

Fuel-Air Mixing Characteristics of DI Hydrogen Jets

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ABSTRACT

The following computational study examines the structure of sonic hydrogen jets using inlet conditions similar to those encountered in direct-injection hydrogen engines. Cases utilizing the same mass and momentum flux while varying exit-to-chamber pressure ratios have been investigated in a constant-volume computational domain. Furthermore, subsonic versus sonic structures have been compared using both hydrogen and ethylene fuel jets. Finally, the accuracy of scaling arguments to characterize an underexpanded jet by a subsonic "equivalent jet" has been assessed. It is shown that far downstream of the expansion region, the overall jet structure conforms to expectations for self-similarity in the far-field of subsonic jets. In the near-field, variations in fuel inlet-to-chamber pressure ratios are shown to influence the mixing properties of sonic hydrogen jets. In general, higher pressure ratios result in longer shock barrel length, though numerical resolution requirements increase. While no scaling investigated in this work demonstrated ideal data collapse for penetration rates, the most effective scaling parameter included consideration of inlet-to-chamber density-ratio effects and pressure-ratio effects.

INTRODUCTION

Hydrogen is an attractive fuel for internal combustion engines because of its clean-burning properties relative to conventional hydrocarbon fuels. Several approaches to introduction of fuel into the combustion chamber have been employed in engines, including: carburetor, throttle body-injection, intake port injection, and direct in-cylinder injection (DI). Direct injection is particularly attractive in the case of hydrogen engines because it avoids the air displacement effect in the intake manifold. Such effects result in power loss and are more pronounced when using hydrogen rather than a typical engine fuel which possesses much greater energy density per unit volume. Additionally, DI permits greater control over the combustion process, thereby potentially allowing for circumvention of unpleasant combustion phenomena, such as pre-ignition and backfire. Backfire, which can occur in engines using premixed charge aspiration, happens when the fuel-air charge is ignited during the intake cycle and causes combustion in the intake manifold. A pre-ignition event is commonly defined as combustion taking place

prior to spark initiation in a spark-ignition (SI) engine. Generally, local high temperature regions are responsible for such occurrences.

Research efforts on optimization of DI hydrogen engines are ongoing. Part of the issue with such engines is that a number of properties of hydrogen are very different from those of conventional fuels. Thus, previous results from the existing body of literature on hydrocarbon fuel-burning engines do not necessarily hold true when considering hydrogen-air combustion. For example, the low ignition energy of hydrogen can cause pre-ignition and backfire [1]. Another unique property of hydrogen is its small surface quenching distance, as compared to that of hydrocarbon flames. This is one of the reasons why in SI engines hydrogen-air combustion employs a smaller spark gap [2]. A small quenching distance can also cause greater heat transfer to flame-impinging surfaces. Commonly, high local temperatures occur at places like the electrodes of a spark plug, exhaust valves, and at surface carbon deposits resulting from pyrolysis of lubricating oil. Such combustion chamber hot spots can result in pre-ignition. Thus, the small surface quenching distance of hydrogen increases the risk of pre-ignition in this sense, since this will cause the surface temperatures at the walls to be higher than observed with hydrocarbon fuels [1]. The third unique property of hydrogen worth noting is its wider flammability limits, which allow engines to run quite lean. This acts to control NO_x formation, which can be prohibitively high in stoichiometric hydrogen engines. Additionally, for equivalence ratios above 0.5 and boosted intake charge pressures Natkin et al. [3] found susceptibility to pre-ignition, providing an additional reason to take advantage of the extended lean flammability limit of hydrogen. In light of these facts, investigations on the characterization of mixing specifically for hydrogen are important.

Two parameters observed to have a significant influence on mixing in DI hydrogen engines are injection timing and pressure. One strategy for controlling pre-ignition in DI engines is to delay start of injection (SOI). However, this is hard on the injection system, which must then endure a severe thermal environment in addition to injecting into a high pressure chamber [1, 4]. Also, when using late injection strategies to avoid pre-ignition, the charge will be

more stratified the later SOI occurs. If the charge remains significantly heterogeneous at ignition, incomplete combustion can occur. Locally richer regions can lead to formation of significant amounts of NO. In the recent work of Wallner et al. [5] the effect of injection timing on mixture distribution in a hydrogen engine and the resulting effects on emissions and engine efficiency have been investigated. At low engine loads, late injection has been found to increase NO_x, while lower NO_x levels are observed using early injection. At higher loads it is suggested that this trend is inverted. Higher amounts of unburned hydrogen are shown for increasing stratification in the study, though indicated efficiency remained virtually unchanged with delayed SOI. However, optimization of nozzle design has been shown by the authors to mitigate NO_x emissions while maintaining efficiency. Another study detailing the challenges of mixture formation with late injection has been presented by White [6]. These qualitative experimental investigations examine the consequences of varying the injection pressure from a choked flow nozzle. It was observed that both injection timing and injection pressure are significant parameters, and are important in predicting mixture distribution in a hydrogen engine. Koyanagi et al. [7] have shown that using higher injection pressures in a hydrogen DISI engine results in more stringent conditions for spark plug placement. This is due to a reduction in the “window of opportunity” for spark initiation. Hydrogen diffusion in the radial direction was diminished near the spark gap location with increasing injection pressure, resulting in hydrogen concentrations approaching the upper flammability limit more rapidly. Also, higher jet penetration was observed with increasing injection pressures. Aside from injection timing and pressure, other parameters shown to significantly influence mixing of hydrogen jets are nozzle geometry and placement. In conclusion, the mixing characteristics of DI hydrogen engines with regards to optimization of engine efficiency are a subject of ongoing interest.

It is difficult to isolate the various effects on mixing in an engine, where the chamber pressure and temperature conditions change during the period of injection and combustion. Therefore, many jet studies investigate mixing in constant-volume chambers. Among such studies, there has been extensive work on examining the fundamental mixing characteristics of transient turbulent jets, particularly entrainment [8-12]. Several different methods for calculation of entrained mass have been presented in these studies. In the work of Tomita et al. [12] the authors examined both combusting and non-combusting hydrogen jets issuing into ambient air. It was found that a transient jet can be separated into two portions: a head vortex region downstream and a quasi-steady portion upstream. The rate of mass entrainment of the head region has been noted to decrease with time, while that of the quasi-steady part remains constant. Total mass entrained using the presented theory agreed well with the experimental results the authors obtained.

While the classical theory of jets issuing into quiescent air is useful for application to DI engines in general, an additional consideration arises when applying such studies to hydrogen engines. In the review paper by White et al. [13], the authors draw attention to the fact that hydrogen injection is usually designed to be sonic with high mass flow rates due to the need for rapid mixing, and to compensate for late injection strategies. Capturing the details of an underexpanded jet is difficult computationally, since there are such a wide range of flow scales to be considered. In the modeling work of Johnson et al. [14] on hydrogen jet injection and combustion, the ratio of length scales in their consideration of underexpanded jets was approximately 4,000. Similarly, it is difficult to capture the range of small/large scale effects experimentally as well.

The generalized configuration of the near-field of an underexpanded jet is well documented [14-24], a simplified model of which is presented in Fig. 1. Notice the various structures, some of which require 3-D modeling in order to provide a truly accurate representation. The flow at the exit plane of the nozzle is assumed to be choked, i.e. $Ma=1$. Immediately upon exit from the nozzle the high ratio of exit pressure to surrounding pressure causes expansion of the gas. Flow subsequently accelerates, thereby generating expansion waves. When these expansion waves meet at the outer boundary they are reflected as compression waves. Finally, these compression waves coalesce to form an oblique shock structure of barrel shape. This structure encloses a supersonic flow region termed the “zone of silence”, wherein it is assumed that no entrainment takes place, i.e. the mass flux at the nozzle exit is conserved throughout this region. For an exit pressure to ambient pressure ratio above approximately 2, the barrel shock culminates in a disk-shaped normal shock called a “Mach disk” and a reflected shock [20]. At sufficiently high pressure ratios this process may repeat several times, resulting in a succession of barrel and normal shock structures. Downstream of the final Mach disk the flow is subsonic, with the adjacent flow from the reflected shock remaining supersonic.

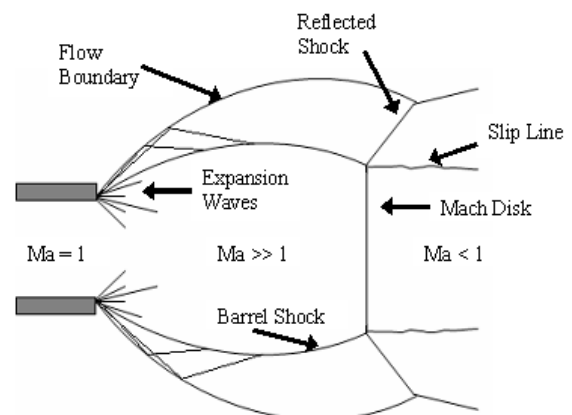


Figure 1. Principal regions around nozzle exit for an underexpanded jet.

Following the abrupt change of density after the Mach disk, pressure in the subsonic flow is assumed to be consistent with that of the surroundings. In the computational study by Mate et al. [15], a trapped vortex with a recirculation zone was observed beyond the Mach disk. It was theorized that the sudden outward deflection of flow from the normal shock at their symmetry axis was responsible. However, it remains unclear whether this structure was due to the computational setup of their axisymmetric model formulation. Beyond the Mach disk and after the flow becomes subsonic the jet behavior begins to conform to expectations based on subsonic flow theory. A potential core region emerges, followed by a transitional section, and finally a fully-developed flow conforming to well-known similarity solutions for classical free jets.

From the previous discussion it is apparent that accurate computational prediction of an underexpanded jet is difficult due to the widely divergent scales of the problem. Various techniques have been employed to overcome this problem, including: a “divide and conquer” approach, use of scaling arguments based on conservation equations, and combinations of scaling arguments employed in conjunction with classic free jet theory. The “divide and conquer” technique was used by Johnson et al. [14] in his computational modeling of choked-flow hydrogen jets. This procedure involves dividing the flow into sections, where the inflow parameters of a later section are obtained from the outflow of the previous section. In their study, separate computations for flow within the nozzle, the expansion and cooling in the near-field region, and the subsequent subsonic processes were carried out. This acted to remove the smallest length scales from the far-field jet penetration and combustion problem that was of primary interest.

The approach taken by Ra et al. [23] in regards to underexpanded jets was to computationally solve only for flow a certain distance downstream from the Mach disk. In the expansion region scaling properties are used that are based on the assumption that the pressure is the same as that of the chamber, and temperature at the exit of the Mach disk is the same as that in the nozzle. The authors then employed a theoretical gas jet model to estimate flow variables immediately following the Mach disk in order to begin their simulations with a subsonic jet of relatively larger diameter, thereby reducing the length scale ratio of the problem. Although it was shown that computed penetration lengths agreed reasonably well with experiments for this setup, in the work of Johnson et al. [14] a temperature decrease of about 12% in the expansion region has been reported previously. Thus, neglecting temperature change in the expansion region can limit the effectiveness of such an approach, since it may significantly alter the ignition properties.

By far the most popular technique for dealing with the expansion region in underexpanded jets is to use scaling based on conservation principles in the expansion region to define inlet flow conditions for a subsonic “equivalent jet”. This is an improvement on the previous method in

that, except for the expansion region, the jet structure is resolved and computationally computed. Experimental studies have used this approach to compare variables such as penetration and axial velocity decay in the downstream region from a choked nozzle [16, 17, 20, 22, & 24]. Likewise, computational studies use this “equivalent jet” idea to compute theoretical inlet conditions for a sonic jet to be used in subsonic calculations [21, 19]. One problem which arises with this method is estimating the downstream distance at which the scaled inlet conditions hold. While experimental data may be fit to classical jet theory through visual examination, for good accuracy it is necessary to know this a priori when setting up computational simulations. Empirical relations for barrel lengths have been proposed, however, such relations are of questionable global accuracy and do not take into account the fact that multiple shock structures may exist for a given exit-to-chamber pressure ratio.

Scaling theories characterizing an “equivalent jet” used in an effort to neglect the expansion region of sonic jets vary in the literature. Simple conservation of mass and momentum has been used heavily in the past under a range of temperature and pressure assumptions in the expansion region [17, 19-24]. However, in the work by Yuceil et al. [16] the authors express concern with these studies since they do not take into account enthalpy change through the expansion region. Also, studies which provide scaling only for the diameter of the “equivalent jet” without attention to other gas parameters such as temperature are called into question. A new scaling technique more rigorous in nature has been proposed [16]. Using this, theoretical centerline parameters for an “equivalent jet” have been successfully compared by the authors to results obtained experimentally. This method, along with previous scaling techniques, will be revisited later in the current work. Additionally, the importance of capturing the near-field for prediction of downstream structure will be addressed.

It has been discussed here that there is currently a need for greater understanding of the mixing process undergone by sonic hydrogen jets. The most obvious application of such studies is in DI internal combustion engines. The character of the mixture within the combustion chamber has ramifications on the ignitability at any given region. However, the discussion of sonic hydrogen jets is not limited to engine applications only. Harstad and Bellan [25] provide a detailed discussion on the safety implications of gaseous hydrogen leaks from high pressure vessels. Challenges to such work remain for the reasons discussed above.

In the present study we compare mixing, penetration, and spreading of hydrogen and ethylene jets in a constant-volume chamber. Parameters that are varied include the injection pressure and fuel. Mixing has been characterized herein by examining the evolution of lean, flammable and rich fractions of fuel, and their spatial distribution in the chamber. Penetration length and axial decay of velocity are examined.

The following section provides a description of the problem setup and solution methodology employed. Subsequently, results for a sonic hydrogen jet computation using different domain resolutions are discussed. A comparison of sonic hydrogen jet simulations having three different exit-to-chamber pressure ratios is then presented. Next, investigation into the effect of fuel type, specifically hydrogen versus ethylene, and exit Mach number on results is carried out. Finally, comparison of case results using various “equivalent jet” scaling techniques is undertaken. The paper closes with highlights of major findings.

COMPUTATIONAL SETUP

Computations have been performed in a constant-volume chamber using an axisymmetric version of a multidimensional code with sub-models for turbulence and wall boundary layers [26]. The code solves the RANS equations for compressible flow using a semi-implicit finite-volume method. Time derivatives are approximated using a first-order backward-difference method. Spatial derivatives for diffusion terms use a second-order accurate central-difference approximation, while spatial derivatives for the convective terms use a first-order upwind-difference method. The standard k-turbulence model with wall functions for heat and momentum fluxes at the wall is employed herein. All flows are modeled as gaseous, non-reacting in the current work. Mixture-averaged diffusion coefficients are used for the species diffusion model.

The computational domain, illustrated by Fig. 2, has been specified as an axisymmetric, constant-volume chamber of dimensions 24 cm by 5 cm in the axial and radial directions, respectively. A 1-degree slice is considered in the azimuthal direction. The orifice, shown at the bottom of the left wall, is set up as an inflow boundary. The remaining portion of the left boundary, as well as the top boundary, are no-slip wall surfaces. The axial line of symmetry is located at the bottom of the domain. The remaining right-hand boundary has outflow conditions imposed.

The grid is structured and stretched in both the axial and radial directions. The aspect ratio of the grid cells varied based on stretching, but did not exceed 60 and 32 in the axial and radial directions, respectively. With the exception of resolution studies, the grid is comprised of 160 cells axially and 60 cells radially. The number of cells in the orifice varied. However, resolution in the region has been held to be approximately 0.1 mm in all simulations (save the resolution studies). At least two cells resolve the orifice radius in all cases. Although resolution studies have been undertaken, it is not the intention of this study to fully resolve the expansion region of the underexpanded jets considered herein. Thus, shocks appearing in these regions are expected to be smeared in nature.

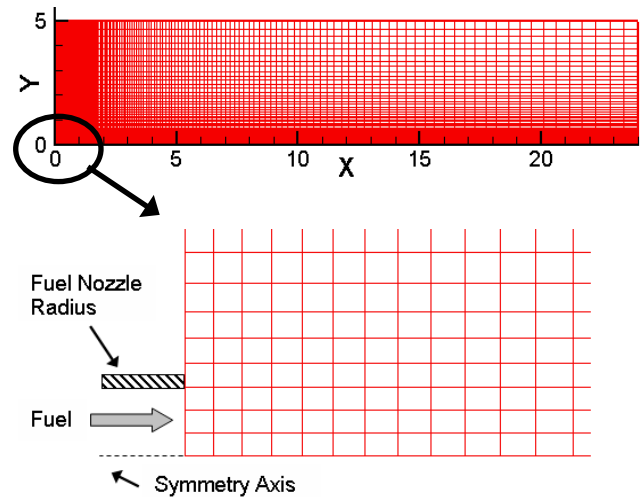


Figure 2. Axisymmetric computational domain employed – dimensions shown in units of centimeters.

Initial conditions within the chamber are identical throughout all of the cases considered herein. Quiescent air at a temperature of 330 K and density of 10 kg/m³ is prescribed. Note that the inflow pressure of subsonic jets has necessarily been set to equal that of the chamber.

It is the intention of this study to compare simulations having equal mass and momentum flow rates at the inlet of the orifice. Mass flow rates between cases are calculated according to Eq. (1), while momentum flow rates are computed through Eq. (2), noting that the velocities in the surroundings are zero initially. The variables ρ , V , and A represent density, velocity, and area, respectively. Subscripts 1 and 2 designate different simulations, while e and a represent conditions at the nozzle exit and in the surroundings, respectively. A 3-millisecond injection duration is taken for all cases, whereupon the fuel inlet is closed and the existing jet continues to penetrate into the domain. The orifice diameters are therefore different among the cases.

$$\rho_{e,1} V_{e,1} A_{e,1} = \rho_{e,2} V_{e,2} A_{e,2} \quad (1)$$

$$\rho_{e,1} V_{e,1}^2 A_{e,1} + A_{e,1} (P_{e,1} - P_a) = \rho_{e,2} V_{e,2}^2 A_{e,2} + A_{e,2} (P_{e,2} - P_a) \quad (2)$$

Ideal gas behavior is assumed in all calculations. However, it should be noted that theoretical inaccuracy results from representation of near-field sudden expansion of hydrogen under the ideal gas assumption. A unique property of hydrogen is its low inversion temperature, the point at which the Joule-Thompson (JT) coefficient equals zero. For temperatures higher than the inversion temperature of a given gas the JT coefficient is negative, and thus temperatures increase as gas expands in a throttling process. This means that in reality hydrogen gas exiting from a blowdown tank initially heats, rather than cools as suggested by the ideal gas equation of state. For atmospheric and 5000 psi (~ 345 bar) pressures the inversion temperature of

hydrogen is approximately 202 and 125 K, respectively [27]. All of the nozzle exit conditions employed in this paper fall within this range. Therefore, it is expected that temperature representations very near the nozzle exit will have errors related to the ideal gas assumption. Nevertheless, according to Schefer et al. [22], to a good approximation hydrogen jets issuing from a high pressure reservoir may be treated as ideal with regards to using the isentropic relations – for reservoir pressures up to approximately 172 bar. Thus, exit pressures have been held below this value in the current work to reduce the level of error. However, since spatial resolution near the nozzle is known to be inadequate for capturing details of the shock-containing near-field anyway, error in temperature field measurements is already known to exist in this region.

RESULTS AND DISCUSSION

This section presents results for the jet mixing cases outlined in Table 1. Recall that all of the 8 cases deliberately employ the same inlet mass flux. Also, the first 5 cases have the same inlet momentum flux, while the last 3 have 2 ½ times that of the previous 5 cases. Due to the disparity in molecular weights of the two fuels considered, i.e. hydrogen and ethylene, for some cases it is necessary to have a high inlet temperature in order to match the mass and momentum inlet conditions between simulations. While it is physically inaccurate to assume that no reactions take place at elevated temperatures, such as those of Cases 5 and 7, for all simulations a non-reacting flow is assumed in order to offer mixing comparisons for jets with equivalent mass and momentum flow rates.

Discussion of the data begins with an examination of resolution effects for the first sonic hydrogen jet case listed in Table 1. Following this, the consequences of variation of exit-to-chamber pressure ratio on sonic hydrogen jets is considered. The third portion of this section contrasts the behavior of hydrogen jet mixing with that of hydrocarbon jets, specifically ethylene, using different exit Mach numbers. Finally, various existing scaling theories for characterization of sonic jets have been compared.

SONIC HYDROGEN JET - RESOLUTION STUDIES

In this section results for a sonic hydrogen jet with a nozzle exit-to-chamber pressure ratio (i.e. P_e/P_a) of 5.56 will be compared for three cases employing different resolution. Details of the inlet conditions are given in Case 1 shown in Table 1. A baseline simulation, having a cell size of 0.1 mm near the fuel inlet, is initialized with 160 x 60 cells in its domain. A fine resolution case employing a 50% increase in mesh density has been set up with a cell size of 0.075 mm near the inlet. Finally, a coarse resolution case, whose near-orifice cell size is increased to 0.2 mm, is carried out. Multi-dimensional computations in engine chambers typically employ even coarser resolution. Comparisons will first be made in the far-field in order to assess variation in the self-similar region. This will be followed by a comparison in the near-field region, which contains a shock structure.

Penetration of the jets was computed 2 ms into the simulation during the period of constant fuel injection. Note that the method of defining axial penetration employed herein makes use of the expected theoretical steady-state profile for the centerline velocity normalized by the inlet velocity, as shown in Eq. (3),

$$\frac{U_{centerline}}{U_{inlet}} = \frac{C}{x/d_e} \quad (3)$$

Penetration is taken at the axial location where the velocity becomes 70% of the theoretical centerline velocity for a steady jet. In Eq. (3), C denotes a constant, x is the axial distance from the jet, and d_e is an effective diameter, which weights the value of the inlet diameter to account for the density ratio of the inlet fluid to the ambient gas, i.e. $d_e = d_{exit}(\rho_{exit}/\rho_a)^{0.5}$. Suggested values for the constant, C, have been estimated from both experimental and computational fits to data, with reported values ranging from 5.1 to 8.6 [11, 28-30]. For the three cases considered here a value of approximately 8 was found to produce the best fit to the velocity data profiles.

Table 1: Cases with specified fuel nozzle exit conditions: pressure, Mach number, temperature, density, velocity, and diameter.

Case Description	Pressure/Mach Number	Temperature	Density	Velocity	Diameter
1. Sonic H ₂	P _e =52.66 bar	249 K	5.128 kg/m ³	1203 m/s	0.06 cm
2. Sonic H ₂	P _e =21.47 bar	320 K	1.63 kg/m ³	1363 m/s	0.10 cm
3. Sonic H ₂	P _e =113.5 bar	229 K	12.04 kg/m ³	1153 m/s	0.04 cm
4. Subsonic H ₂	Ma=0.890	788 K	0.292 kg/m ³	1903 m/s	0.20 cm
5. Sonic C ₂ H ₄	P _e =56.65 bar	3527 K	5.42 kg/m ³	1139 m/s	0.06 cm
6. Sonic C ₂ H ₄	P _e =25.24 bar	700 K	12.17 kg/m ³	507.2 m/s	0.06 cm
7. Subsonic C ₂ H ₄	Ma=0.858	2150 K	1.486 kg/m ³	762.9 m/s	0.14 cm
8. Subsonic H ₂	Ma=0.805	154.5 K	1.486 kg/m ³	762.9 m/s	0.14 cm

Note that since the barrel lengths of the shock structures, as well as that of the potential core, were found to differ in the near-field region it was necessary to shift the subsonic theoretical velocity profile to the right in order match the computational data. This is demonstrated in Fig. 3, where the normalized velocity profile of the steady jet has been adjusted to fit the transient profiles of the baseline and fine resolution cases in the self-similar region. Also shown in Fig. 3 is the line denoting 70% of the steady velocity profile, from which the penetration length is estimated. Adjusting the axial start location of the steady jet to conform to that of the transient profiles, analysis shows that penetration is 1.3% higher for the fine resolution case compared to the baseline case at 2 ms; while the simulation employing coarse resolution varies less than a percent from that of the baseline case when a corrected steady jet profile is employed.

Aside from penetration rate, another parameter of interest in the self-similar region of the jet is the spreading rate. This is computed as the change in the value of the half-width, $r_{1/2}$, with x , where $r_{1/2}$ is the radial distance at which the velocity is half of the centerline velocity. Table 2 presents the results for the average spreading rate dependency on resolution effects during the period of injection. The coarse resolution case is 8.6% below the baseline case, whereas the fine resolution grid is about 7% higher. Use of the standard $k-\epsilon$ model to compute spreading rates in round jets has historically been shown to over-predict measured values, which lie within the range of 0.086-0.096 [31]. It should be noted that the values shown in Table 2 under-represent the expected solution from a self-similar round jet with $k-\epsilon$ model turbulence representation. In an effort to understand this, initial values for the kinetic energy and dissipation rate were varied up to an order of magnitude. However, no significant deviation from the spreading rates represented below was observed. In the work of Magi et al. [32] the spreading rates of a round jet computed using the standard $k-\epsilon$ model were found to increase by 10% when the resolution was tripled near the nozzle exit. Variation in spreading ranged from 0.102, with 12 cells resolving the orifice, to 0.110, for 36 cells located within the diameter of the nozzle. Thus, it is thought that the lower values observed here may be due to low resolution effects (even for the “fine resolution” case).

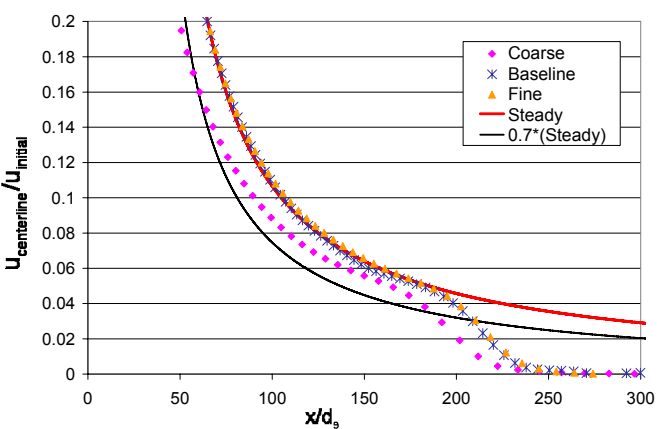


Figure 3. Centerline-to-inlet velocity ratio comparison of three resolution cases at 2 ms, along with normalized velocity profiles of a theoretical steady jet and 70% of the steady jet magnitude. Note that the steady jet has been adjusted axially to conform to initial profiles of the baseline and fine resolution cases in the present plot.

Table 2: Average spreading rate dependency on resolution – computed 2 ms after SOI.

Resolution	Grid Resolution	Spreading Rate
Coarse	80 x 30	0.0821
Baseline	160 x 60	0.0898
Fine	240 x 90	0.0961

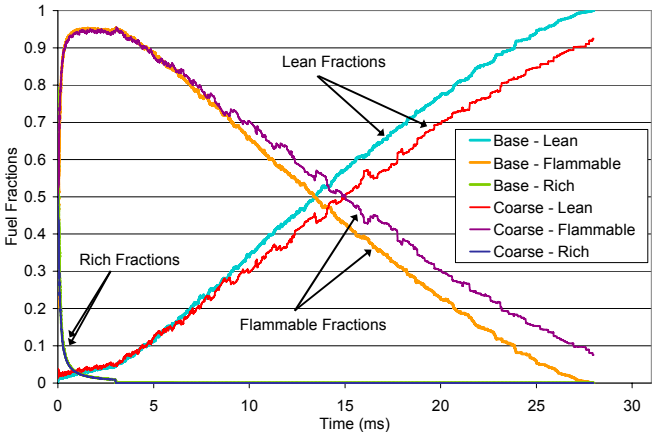


Figure 4. Temporal evolution of fuel fractions within domain for baseline case compared with coarse resolution case.