EXAMINATION OF INITIALIZATION AND GEOMETRIC DETAILS ON THE RESULTS OF CFD SIMULATIONS OF DIESEL ENGINES

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ABSTRACT
Computational Fluid Dynamic (CFD) simulations using the AVL Fire and Kiva 3v codes were performed to examine commonly accepted techniques and assumptions used when simulating direct injection diesel engines. Simulations of a steady state impulse swirl meter validated the commonly used practice of evaluating the swirl ratio of diesel engines by integrating the valve flow and torque history over discrete valve lift values [1]. The results indicate the simulations capture the complex interactions occurring in the ports, cylinder and honeycomb cell impulse swirl meter. The commonly adopted axisymmetric assumption for an engine with a centrally located injector was tested by comparing the swirl and emissions history for a motored case and a double injection low temperature combustion case. Consideration of the detailed engine geometry including valve recesses in the piston and the head lowered the peak swirl ratio at TDC by approximately 10% compared to the simplified no-recess case. The corresponding combusting cases also had different heat release and emissions predictions but could be partially compensated for by lowering the initial swirl ratio for the axisymmetric case.

INTRODUCTION
CFD has gained acceptance as a tool for engine design and to evaluate changes to engine operating parameters. In order to save computational time, an axisymmetric combustion chamber can be assumed if the engine has a centrally located injector with a prescribed number of equally spaced holes. However, this assumption necessitates sacrificing details of the engine geometry. For example, machining done to the piston and cylinder head to accommodate the valves is not laid out in an axisymmetric fashion. The additional volume created by these features also contributes to the volumetric compression ratio. The clearance between the piston and the head at TDC, referred to as the squish height, is often not constant in actual engine geometry. To be able to make the axisymmetric assumption some compromise must be made to adequately account for the squish height since its value has a significant effect on the squish flow created when the working fluid moves from the outer edges of the cylinder into the smaller bowl diameter during the compression process. The same phenomenon is responsible for the increase in swirl as the total volume decreases and the corresponding reduction in swirl as the volume increases in the expansion stroke.

Simulations require extensive knowledge of the operating conditions in order to give the best opportunity for accurately duplicating the physics occurring in the engine. Of particular importance are the thermodynamic considerations of the working fluid such as inlet temperature, pressure, and species composition including the amount of recirculated exhaust (EGR). The inlet oxygen composition is a primary driver to achieving low temperature combustion [2]. The benefits of low temperature combustion include the ability to meet legislated soot and NOx emissions but possibly with a concomitant increase in the amount of unburned hydrocarbons and carbon dioxide.

In addition to the thermodynamic considerations, the initialization of the flowfield is also important. In a study of varying inlet conditions and swirl ratio, Miles, et al. [3] showed an optimum swirl and injection timing for this type of operating condition. The optimal injection timing was found when the injected plume was targeted at the corner of the bowl lip. Simulations of the corresponding operating condition showed that a double vortex structure appeared in the piston bowl which appeared when the swirl was varied to the optimal value.

The swirl flow therefore is an important operating parameter to consider when initializing a CFD simulation of diesel engine combustion. Often full optical characterization of the flowfield is not available. Although studies using PIV [4,5], LDV [6] and hot wire anemometry [1] are available for
particular engines, initial swirl conditions for CFD simulations are often derived from steady-state flow bench experiments. Here the head is mounted to a cylindrical section which matches the bore size and ranges from 1 to 1-1/2 bore diameters in length. An impulse swirl meter converts the angular momentum of the flow to a torque and is located at the bottom of the cylindrical section. The valve lift is then varied over its operating range and the corresponding flow and torque numbers are integrated over the lift profile and a composite swirl number is determined [1].

This paper examines the following details of the axisymmetric assumption and the swirl initialization. First a steady-state simulation of a flowbench case was used to validate the CFD code’s ability to predict the global swirl behavior. Then, a series of motored simulations were run to determine the effect of the real engine geometry on the swirl history. Combusting cases in both detailed and axisymmetric geometries were used to determine real engine geometry effects. Finally, a low temperature combustion sector mesh case with a lower swirl ratio that more closely matches the swirl history was compared.

The GM 1.9L single-cylinder engine was examined in this study. Its geometric parameters are summarized in Table 1 and the engine is shown in Figure 1.

### Table 1 Geometric parameters for GM 1.9L engine

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>82.0 (mm)</td>
</tr>
<tr>
<td>Stroke</td>
<td>90.4 (mm)</td>
</tr>
<tr>
<td>Displacement/cylinder</td>
<td>0.48 l</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>16.6</td>
</tr>
<tr>
<td>Valves</td>
<td>2 intake, 2 exhaust</td>
</tr>
<tr>
<td>Intake ports</td>
<td>directed, helical</td>
</tr>
<tr>
<td>Bowl</td>
<td>re-entrant</td>
</tr>
</tbody>
</table>

**NUMERICAL SETUP COMBUSTING, MOTORED CASES**

The CFD code used in the present simulations is a version of the KIVA-3V Release 2 code [7] with improvements in various physical and chemical models developed at the Engine Research Center, University of Wisconsin-Madison. The properties of tetradeacane were used to simulate the physical properties of diesel fuel and the chemistry was simulated by a 54 reaction reduced n-heptane chemistry mechanism [8]. The KIVA code was coupled with the CHEMKIN II code [9] to solve for the detailed diesel fuel chemistry during the multidimensional engine simulations.

The RNG k-ε model [10] was used for in-cylinder turbulence simulation. The Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) hybrid breakup model [11] was used to calculate the droplet breakup process of high pressure solid-cone spray injections. An advanced unsteady vaporization model was applied to predict the droplet evaporation process [12].

Since mesh density was a key issue for this study, a recently developed gas-jet model was used for the calculation of the relative velocity between the droplets and the gas phase in the unresolved region near the nozzle. This spray model has been shown to reduce the effect of grid density on spray calculations [13].

**STEADY STATE INTAKE FLOW SIMULATION**

The simulation was performed using AVL FIRE release 8.52. The turbulence model based on the RANS (Reynolds Average Navier Stokes) method is the two-equation K-ε model, which takes the effects of turbulence in the mean flow into account.

The honeycomb of the impulse swirl meter and the engine domain were meshed separately with boundary-fitted grids consisting of only hexahedral cells. The grids were then joined together to form one single mesh by means of the arbitrary-connection tool of Fire software.

The torque was calculated considering the pressure and shear forces acting in each face of the honeycomb wall in Figure 2.
Figure 2  Honeycomb cross section of impulse swirl meter

The comparison between numerical and experimental data (Figure 3) shows a good agreement. The torque is predicted with CFD with an error of 8% and the mass flow rate with an error of 16% demonstrating the consistency of this model to predict the swirl ratio.

Figure 3 Mass flow and torque comparison between numerical and experimental results

MOTORED SWIRL HISTORY

MESH SENSITIVITY

A mesh sensitivity study was conducted to determine the proper cell size for the motored swirl ratio history. The coarsest mesh has approximately 40,000 cells, the Medium mesh which was also chosen for further study has approximately 115,000 cells and finally the Fine mesh has 420,000 cells.

Figure 4 Swirl history for the detailed geometry at refined, coarse and medium mesh sizes.

Figure 4 shows the results of the mesh sensitivity study. The coarse mesh exhibits some amount of waviness in its response and a lower maximum value than the value seen at TDC for the refined and baseline Medium grid.

INFLUENCE OF THE GEOMETRY DETAILS IN THE FLOW FIELD

In order to test the effects of the different possibilities for geometrical features on the results, a series of tests with different grid details were used:
1. Detailed geometry with head and piston valve recesses
2. Piston and head valve cutouts removed (flat head/piston)
3. Piston valve pockets removed
4. Head valve recesses removed.

Figure 5 shows the swirl history for the four different geometries referenced above for initial swirl ratio of 2.2. Observe that the total swirl is not recovered after the swirl spin up (compressing) and spin down (expanding) processes due to viscous effects. As expected, the geometry with the fewest geometric details exhibited the highest swirl ratio at TDC. The geometry with the most detail has the lowest swirl ratio, indicating that details of the valve recesses in the head and piston impede the flow to a greater extent than the detail in the piston geometry thereby changing the swirl history. The next lowest swirl is the one without head crevices indicating that the valve cutouts in the piston had a lesser affect than those in the head.
ALTERNATE SWIRL HISTORY ACCOMODATIONS

Since computational cost can be a significant consideration when conducting modeling studies of combusting flow, alternatives to using the full 3d geometry will be discussed. Two principal strategies will be discussed for simulations in sector meshes. The first is simply to lower the initial swirl level such that the maximum swirl reached by the detailed and sector mesh cases match. The second will be to include additional geometry in the grid. This is illustrated in Figure 6.

A groove was placed perpendicular to the swirl direction such that the flow could decay with a similar mechanism as the detailed geometry above. The compression ratio was matched by changing the clearance height so the thermodynamic conditions remain constant in the combusting cases. The depth of the groove was estimated from the valve crevice. The length of the groove was also estimated by summing up the circumference of the valve crevice and dividing that number by the holes in the injector – 7 in this case. The placement of the groove in the azimuthal direction was determined such that the groove would have minimal interaction with the spray plume. The groove was placed upstream to the swirl from the symmetric location in the middle of the mesh assuming the spray plume would be deflected downstream to the swirl.

The results are shown in Figure 7. The groove has the intended effect in that it slows the swirl at TDC by approximately 14% from the smooth sector geometry. As can be seen in Figure 7, the swirl history for the sector mesh (axisymmetric) and 3d geometry with flat head and piston geometry are essentially identical. The swirl history for the groove and 3d detailed case do not match identically. Despite the swirl being lowered significantly, it is not decreased to the same extent as the detailed case particularly later in the expansion stroke. This outcome was satisfactory as the modifications to the sector grid were based on real geometry considerations and the difference seen at TDC was less than 4%.

Figure 8 compares the swirl history of a smooth (flat) sector mesh with the baseline swirl ratio, a lowered initial swirl ratio, and the grooved sector mesh. The TDC swirl of the smooth geometry with lowered initial swirl and the grooved geometry with the baseline swirl ratio match at TDC. These different approaches to altering swirl history will be compared later in the combusting cases.
Figure 8 Swirl history for sector mesh cases with varying detail

EFFECT OF DETAILED GEOMETRY ON COMBUSTION

Having shown that the details of the geometry affect the swirl history and ways for compensating for this effect in the sector meshes, simulations were run at two low temperature combustion operating points from the work of Koci [14], as summarized in Table 2.

Low temperature combustion is often associated with decreased combustion efficiency and higher levels of CO compared to traditional diesel combustion [3]. These operating conditions were chosen to illustrate the importance of the change in swirl brought about by geometric changes at different operating conditions. The cases simulated are summarized in Table 3.

Table 2 Operating conditions for combusting cases [14]

<table>
<thead>
<tr>
<th>Operating Condition 1</th>
<th>IMEP (bar)</th>
<th>6.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intake O2 %</td>
<td>9.8 %</td>
<td></td>
</tr>
<tr>
<td>Injected Fuel mass (mg)</td>
<td>13.6</td>
<td></td>
</tr>
<tr>
<td>Air-Fuel Ratio</td>
<td>18.5</td>
<td></td>
</tr>
<tr>
<td>RPM</td>
<td>2000</td>
<td></td>
</tr>
<tr>
<td>First injection start</td>
<td>-12.2°</td>
<td></td>
</tr>
<tr>
<td>duration</td>
<td>5.5</td>
<td></td>
</tr>
<tr>
<td>first injection pressure</td>
<td>860 bar</td>
<td></td>
</tr>
<tr>
<td>Second injection start</td>
<td>-28.2°</td>
<td></td>
</tr>
<tr>
<td>duration</td>
<td>5.5</td>
<td></td>
</tr>
<tr>
<td>second injection pressure</td>
<td>860 bar</td>
<td></td>
</tr>
<tr>
<td>Nozzle diameter</td>
<td>140 micron</td>
<td></td>
</tr>
<tr>
<td>Included angle</td>
<td>155°</td>
<td></td>
</tr>
</tbody>
</table>

Table 3 Combusting case additional details

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Swirl Ratio at IVC</th>
<th>IMEP (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sector Smooth</td>
<td>2.2</td>
<td>6.0</td>
</tr>
<tr>
<td>Sector Smooth</td>
<td>1.9</td>
<td>6.0</td>
</tr>
<tr>
<td>Sector Groove</td>
<td>2.2</td>
<td>6.0</td>
</tr>
<tr>
<td>3-d (Detailed)</td>
<td>2.2</td>
<td>6.0</td>
</tr>
<tr>
<td>Sector Smooth</td>
<td>1.9</td>
<td>10.5</td>
</tr>
<tr>
<td>Sector Groove</td>
<td>2.2</td>
<td>10.5</td>
</tr>
<tr>
<td>3-d (Detailed)</td>
<td>2.2</td>
<td>10.5</td>
</tr>
<tr>
<td>3-d (Flat Head Piston)</td>
<td>2.2</td>
<td>10.5</td>
</tr>
</tbody>
</table>

The previous section demonstrated the effect of detailed geometry on the swirl history of a motored condition. The first purpose in studying combusting cases is to assess the impact of geometrical details on the emissions results. The second purpose is to see if any modified initial conditions can be used to improve the fidelity of the simplified calculations in a sector simulation. Figure 7 showed that an approximate 14% difference was seen in the peak swirl ratio when the detailed and simplified simulations were compared. Further tests were conducted with a 51.4° (considering 7-hole nozzle geometry) sector mesh with reduced swirl levels and increased geometry detail (groove) to assess the affect of total angular momentum on the results of the simulations.

Figures 9 and 10 summarize the numerical simulations of the various levels of detail for the 3d cases at operating condition 2. Figure 9 shows that the ignition delay is essentially identical for all cases. Only results for flat head/piston and detailed are shown for brevity. The detailed geometry case shows a greater amount of heat release during the main combustion event. Also noteworthy is the fact the CO emissions follow the same trend as the swirl history. The cases with the highest swirl have the highest CO and the case with the lowest swirl had the lowest CO.

Also shown in Figure 10 are the CO emissions results for the sector mesh cases at the high load operating condition (operating condition 2). It can be seen there is some difference...
between the sector mesh and 3d cases. This is due to differences in jet penetration due to the different mesh types between the two simulations. Sector meshes tend to have smaller cells near the nozzle and therefore affect the spray penetration process. Further research is being done to attenuate these mesh type dependencies [15]. For the purposes of this study, the important thing to note is the lower swirl ratios of the detailed (3d and sector groove) or lowered initial swirl caused the same change (lower) in the CO emission.

Figure 9 Pressure and heat release for IMEP 10.5 bar case with 3d geometry

Figure 10 CO emissions for sector mesh and 3d cases at 10.5 bar IMEP.

The use of initial swirl and additional groove geometry as a means to compensate for the differences in swirl history can also be seen in Figure 11. The change in swirl history does not have a strong effect on global parameters such as pressure and heat release for the 6.0 bar IMEP load. In Figure 11 changes in the CO emission for the sector mesh simulations does not change significantly as this operating condition appears to be less sensitive to swirl history with regard to the emission of CO. Figure 10 shows this is not the case for the 10.5 bar load point. For the 3d cases the CO emission decreases by 75 g/kgf when going from smooth to detailed geometry. A similar trend is seen for the sector mesh cases as both strategies (lower initial swirl and groove) for lowering the swirl lower the CO emission by approximately the same amount. This illustrates that either strategy may be used to compensate for geometry affects or that it is the total angular momentum at TDC that affects the emissions results the most for this operating condition. The groove geometry is a closer physical analog and is computationally inexpensive.

Figure 11 CO emissions for Operating Condition 1 with sector mesh geometries

CONCLUSIONS

A numerical study that examined common modeling practices for diesel combustion was conducted. A steady-state swirl torque meter was modeled and revealed that the CFD code was capable of replicating the mass flow and torque seen in the experiments used to characterize the swirl and often used to initialize the flowfields of numerical simulations.

The swirl histories of several different permutations of engine geometric detail obtained by removing the valve cutouts in the piston and/or the crevices in the head showed that the details generally slow the swirl down and that the head crevice region is most responsible for the slowdown in swirl.

Two different strategies to accommodate for swirl history changes due to geometry details were tested for sector meshes.

1. Lowering the initial swirl
2. Including a groove in the head to simulate the effect of valve crevices.

Both strategies showed a similar effect on the CO emissions indicating the emissions is controlled by the total angular momentum at TDC for this operating condition.
Compensating for the effect of the detailed geometry on the swirl history by lowering the initial swirl for the sector cases lead to emissions changes in the direction (lower) of the detailed geometry results.

The sensitivity of the CO emissions results to swirl history increased with increasing load.

ACKNOWLEDGMENTS

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