

NUMERICAL INVESTIGATION OF NATURAL GAS DIRECT INJECTION PROPERTIES AND MIXTURE FORMATION IN A SPARK IGNITION ENGINE

by

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In this study, a numerical model has been developed in AVL FIRE software to perform investigation of direct natural gas injection into the cylinder of spark ignition internal combustion engines. In this regard two main parts have been taken into consideration, aiming to convert an MPFI gasoline engine to direct injection natural gas engine. In the first part of the study of multi-dimensional numerical simulation of transient injection process, mixing and flow field have been performed via three different validation cases in order to assure the numerical model validity of results. Adaption of such a modeling was found to be a challenging task because of required computational effort and numerical instabilities. In all cases present results were found to have excellent agreement with experimental and numerical results from literature.

In the second part, using the moving mesh capability the validated model has been applied to methane injection into the cylinder of a direct injection engine. Five different piston head shapes along with two injector types have been taken into consideration in investigations. A centrally mounted injector location has been adapted to all cases. The effects of injection parameters, combustion chamber geometry, injector type, and engine rpm have been studied on mixing of air-fuel inside cylinder. Based on the results, suitable geometrical configuration for a natural gas direct injection engine has been discussed.

Key words: *compressed natural gas direct injection, spark ignition, mixture preparation, engine revolution per minute*

Introduction

In general, flow field inside the cylinder is quite complex. Direct injection of fuel makes it even more complex, and the situation turns more complicated with gaseous fuels. In fact mixture formation with natural gas due to its low density is more critical in comparison to liquid fuel engines. The reason is even very high injection velocities produce low fuel penetration, and consequently poor mixture formation. Thus mixture formation in gas engines depends more on in-cylinder charge motion than in gasoline engines [1].

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To enhance natural gas (NG) fuel penetration in cylinder, very high fuel rail pressures of up to 200 bar are used. Such an elevated pressure can also help increase the turbulence level of mixture and the overall fuel-air mixing.

Very high pressure ratios between fuel rail and in-cylinder cause the flow at injector exit to be typically under-expanded. That means the flow becomes sonic at nozzle exit and undergoes a complex pattern of shock-expansion waves downstream from the nozzle exit.

Accurate capturing of such a pattern in the near field has been shown to strongly affect the complete jet shape and mixture formation downstream from the nozzle [2]. Huang *et al.* [3-6] conducted a set of experimental studies on different injection and combustion characteristics of NG using a rapid compression machine and also a NG fuelled engine.

Numerical investigations of the flow in these engines have been focused on different challenges of modeling. Multi-dimensional modeling with focus on turbulence modeling has been performed in [7-9]. The evolution of gas jet injection is studied in [7, 10, 11].

Li *et al.* [2] have conducted a 2-D numerical modeling as well as method of characteristics to study under-expanded gas injection into the cylinder of a large bore engine. In the study, it has been reported that main parameters determining the type of flow exiting from a sonic nozzle are the pressure expansion ratio and the nozzle geometry. It has been mentioned that accurate computation of the flow at the nozzle exit is of main importance because it controls the jet mixing downstream from the nozzle.

In the same study and also in [11, 12] the grid density at the nozzle exit has been discussed. It has been reported that a minimum of about 10 cell layers is necessary for accurate capturing of flow field in the near field.

Ouellette and Hill [11] have studied turbulent transient methane and air injection into a constant volume chamber. A multi-dimensional numerical as well as experimental investigation has been performed on subsonic and sonic jets emerging from a single nozzle into the chamber. Numerical modeling tool used in the study has been the KIVA code and jet shape and penetration have been presented in different cases.

A virtual nozzle approach has been used in modeling the injection instead of computing the detailed near field flow in [10, 13-15]. Such cases have their inlet boundary condition set at the mach disc in nozzle exit, and thus the inside injector space is eliminated. This method results in decreased grid density at nozzle exit but is limited to two dimensional slot and hole injector geometries. It also requires accurate data about mach disc size and location.

In [1] an idea of fictive gas droplets has been introduced into a numerical model in Quicksim software to reduce the grid number requirements of the modeling. Also in [16] a phenomenological model has been implemented along with KIVA code to predict the quantities of the flow in the near field.

It could be concluded from the literature that the most accurate approach is to include inside-injector space into computations. Such an approach is followed by [17-20]. In [17] a multi-dimensional modeling approach has been undertaken using STAR-CD software. A centrally mounted outwardly-opening Injector has been implemented in the model and injection and mixing has been studied in different poppet-valve chamber geometries. The injection process has also been studied in a type of single-cylinder research engine.

In authors previous publications [19, 20] the evolution of gas jet into the cylinder of a direct injection engine has been studied using AVL FIRE software. The effects of injection and combustion chamber geometry have been investigated in these studies using different types of

injectors. Different injection variables have been studied and suitable configuration for each case has been discussed.

Present work

It has been intended to convert an existing 1800 cm³ MPFI gasoline engine to direct injection NG engine with minimum modifications. In this regard an extensive numerical modeling has been performed on the transient injection process, mixing and flow field. Table 1 illustrates the basic characteristics of the engine and a view of the base engine geometry has been shown in fig. 1. The objective has been to determine a suitable configuration for the piston head geometry with regard to injector location and also to investigate the effect of injector type for the application.

In order to perform modeling, two injector types of single-hole and multi-hole have been chosen. The multi-hole injector has 6 equally spaced nozzles with a 30° bend angle to the axis. Both injectors are centrally-mounted and exhibit inwardly opening needle. It has been intended to use stratified charge mixture preparation strategy in the modifications to achieve better fuel economy as declared in [1, 17].

The study has been conducted through two main parts. Firstly, a couple of validation cases have been performed in order to make sure the numerical model can predict the injection and flow physics adequately. Secondly, flow inside a real engine cylinder has been studied aiming to get a flammable stratified mixture. In this part different combustion chamber geometries along with the two injector types have been considered and injection and mixture formation in each case has been investigated. Finally, to determine the effects of engine speed on mixture preparation, a set of investigations have been performed on selected combustion chamber geometries at different engine speeds.

Mixing performance of any injector-geometry configuration is obtained by realization of flammable mass fraction inside cylinder [19]. The values of 0.8 and 1.4 on RAFR have been chosen for flammability limits as suggested in the same study. The mixture in each cell is categorized in three different levels of lean, flammable, and rich. Flammable mass fraction is defined on this basis.

Numerical model development

Generally the NG injector holes are of very small diameters of typically less than 1 mm. Such a small diameter could lead to a staggering difference of order 1000 between nozzle and cylinder length scales. Detailed numerical calculation of flow inside such a small nozzle requires a significant computational effort. One of the most important variables which affect the numerical model ability in correct flow prediction is the number of grid points across nozzle diameter. The study of Chiodi *et al.* [1] has been taken into consideration to investigate this effect. The modeling conditions are shown in tab. 2. In this case a couple of numerical models with different number of grid points across the nozzle diameter have been generated.

Table 1. The base engine characteristics

Bore	83 mm
Stroke	81.4 mm
Displacement volume	440 cm ³ /cyl.
Connecting rod length	150.15 mm
Compression ratio	9.5



Figure 1. A view of base engine geometry and ports

Table 2. Injection conditions [1]

Injected fluid	Methane
Chamber fluid	Air
Fuel rail pressure	8 bar
Chamber pressure	1 bar
Chamber temperature	300 K
Duration of injection	1.2 ms
Fuel mass flow	270 mg/s

The results for jet penetration and mach disk location for time 0.1 ms after start of injection (SOI) have been plotted against number of grid points across the nozzle for all cases. The most critical flow phenomena occur near the nozzle exit so variables at first time step have been checked for grid independency. In the first time step the flow has not been developed into the cylinder and most of the fuel is in the near field of injector exit. Figure 2(left) shows penetration in different cases for this test. The mach disk location has been measured on cylinder axis downstream from the nozzle exit and is depicted in fig. 2 (right).

It could be seen from fig. 2 that penetration shows increases with increase in number of grid points up to 10 layers; after which the difference in penetration is not significant. Similar trend could be seen in the variations of mach disk location. This indicates that 10 cell layers are the adequate resolution for grid-independent numerical simulation of compressed natural gas (CNG) injection which agrees with results of [2].

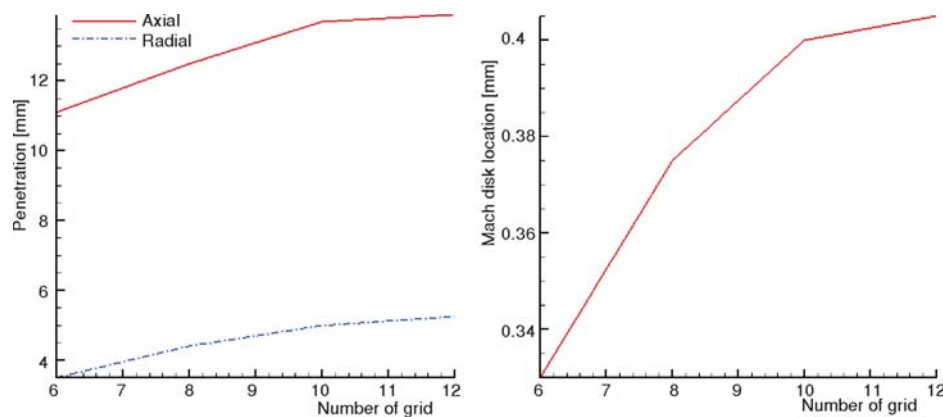


Figure 2. Variations of jet properties using different number of grid points across the nozzle diameter; left: axial and radial penetration, right: mach disk location

It is necessary to have very fine grids near the nozzle exit and coarser grids far from the nozzle to have reasonable total grid number. So it is very important to vary the cell size between these levels smoothly. That means any jump in cell size should be controlled at a reasonable level. To avoid numerical instability the “transition layer” should be located at least 8~10 times the nozzle diameter downstream from the nozzle. A graphical representation of the transition layer is shown in fig. 3.

It has been found that locations of transition layers for successive coarsening of the cell size have little effect on numerical stability. Also the first transition layer in radial direction should be located 2.5~3.5 times the nozzle diameter measured from the cylinder axis. On the other hand inlet boundary should be located far upstream from the nozzle exit to avoid critical condition. This condition is more realized in under-expanded nozzles.

To assure the model accuracy and robustness in injection calculations three cases of validation have been performed based on literature available data. These validation cases have been chosen to test the numerical model ability to comply with different injection conditions and different geometries. Such differences necessitate the use of different grid size and topology for each case.

Validation case 1

A constant volume chamber with a centrally mounted injector similar to that of Ouellette *et al.* [11] has been used to build up a numerical model. A total number of about 380000 hexahedral/hybrid grid cells have been generated. Three transition layers have been used to coarsen the mesh inside the chamber. The injection conditions are listed in tab. 3 and boundary conditions are set based on data. The numerical model with the given condition has been developed in AVL FIRE software and injection modeling of methane gas into air has been undertaken. A snapshot of flow field near nozzle exit is shown in fig. 4 (right). One can easily see the complex pattern of flow with a mach number about 1.0 at the inlet boundary and a maximum mach number of 3.24 about one millimeter downstream of the nozzle exit. The flow field captured agrees with the graphical representation presented in Ouellette and Hill [11] as shown in fig. 4 (left).

It has been found that a minimum of eight times the nozzle diameter, *i. e.* 4 mm in this case, is necessary for the injector length to avoid critical conditions at inlet in under-expanded

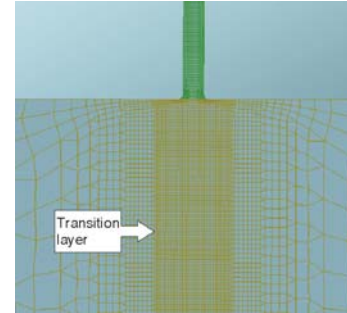


Figure 3. Transition location of transition layer and Inlet boundary with respect to nozzle

Table 3. The injection conditions for first validation case [11]

Chamber dimensions	Radius: 20 mm, Length: 90 mm
Injection pressure and temperature	$P_{0,inj} = 15 \text{ MPa}$, $T_{0,inj} = 350 \text{ K}$
Chamber pressure and temperature	$P_{0,ch} = 5 \text{ MPa}$, $T_{0,ch} = 850 \text{ K}$
Wall temperature	$T_w = 450 \text{ K}$
Nozzle diameter	$d_N = 0.5 \text{ mm}$
Injected mass	3.5 mg
Turbulence level	$1.5 \text{ m}^2/\text{s}^2$

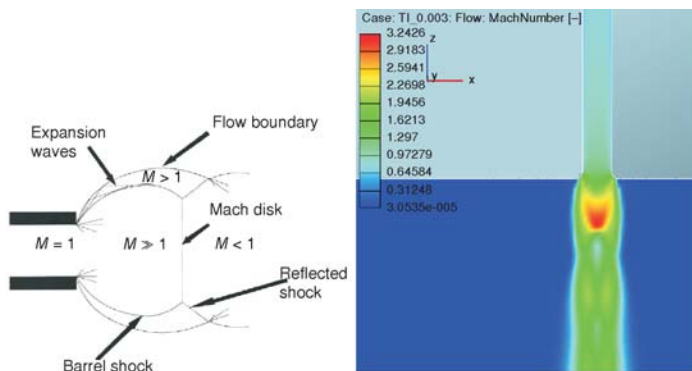


Figure 4. Flow pattern in under-expanded flow; graphical representation (left) [11], calculated representation (right)

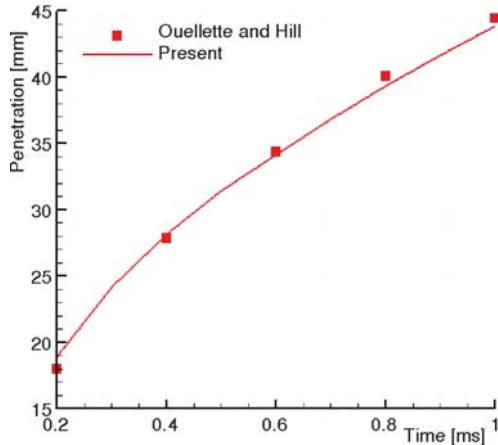


Figure 5. Comparison of jet penetration for first validation case

Table 4. The modeling conditions for the second validation case [16]

Injector diameter	0.82 mm
Mean injection pressure P_{inj}	4.94 bar
Injection temperature	298 K
Environment temperature	295 K
Environment pressure	1 bar
Environment fluid	Air
Wall distance from nozzle	15.5 mm
Injected fluid	Air
Reynolds number	60000
Chamber dimensions	100 × 100 × 15.5 mm

A numerical model has been developed in AVL FIRE and air injection into a chamber filled with air has been modeled. Nearly 450000 grid cells were generated. The results of jet penetration across the plate are shown in fig. 6. It could be seen that there is excellent agreement between the results.

Validation case 3

In order to check the numerical model in a real injection process it was decided to model the case of direct methane injection in set-up of [1]. The gas has been injected into a pressure

flow cases. Figure 5 shows a comparison of the results for jet tip penetration along injection axis for this case. As it could be seen there is very good agreement between the results.

Validation case 2

In direct injection of CNG into the cylinder impingement of jet to the piston head is inevitable. The impingement of jet to piston head affects the jet shape and its induced flow field inside cylinder. It also makes a radial motion of flow towards cylinder walls. This can make the flow quite different and it would be necessary to study the effects of gas jet impingement to the walls. In this regard the numerical study of Andreassi *et al.* [16] and experimental study of Tomita *et al.* [21] have been considered. 10 grid cells in the nozzle throat have been used and grids are coarsened in 3 stages downstream of the injector nozzle. The injection conditions in this case are shown in tab. 4.

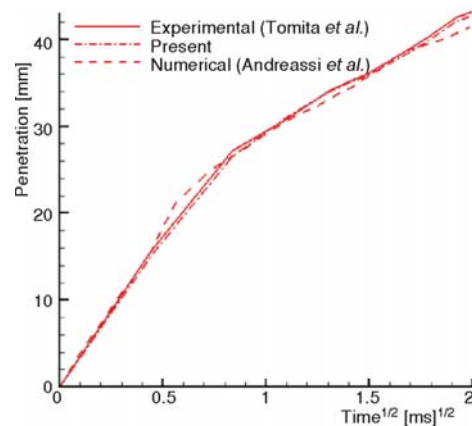


Figure 6. Comparison of jet penetration for different cases in second validation case

chamber with simple cubic geometry of 200 mm in edge length. The chamber is filled with air. The modeling conditions are presented in tab. 2. A total of approx. 290000 computational cells have been generated.

The case has been developed in AVL FIRE and methane jet penetration into the media has been measured. Figure 7 shows a comparison of jet penetration downstream from the nozzle in all cases. It could be seen that there is excellent agreement between the experimental and numerical results.

Model application and results

The 3-D validated numerical model has been applied to the simulation of methane direct injection into different engine combustion chambers with real-like moving piston. In this context the effect of two injector types of multi-hole and single-hole as well as five piston-cylinder head configurations has been studied on mixture homogeneity and air-fuel ratio distribution into the cylinder. A centrally mounted injector location has been adapted to all cases. To better understand the phenomena, the effect of different engine speeds has been also conducted in the study.

In tab. 5 the investigated combustion chamber geometries are summarized. To focus only on injection and piston geometry a flat cylinder head has been used for all cases in this step. Grid generation for different cases has been performed resulting in approximately 700000 cells in multi-hole injector cases and about 200000 cells in single-hole injector cases.

The total injected fuel has been set to form a generally lean mixture of air and fuel inside cylinder after end of injection (EOI). Injection duration has been kept constant in all cases to 90 degrees of crank angle. The effect of injector needle has been accounted for by application of variable fuel rate at inlet boundary condition with a maximum fuel rate of 2.1 grams per second at 2000 rpm. The chamber pressure at the start of calculation is set to standard air conditions. The start of injection (SOI) timing for all the simulated cases is 120° bTDC firing. The engine speed has been considered to be 2000 rpm in all basic cases. Also the compression ratio has been kept constant at 9.5 which is the same as base engine.

In fig. 8 the effect of different piston head shapes on mixture formation and jet development inside cylinder for single-hole injector has been shown through some snapshots of inside cylinder flow at a crank angle near spark timing. All of the presented figures correspond to 40° bTDC firing. As it could be easily seen even small changes as rounding up the edge of combustion chamber can have a major effect on fuel jet shape inside cylinder.

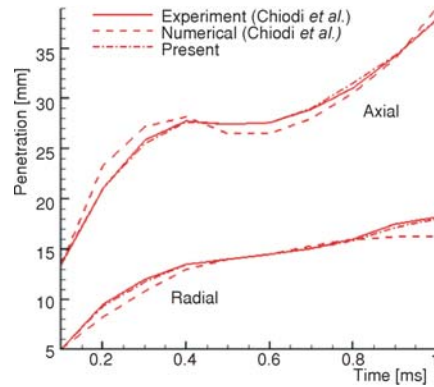


Figure 7. Comparison of jet penetration in axial and radial directions for third validation case

Table 5. Main characteristics of selected combustion chambers

Piston configuration	Bowl diameter [mm]	Bowl depth [mm]
Flat	–	–
Base	65	4
Narrow bowl	38	10
Large bowl	59	5
Large bowl modified	59 (fillet)	5

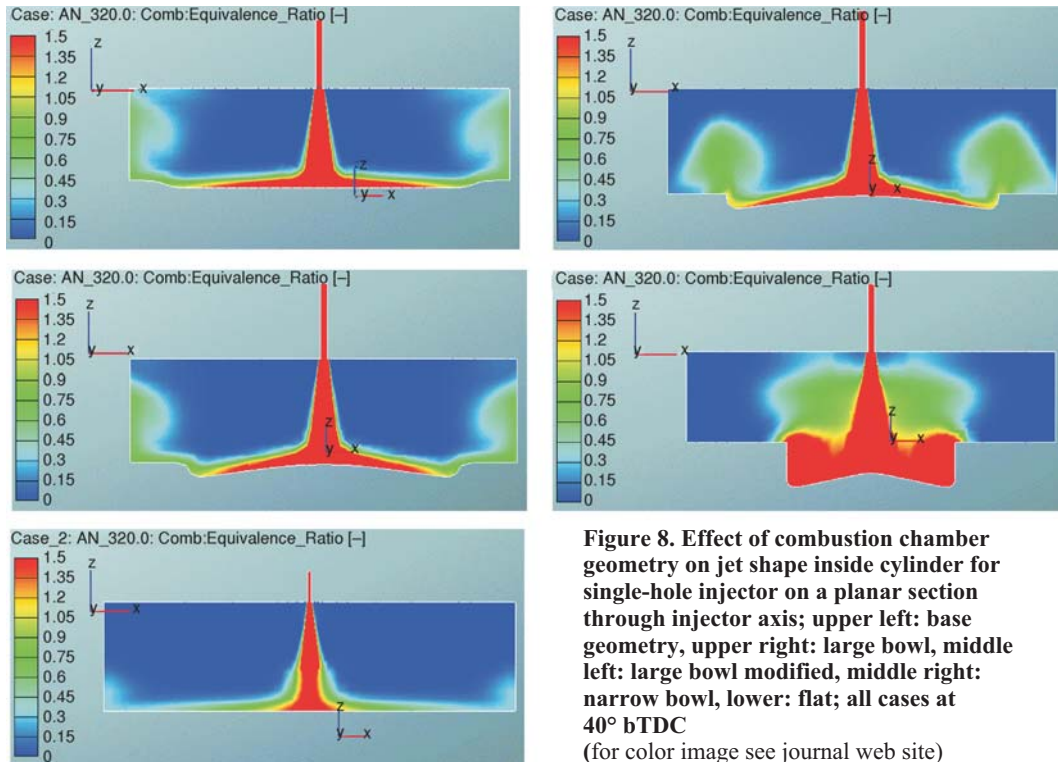
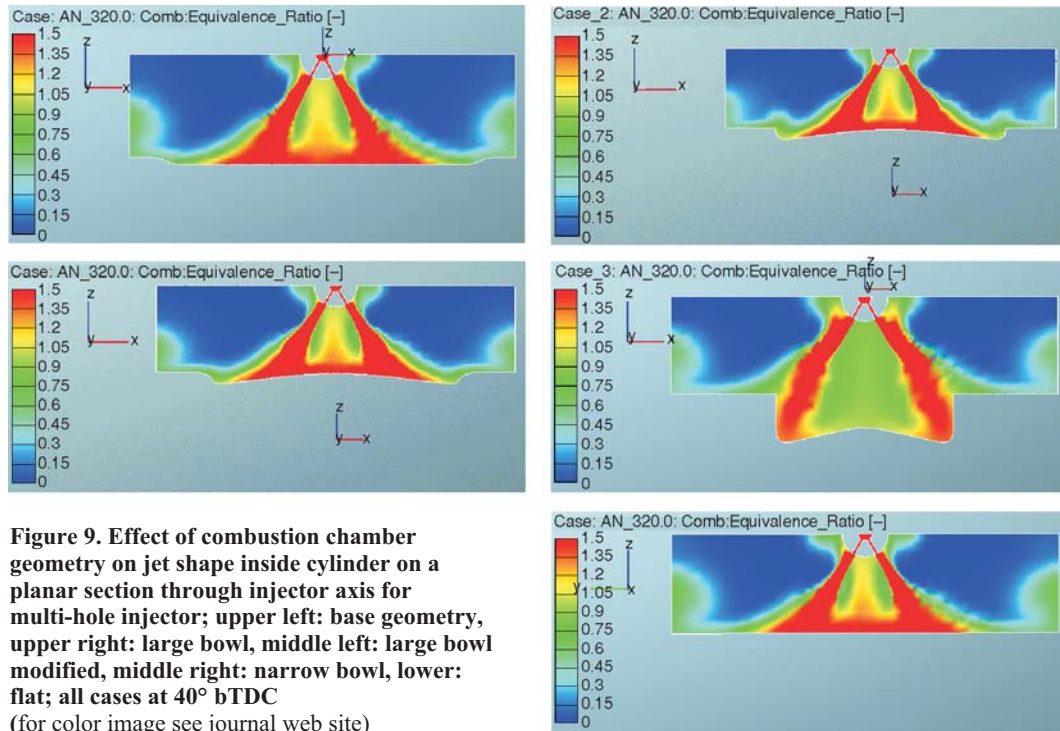


Figure 8. Effect of combustion chamber geometry on jet shape inside cylinder for single-hole injector on a planar section through injector axis; upper left: base geometry, upper right: large bowl, middle left: large bowl modified, middle right: narrow bowl, lower: flat; all cases at 40° bTDC (for color image see journal web site)

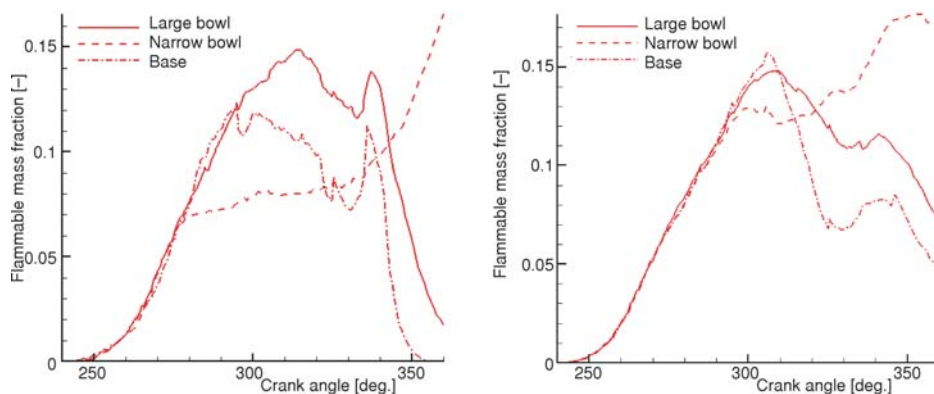
As it could be seen in the figures flat piston shape causes the flow to be driven to cylinder edges. But narrow bowl combustion chamber causes the flow to recirculate and generates a kind of tumble flow inside cylinder resulting in a narrower jet shape and more stratification. It has been found that even small changes as rounding up the edge of combustion chamber can have a major effect on fuel jet shape inside cylinder. Despite that difference in flow field the large bowl and large bowl-modified combustion chambers showed generally similar characteristic as the base engine geometry. All these cases have been realized to develop a wide and weak tumble effect in the combustion chamber and lower stratification of in cylinder charge. Despite flat combustion chamber these shapes tend to avoid jet from penetration towards cylinder edges and thus make a more compact jet shape in comparison to flat piston head shape.

Same flow and jet development pattern has been observed in the cases using multi-hole injector as shown in fig. 9. As it could be seen the general pattern of mixture development inside cylinder is the same as single-hole injector for each case. But in these cases the developed jet has a generally wider cone angle which leads to more mixing inside cylinder and lower stratification.

In order to get better understanding of mixture preparation inside cylinder a quantitative comparison could be easily done based on flammable mixture definition. As stated earlier flammability limits of 0.8 and 1.4 on RAFR has been considered for stable combustion based on the literature. So a flammable mass fraction could be obtained based on these limits. Flammable mass fraction is simply the fraction of flammable mass of mixture to the total mass of mixture. Similarly, rich mass fraction is the fraction of rich mixture mass to the total mass of mixture.



Temporal evolutions of flammable mass fraction for different cases are shown in fig. 10 using single-hole injector (left) and multi-hole injector (right). To make comparisons easier three geometries have been considered. It could be seen that as more fuel is injected into the cylinder flammable mass fraction increases. This value shows a maximum in the case of large-bowl and base geometries. A decrease in the level of flammable mass fraction is experienced after that point because of the motion of mixture towards walls. After EOI timing the flammable mixture in these two cases rapidly decreases to near zero values, which shows over mixing of fuel and air.



Unlike these two cases the flammable mass fraction in narrow-bowl geometry shows a constant increase. This trend is more realized near the EOI timing, at which a rapid increase in flammable mass fraction occurs for both injector types.

Similar trends could be easily found in the temporal evolution of rich mass fraction as shown in fig. 11 for injector types of single-hole (left) and multi-hole (right). In fig. 11 (left) narrow-bowl geometry case seems to show completely different characteristics in comparison to other two cases. As the narrow-bowl geometry tends to keep the whole mixture in a “trapped” region for a while, both flammable and rich mixture fractions show rapid increase in this case. Finally the mixing between trapped region and outside air causes the rich mass fraction to decrease after EOI timing in this case.

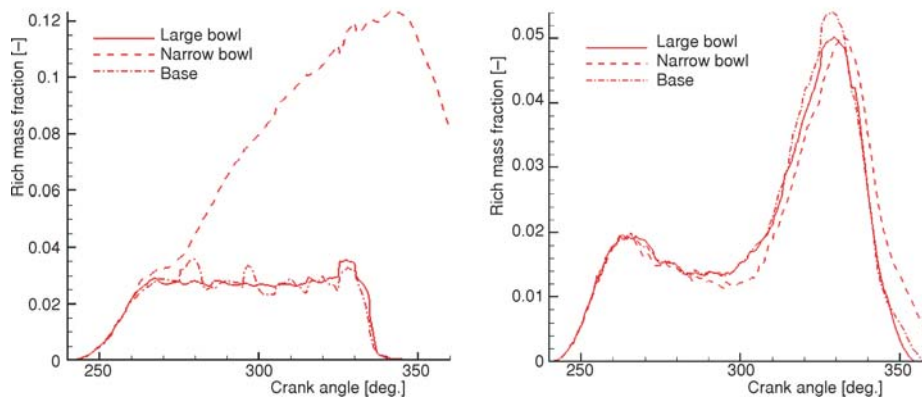


Figure 11. Temporal variations of rich mass fraction for different combustion chamber geometries; left: single-hole injector, right: multi-hole injector

Rich mass fraction variations for the geometries with multi-hole injector are much similar to each other as depicted in fig. 11 (right). All cases show an initial increase after SOI, a slight decrease because of stronger tumble motion and a rapid increase near EOI due to the lack of available air for mixing. Mixing between fuel and outer air makes the rich mass fraction decrease steeply after EOI. However a slight difference in rich mass fraction variations could be realized in the figure 11(right) as it shows generally a higher value in large-bowl and base cases.

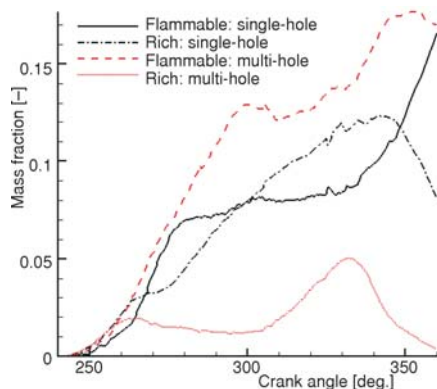


Figure 12. Comparison of flammable and rich mass fractions using different injectors for narrow-bowl case

Temporal evolutions of flammable and rich mass fractions are plotted in fig. 12 for both injector types in narrow-bowl piston head case. The general trends for different mass fraction variations are roughly the same for both injectors. But an obvious difference in the values for both flammable and rich mixtures could be easily seen in the figure. The flammable mass fraction in multi-hole injector case seems to increase more rapidly and experience higher values compared to that of single-hole injector case. Rich mass fraction variations show an early increase and then decrease appropriately. The

reason in the difference could be realized regarding the tendency of multi-hole injector to create a wider jet and thus more mixing.

On the other side, a slight decrease in the flammable mass fraction for multi-hole injector case could also be related to over-mixing of fuel and air inside cylinder. Same properties could be seen in the decrease of rich mixture fraction towards zero for multi-hole injector case. However the final values of flammable mass fraction for both injectors are approximately the same. This suggests the multi-hole injector could deliver a slightly higher quality mixture towards the end of compression stroke.

To sum up, the presented results show that narrow combustion chamber geometry promises better characteristics for mixture preparation. On the other hand using multi-hole injector seems to give wider spaced jet shapes and smoother equivalence ratio variations compared to single-hole injector. However accurate matching of injection timing, combustion chamber geometry, injector type and its location is necessary to get better combustion characteristics for the engine.

Using centrally mounted inwardly-opening single-hole injector with narrow-bowl head shape tends to create a narrow jet near the cylinder axis. This position is important regarding spark plug location. So this shape is chosen for further modification and studies.

Effect of engine speed

One other variable which affects the mixture preparation time is engine speed. All the presented results have been performed at constant engine speed of 2000 rpm. In order to get better understanding of jet shape development inside cylinder, it is inevitable to study the injection process in different engine speeds.

The first variable which is affected by the variation of engine speed is the time available for the fuel injection and thus for mixing process. It is necessary to use elevated fuel rail pressures to acquire the same RAFR as base case at higher engine speeds. In fig. 13 the variation of fuel rail pressure versus engine speed for two types of injectors with narrow combustion chamber has been shown. It could be seen that increasing engine speed the fuel pressure needed to complete the injection process increases. The injection time is reduced at higher engine speeds and consequently higher fuel rail pressures are needed to inject the same amount of fuel in less time.

Another interesting result out of fig. 13 is the higher fuel pressure needed by multi-hole injector compared to single-hole injector. This could be related to more loss experienced in multi-hole injector for injecting the same amount of fuel in constant time periods.

As the engine speed is increased, the time available to inject the fuel into cylinder becomes less and less until finally there might not be enough time for the air-fuel mixture to form a flammable mixture. So advancing the SOI at higher engine speeds may be realized to give more time for mixture preparation.

Some snapshots of flow field inside cylinder for single-hole injector case at a same crank angle degree for different engine speeds are shown in fig. 14. It could be inferred from the figures that higher engine speed cases clearly show less-developed jet shape. This point indicates again the need for more time to prepare a flammable mixture inside cylinder at higher en-

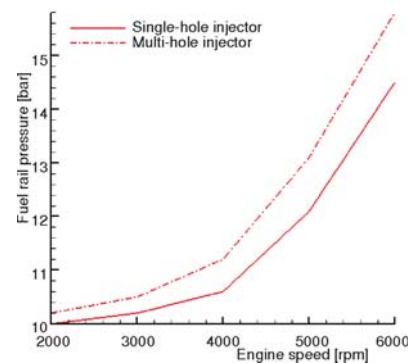


Figure 13. Comparison of fuel rail pressure needed by different injectors

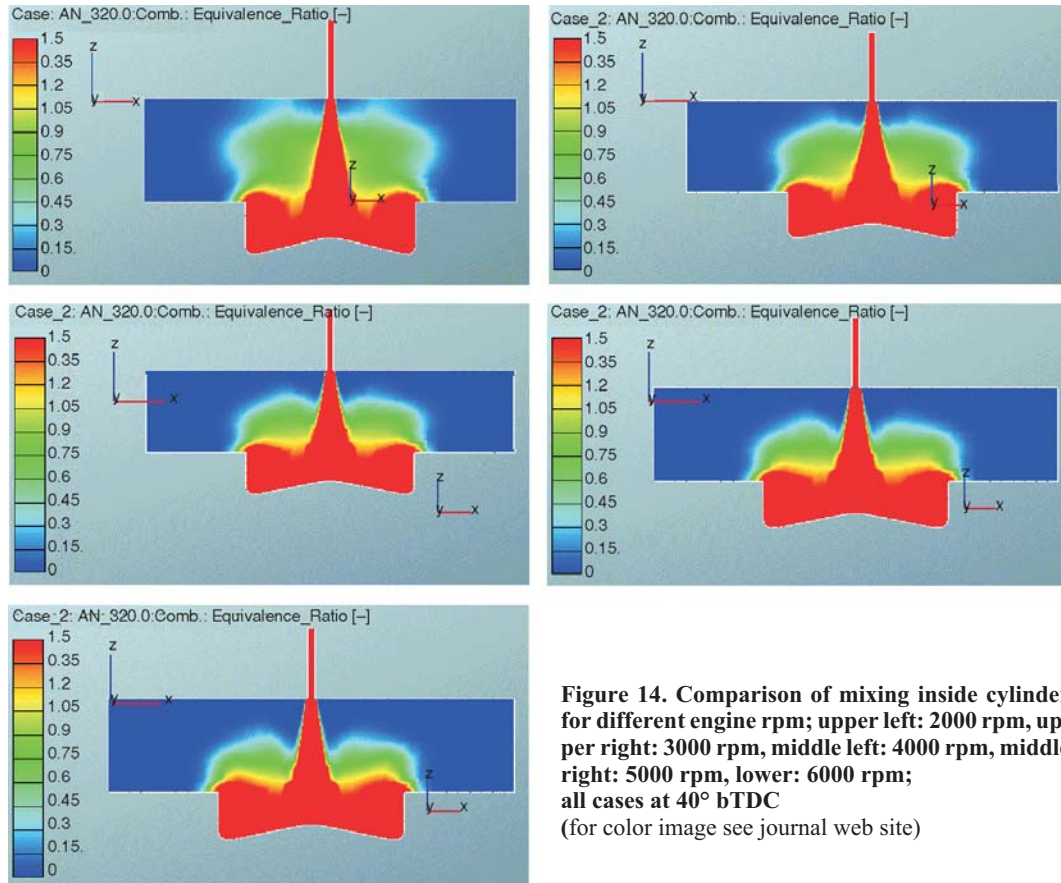


Figure 14. Comparison of mixing inside cylinder for different engine rpm; upper left: 2000 rpm, upper right: 3000 rpm, middle left: 4000 rpm, middle right: 5000 rpm, lower: 6000 rpm; all cases at 40° bTDC (for color image see journal web site)

engine rpm. The amount of advance in injection timing could only be defined through a study regarding combustion period.

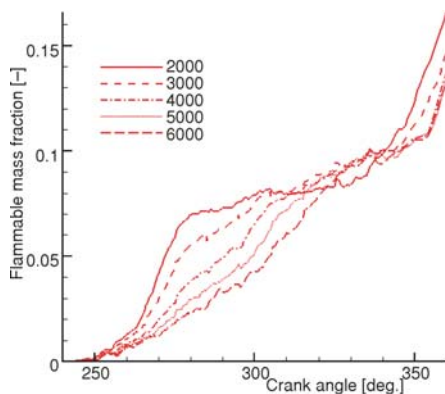


Figure 15. Temporal variations of flammable mass fraction at different engine speeds

The variation of flammable mass fraction inside cylinder for different engine speeds is shown in fig. 15. The general trend for the variations is the same as previous cases. As the available time for mixture preparation decreases with increase in engine speed, formation of a high quality mixture is delayed and the level of flammable mass fraction decreases. This decrease is more pronounced at initial stages of injection. The proper mixing between fuel and air is delayed until timings near the EOI at which level of flammable mass fraction at higher speeds increases. Even after this point lower engine speed cases show higher values. This agrees with the trend observed in the fig. 14.

Conclusions

Based on the discussions presented in previous sections, there are some main conclusions summarized as follows:

- The results are very sensitive to mesh, especially number of grid points across the nozzle.
- A minimum of 10 cell layers across the injector nozzle is needed to avoid numerical instability. Also transition layer should be located at least 8~10 times the nozzle diameter downstream from the nozzle.
- The modeling results were shown to have very good agreement with validated experimental and numerical results from literature.
- Five bowl-in-piston configurations were chosen to study the effect of piston head geometry. Narrow-bowl geometry showed the best characteristics in terms of mixture stratification.
- Representation of results show that even a small difference in combustion chamber geometry could cause quite different jet shape and mixture properties inside cylinder.
- Generally wider bowl geometries tend to spread the mixture towards the cylinder walls, while narrower bowls tend to “trap” the fuel jet in a compact area. Keeping the flammable mixture in a compact area seems to be an important characteristic for stratified charge operation.
- Narrow-bowl geometry seems to have completely different effect on temporal evolution of flammable and rich mixture fractions inside cylinder in comparison to all other cases. Such effects are considered to be related to more mixture stratification.
- It was found that cases with multi-hole injector could produce less amount of rich mass fraction and a slightly more amount of flammable mass fraction in comparison to geometries exhibiting single-hole injector. However the value of the flammable mass fraction at the end of compression stroke was found to be almost the same for both injector types.
- The multi-hole injector needs more fuel rail pressure to inject the same amount of fuel into cylinder compared to single-hole injector. Both injector types exhibit useful characteristics for mixture stratifications.
- Increasing engine speed was found to reduce the mixing quality inside cylinder and increase fuel rail pressure needed by the Injector.

Acknowledgement

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Abbreviations

BDC	– bottom dead center	MPFI	– multi-point port fuel injection
bTDC	– before top dead center	RAFR	– relative air-fuel ratio
CNG	– compressed natural gas	SCRE	– single cylinder research engine
DI	– direct injection	SI	– spark ignition
EOI	– end of injection	SOI	– start of injection

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