complex geometries.

Another modification was made of the implementation of the k-ε model that had no effect on the results of the turbulence model but significantly improved its

convergence. Number of iterations of the semi-implicit solution of the k-ε equations were observed to be 15 to 22. The difficulty in the convergence was found to be localized unrealistic negative values of k and ε. Rigidly imposed floors on the values of k and ε were implemented corresponding to the minimum turbulent energy density expected in the problem and the correspondingly largest length scale, the bomb diameter, which when combined with the smallest k value gave a minimum value for ε. The number of iterations were reduced to 3 to 4, with no change in the simulation results.

In Figure 6 the experimental data with combustion are plotted for a gas temperature of 1150 K, along with the most promising simulation results without combustion. A question arises as to how best to determine the penetration of the jet for comparison to the experiments. Plotted in Figure 6 are the penetration as determined by the 1 and 2 percent contours of hydrogen gas density; the penetration based on a 3 percent contour significantly falls below the data at late times. Although either of these penetration determinations by KIVA match the experimental penetration at early times quite well, at later times, the two specifications of the penetration begin to diverge. This trend will continue as the hydrogen front becomes more diffuse. Because the hydrogen jet cannot be observed in these preliminary experiments until combustion has begun, experimental data is not shown at early times.

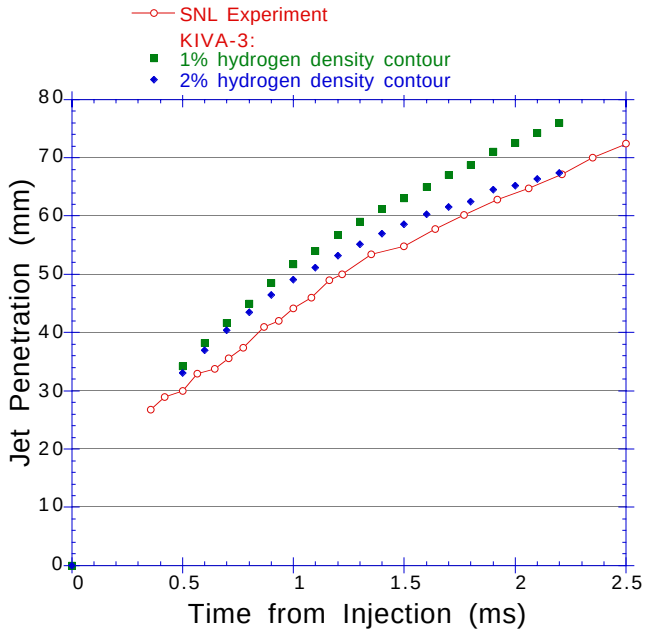


Figure 6. Comparison of the penetration history of the hydrogen jet of the KIVA simulation and the SNL-CA experiments. The penetration in the KIVA simulations is presented for the maximum axial extent of the one and two percent hydrogen density contours.

Because of the inability to monitor the hydrogen penetration before combustion in the experiments, experiments without combustion were not performed. Hence the comparison in Fig. 6 of the noncombusting simulations with the combusting experiments is uncertain to the degree that the combustion affects the penetration. Prior to the analysis of the hydrogen injection, experiments and simulations were performed on the injection of methane (Nabers et al., 1994b), with and without combustion, using the same approach outlined in this paper. The properties of methane allowed for noncombusting penetration to be monitored. Results for KIVA simulations with combustion were obtained using a single oxidation equation with the forward reaction rate chosen to duplicate the autoignition time observed in the experimental pressure rise. For the methane simulations, good agreement with the data was found (Fig. 7), and little difference was observed between the predicted penetration with and without combustion.

The modeling of hydrogen combustion at the conditions in the SNL-CA experiments is not well understood. To assess the accuracy of existing models for the combustion of hydrogen, the KIVA simulations were repeated with the NASP hydrogen combustion kinetics (this 22 reaction set was developed by the National Aero-Space Plane, NASP, Program, NASP Technical Memorandum 1107, 1990). For the intended application, the NASP kinetics are considered to be the minimum set of reactions necessary to describe hydrogen combustion and are

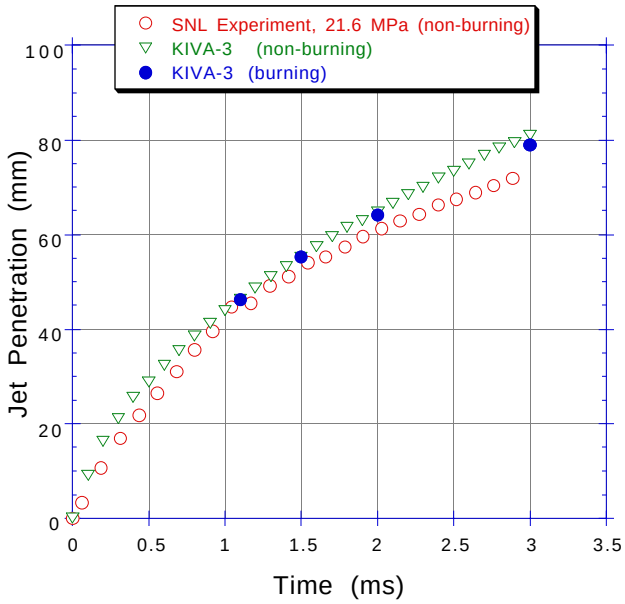


Figure 7. Comparison of the penetration history of the methane jet of the KIVA simulation and the SNL-CA experiments. The penetration in the KIVA simulations is based on the 1% methane density contours. A similar plot of data using 2% contours falls exactly on top of the data at late times.

an industrial standard for all NASP calculations. There are no free parameters in this model to modify to best fit the data.

Using the NASP reaction set, the hydrogen was observed to autocombust at 0.05 ms, in contrast to the experimentally observed value of 0.355 ms. Likely the large discrepancy is because the NASP reaction set is being applied outside of its intended range ( 0.05-5 atm versus 60-70 atm for the SNL-CA data). The discrepancy could also be due to the excessive mixing occurring in the coarse mesh used in the simulation. Until more appropriate kinetics for hydrogen combustion is available, the source of this discrepancy is uncertain.

In order to proceed with the determination of the effect of combustion on the penetration, KIVA was modified to duplicate the experimentally-observed ignition delay of 0.355 ms by preventing the combustion to occur until the desired time. This is a common approach for liquid fuel injection for diesel modeling (Allocca et al., 1994). The following was observed in the simulation: (1) the penetration with combustion is slightly higher than the penetration without combustion and the SNL-CA data (Figure 8), (2) the pressure rise compares well with the SNL-CA experiment to within 10 percent, (3) the flame front reaches steady state conditions very quickly (0.05 ms after ignition) as determined by the amount of unburned fuel, and (4) the 22 reaction set significantly increases the running time for the simulation (an increase of 5 over the simulation with no reaction). We note that the penetration in the simulation in the presence of combustion is difficult to determine. In an attempt to use the same criterion for both the combusting and noncombusting simulations, the total density was used to determine the penetration in the combusting case.

In the absence of an accurate reaction set for hydrogen combustion at the conditions encountered in the SNL-CA experiments, development of a single step kinetic reaction for hydrogen combustion was undertaken. A crude, single reaction may be sufficient for the following reasons. A primary motivation for using a complex reaction set is to describe the autoignition delay time, and it's dependence on operating conditions; but because the best available extended reaction set for hydrogen combustion, the NASP 22 reaction set, did not correctly describe the delay time within the KIVA simulation, there is no advantage in this regard over a single reaction with an enforced experimentally observed delay time. Another reason is that the turbulent mixing controls the combustion at all times except very early in the combustion, and the use of multistep kinetics is not warranted for most of the combustion history. The forward reaction rate in the single step reaction was chosen to best match the pressure rise in the combustion chamber.

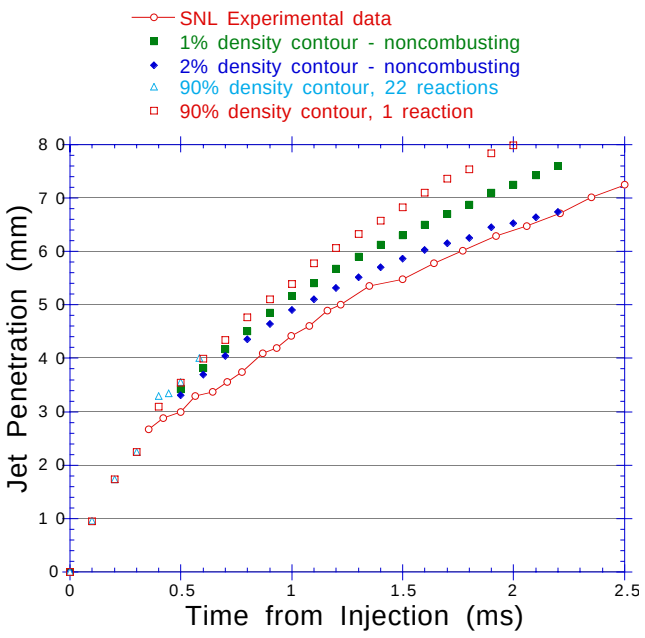


Figure 8. Comparison of the penetration history of the hydrogen jet of the KIVA simulation and the SNL-CA experiments. The penetration for the combusting KIVA simulations is presented for the maximum axial extent of the 90% total density contours. The penetration for the noncombusting simulation is as in Fig. 6.

Simulations with the one-step reaction for hydrogen combustion gave results that were similar to the NASP 22 reaction set (see Fig. 8) but executed 3.2 times faster, enabling the simulation to be extended to later times (the entire calculation took just over 3 hours on a CRAY YMP). The major difference between the two simulations was that the final pressure rise was slightly higher in the single step reaction. This difference can be attributed to the existence of intermediate species in the 22 reaction set that reduces the heat release, and hence the pressure rise. The single reaction simulation did not include the equilibrium chemistry package in KIVA because it is intended for combustion of alkanes. Had a comparable package been used for hydrogen combustion, we expect the pressure rise to be comparable, with little compromise of running time. We also note that although both of the simulations included the $NO_X$ reaction set, the experiments did not include $NO_X$ measurement so no comparisons were made.

Because the single reaction simulation can efficiently be run to a much later time, the question of the effect of combustion on the penetration can now be examined. In Figure 8, it appears that the penetration with combustion is comparable to the penetration without combustion and to the SNL-CA data. This conclusion must be qualified by the observation that the curves for the penetration were found to be dependent on the method used to track the front

of the gas cloud (observe the difference in the 1% and 2% curves in Fig. 6). No similar method could be found for both the combusting and noncombusting runs that was satisfactory, primarily because of the large difference in species concentration and temperature between the two simulations. Our current conclusion is that to within the uncertainty of determination of the penetration, the penetration is comparable. Consequently in future analysis of the penetration of hydrogen, the option is available to simulate the penetration of a combusting experiment with a noncombustion model.

## CONCLUSIONS

The current state of numerical modeling of gas injection is comparable to the early state of modeling of liquid fuel injection for diesel engines in the late 1970's. Given the increased understanding of the liquid injection problems over time, special techniques were developed to model accurately the problem on meshes of practical interest (Amsden et al., 1989). This report describes the comparable challenge of resolving the large disparity of length scales for gas injection and an approach to numerically modeling the problem.

From a simulation and analysis of the dynamics of the exit of the gas from the orifice, significant modifications of the exit conditions of the gas occur at a length scale about 1/200 the size of the combustion chamber and must be included in a realistic simulation of the injection process.

Many fully three-dimensional simulations were made of the SNL-CA experiments with methane and hydrogen injection, with and without combustion. The penetration history is found to be highly sensitive to the mesh refinement and the treatment of turbulence. Overall, the outstanding challenge of the modeling will be the description of the penetration history of the gas jet on poorly resolved meshes. The approach taken in this paper is to remove the details of the jet dynamics upon exit from the orifice and model the expanded jet on a coarser mesh. This approach reduces run times by a factor of 10. Reasonable agreement is obtained with hydrogen jet penetration data with a moderately resolved, three-dimensional KIVA-3 simulation. Current simulations are limited by execution time and computer memory in the duration and complexity of the problem that can be examined.

The combustion of hydrogen is examined using a single-step oxidation reaction and a 22-equation reaction model developed for the National Aerospace Plane program. Both reaction mechanisms require that empirical autoignition delay times be set in order to reproduce the experimental results. From these studies we conclude that: (1) the hydrogen jet penetration with combustion is comparable to the penetration without combustion, (2) the pressure rise and penetration compares well with experiments, (3) the two approaches to combustion perform similarly, with the single-step oxidation running 3.2 times faster and producing a slightly higher total pressure rise, (4) the hydrogen burning rate reached steady-state conditions very quickly and (5) the 22-reaction set without the imposed experimentally observed ignition delay severely underpredicts the autoignition time..

## ACKNOWLEDGMENTS

This work was funded by the Department of Energy Hydrogen Program under the direction of Dr. N. P. Rossmeissl. We wish to thank our colleagues for their insightful assistance: M. Sahota, T. D. Butler, and P. J. O'Rourke.

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