

Pathline Analysis of Full-cycle Four-stroke HCCI Engine Combustion Using CFD and Multi-Zone Modeling

Randy P. Hessel and David E. Foster

University of Wisconsin-Madison

Richard R. Steeper

Sandia National Laboratories

Salvador M. Aceves and Daniel L. Flowers

Lawrence Livermore National Laboratory

ABSTRACT

This paper investigates flow and combustion in a full-cycle simulation of a four-stroke, three-valve HCCI engine by visualizing the flow with pathlines. Pathlines trace massless particles in a transient flow field. In addition to visualization, pathlines are used here to trace the history, or evolution, of flow fields and species. In this study evolution is followed from the intake port through combustion.

Pathline analysis follows packets of intake charge in time and space from induction through combustion. The local scalar fields traversed by the individual packets in terms of velocity magnitude, turbulence, species concentration and temperatures are extracted from the simulation results. The results show how the intake event establishes local chemical and thermal environments in-cylinder and how the species respond (chemically react) to the local field.

Flow is modeled with KIVA3V-MZ-MPI, which is a multi-zone combustion model implementation of KIVA3V that calculates detailed combustion chemistry. Chemical reactions are modeled with a 29-specie, 52-reaction, n-heptane mechanism developed by the University of Wisconsin-Engine Research Center. The engine modeled is the 4-stroke, automotive HCCI research engine of Sandia National Laboratories fueled with n-heptane.

INTRODUCTION

Most CFD analysis is Eulerian, that is, flow is considered as entering, leaving and changing in a control volume. With engines, the control volume is the whole combustion chamber with flow entering and leaving

through the ports. Other times the control volume is one, or a group of computational cells and flow enters and leaves via neighboring cells.

Pathline analysis is Lagrangian. Packets of gases are identified at various times and locations, then the packets are tracked in time and space. Because pathlines run parallel with the velocity vector field, there is no convective flow entering or leaving pathlines. But, the species associated with pathline gases can change along a pathline with time. Pathline gases may travel into regions where they speed up, or slow down, or where they heat up, or cool down. If sufficiently heated, pathline gases react.

A great deal of knowledge about HCCI systems has accumulated using Eulerian analysis. So a fair question to ask is what insights can a Lagrangian approach add to this bed of knowledge? Addressing this question is the main focus of this paper.

ENGINE SPECIFICATIONS

Table 1 lists specifications for the modeled engine. This engine is known as the Sandia National Laboratories Automotive HCCI Research engine. It is a single cylinder engine that can be operated with a variety of components and fuels. For this study a high ring pack, flat aluminum piston and metal liner are used. The high ring pack provides a small piston/liner crevice volume. Its volume is only 1% of the combustion chamber volume at top dead center (TDC).

Figure 1 is the model representation of the engine at TDC-combustion with all valves closed. There is one exhaust and two intake valves. The intake valves are in line with each other.

The TDC volume used in the model compression ratio calculation is the volume visible in figure 1, excluding the port volumes. The bottom dead center (BDC) volume is determined with the piston at BDC and the intake valves slightly open. Volumes above the intake valves are not used in the BDC volume calculation.

To promote a homogeneous charge, n-heptane is introduced upstream of the intake runner. Experiments are run at an equivalence ratio of 0.293 at 1200 RPM. Please refer to [1] for more engine hardware and test equipment specifications.

Table 1. Engine specifications and model input values. When different, model values are given in parentheses.

Bore	92.0 mm	Stroke	95.2 mm
Piston diameter	91.3 mm	Squish height	1.85 (1.7) mm
Piston/liner crevice vol.	0.61 cc	Compress. ratio	11.2
Engine speed	1200 RPM	Equivalence ratio	0.29
Intake surge tank pressure	1 bar	Exhaust surge tank pressure	1 bar
Intake surge tank temp.	332 K	Connecting rod length	166.7 mm
[†] Intake valve open	-372 (-344) deg. atdc	[†] Intake valve close	-134 (-162) deg. atdc
[†] Exhaust valve open	101 (135) deg. atdc	[†] Exhaust valve close	-323 (-363) deg. atdc

[†] The reason that engine and model valve timings differ is that in the model valves are opened and closed at 0.5 mm lift. 0°= TDC combustion.

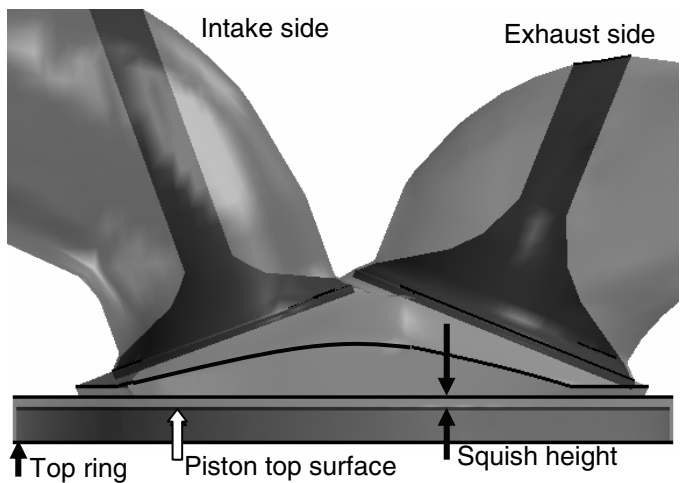


Figure 1. Combustion chamber at TDC.

MODEL SETUP

The CFD code used is based on KIVA3V-Release 1. Code upgrades specifically relevant to this work include

an improved wall heat transfer model [2] and a fully integrated multi-zone combustion model [3].

The term ‘fully integrated’ implies that the multi-zone combustion model is incorporated into the CFD code similar to any other CFD sub-model. That is, at a particular time in the computational loop all of the computational cells have the opportunity to be acted upon. For the multi-zone combustion model, this means that the species in each cell have the opportunity to react (using zones). Other than that, the CFD code can be considered unchanged. Therefore, all other typical CFD calculated processes, like turbulent mixing between cells via the RNG k-ε model, boundary layer formation via the law-of-the-wall, etc. are all calculated just as if any other combustion model were used.

Regarding the time step, kinetics are sub-cycled at a fraction of the fluid mechanics time step. The chemistry solver time step is chosen for the well-mixed reactor ODE solver. Each zone is treated as an independent well-mixed reactor for the duration of the fluid mechanics time step.

There are many good papers that explain the sub-models within KIVA3V [4] and there is a web site with reference material for the interested reader [5]. Let it suffice to say that the version of KIVA3V used for this paper solves the following equations:

- Conservation of mass, momentum and energy.
- Chemical reactions using a multi-zone solver.
- RNG k-ε turbulence equations.
- Ideal gas law.
- Slider-crank mechanism, and valve motion.

The computational domain (figure 2) includes the two intake ports and single exhaust port, a portion of the intake and exhaust runners, all three valves, the complete pentroof combustion chamber and the piston/liner crevice extending from the top of the piston to the top surface of the top ring. The grid was built with ICEM-CFD [6] and then it was further post-processed with in-house programs to correct some flag settings and redistribute port and runner vertices. Table 2 lists the numbers of cells used in each region.

Table 2. Computational cells per region.

Total mesh	140928	Piston/liner crevice	1332
Combustion chamber @ BDC	124772	Combustion chamber @ TDC	29922
Intake ports	9648	Exhaust port	6508

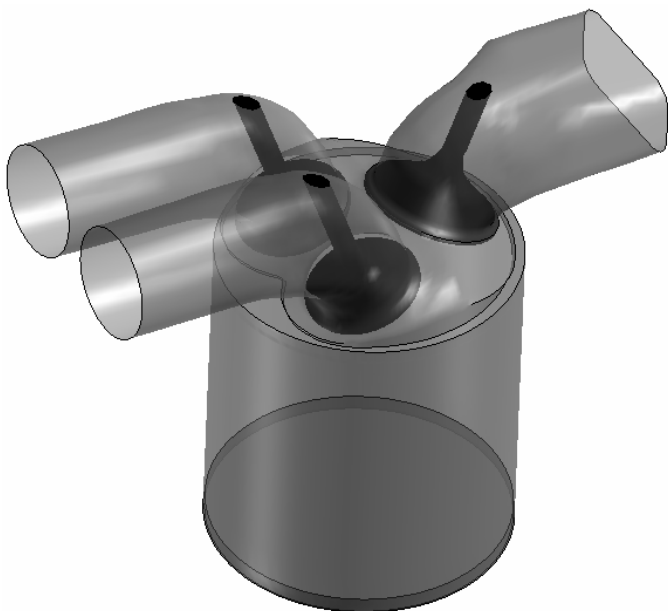


Figure 2. Complete computational domain at BDC.

The grid adjusts to valve and piston motion by first moving the vertices that lie on the combustion chamber surfaces, then moving the interior vertices accordingly in order to maintain good cell quality. The grid adjustment phase is called rezoning.

The grid used in these simulations requires a more robust rezoner than the standard KIVA3V rezoning algorithms, and one has been developed. The standard rezoners produced multiple cell inversions and therefore could not be used for these simulations. The new rezoner allows the grid to run multiple engine cycles with typically only 24 non-convex cells at any given time step.

Simulations are conducted for multiple engine cycles until a stationary condition is reached where subsequent cycles are nearly identical. The results presented in this paper are from the third simulated cycle. Three cycles is found to be sufficient to establish a stationary solution, and by the third cycle the initial conditions, like temperatures, pressures and species concentrations, have little influence on the final results.

Boundary conditions are assigned at the start of the simulation and stay in force throughout all cycles. Therefore, uncertainties in wall temperatures, intake and exhaust pressures and boundary species concentrations can all influence model accuracy.

The simulation start and end times are a matter of choice, since multiple cycles are simulated. Regardless, results will be presented using a reference crank angle of 0° = TDC combustion, unless stated otherwise. The simulation start time is -375° . At this crank angle the exhaust valve is still open and the intake valves are closed. The simulation end time is $-375^\circ + 720^\circ = 345^\circ$. Results at -375° and 345° are not identical, but they are similar enough to be considered cyclic.

In the model, valves close earlier and open later than on the engine. This is because there are computational cells between the top of the valves and the valve seats. If the model valve lifts would go to zero these cell volumes would also go to zero resulting in extremely small time steps and computational instability. Instead, valves are closed when the closing lift profile reaches 0.5 mm lift by constructing a zero thickness wall around the valve peripheries. Valve motion is stopped at 0.5 mm lift. Valves are reopened when the opening lift profile again reaches 0.5 mm. The wall is removed and the valve is again free to move, thus allowing flow between the ports and the cylinder.

Wall temperatures are listed in table 3. In the simulation, different surfaces of the combustion chamber have different temperatures, but temperatures are uniform over any one surface. Surface temperatures are held temporally constant throughout the simulation.

Table 3. Model surface temperatures, K.			
Piston	500 ¹	Liner	494 ¹
Head and ports	444 ¹	Intake valves	400 ²
Exhaust valve	481 ³		
¹ Estimate from Wave [7]			
² Assumption			
³ $0.7 \cdot (T_{\text{exhaust}} - T_{\text{coolant}}) + T_{\text{coolant}}$ [8]			

Combustion is solved with a multi-zone approach. This means that to determine the new species for each computational cell as a result of chemical reactions, rather than calling CHEMKIN for every cell individually, KIVA3V-MZ-MPI gathers the species of cells that are similar in temperature and equivalence ratio into zones, and solves the reactions for these zones. The new zonal species are then mapped back to the cells from which they came and the resulting energy release for each cell is calculated. Approximately 100 zones are used for the simulation. More detailed information about KIVA3V-MZ-MPI can be found in [3].

The engine is fueled by n-heptane. The University of Wisconsin-Engine Research Center n-heptane mechanism [9] is used to predict n-heptane autoignition. The mechanism has 29 species and 52 reactions. Run time for a 720° simulation is approximately three days running in parallel on eight Intel Core2 Duo E6600 processing cores. Note that the multi-zone chemistry solver runs in parallel while the CFD part of the simulation runs on a single processor.

Figure 3 shows a cylinder pressure comparison for this engine at $\Phi = 0.293$ and an engine speed of 1200 RPM. The model does a reasonable job of matching the measured pressure for the purpose of this paper.

As an aside, note that no model tuning has been done to obtain this match. Model initial and boundary conditions are either from measurements, or from engineering

estimates. Often, reaction rates and intake temperatures and/or pressures are adjusted to get a better match to the data. Since the full engine cycle is being modeled, it is felt that tuning is not the appropriate first step to obtain a better match. Instead, the impact of boundary conditions, like uniform and constant temperature walls are being investigated. It has also been observed that the sudden closing of valves with zero thickness walls causes locally high temperatures, which can then determine the start of HCCI reactions. These are areas of current research.

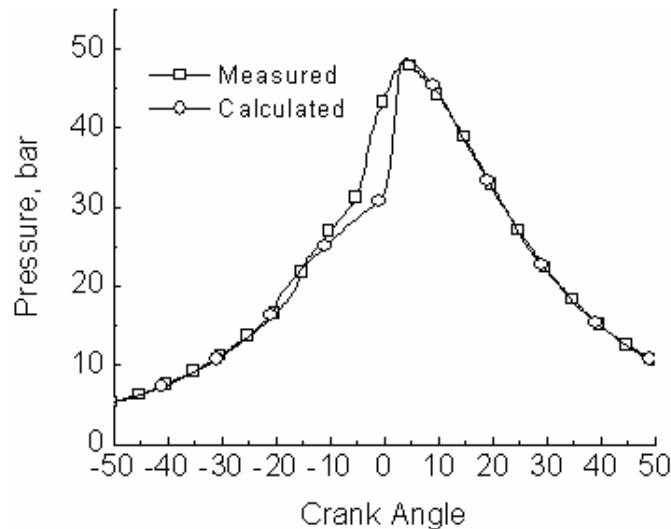


Figure 3. Measured and calculated cylinder pressures. $\Phi = 0.293$, engine speed = 1200 RPM.

PATHLINES

A particle trace portrays a vector field by displaying the path that a massless particle would follow if placed in that field. At each point on the particle trace, the direction of the trace is parallel to the velocity vector field at that point and time. A streamline is a particle trace in a steady-state vector field, while a pathline is a particle trace in a time-varying vector field. [10]

In addition to visualization, pathlines can be used to trace the evolution of species in time and space. Here, pathline analysis follows packets of intake gas in time and space from induction, through compression and combustion. The local scalar fields traversed by the individual packets in terms of species concentration, temperatures, velocity magnitude and turbulence are extracted from the model results. The results show how the intake event establishes local chemical and thermal environments in-cylinder and how the species respond (chemically react) to the local field.

For this study, pathline creation is strictly a post-processing exercise. No modifications have been made to the CFD code to provide them. The commercial software visualization program EnSight [10] is used to

visualize and extract pathline information from the CFD results.

EnSight creates pathlines by integrating the vector field variable over time using a Fourth Order Runge-Kutta method and utilizing a time-varying integration step. The integration step is lengthened or shortened depending on the flow field, but the minimum number of integration steps performed can be controlled [10].

There are at least three resolutions to discuss regarding pathlines, namely spatial, temporal and density resolution.

Spatial resolution is a function of the computational cell size. In KIVA3V-MZ-MPI, distinct velocity values exist at the vertices of each cell. These are the velocities available for pathline creation.

Temporal resolution for pathlines is a function of how frequently CFD results are written as output to files. Where temporal resolution for CFD is typically about 1 microsecond, for pathline creation one crank degree increments are used. Pathline temporal resolution can be increased, but only at the cost of increased file size. The output file from KIVA3V-MZ-MPI (called otape9) is about 35 gigabytes for a 720° simulation when writing with 1° resolution. Such large amounts of data are not practical for processing interactively on typical desktop computers. Instead, the post-processing is done in batch mode.

The third resolution to discuss is density. Density refers to the number of pathlines created within the computed domain. Creating more pathlines provides more information about the flow field, but too many pathlines can produce images that contain so much information that no distinct flow structures or trends can be distinguished. The user must choose a density that sufficiently resolves the features of the flow field while still permitting adequate visualization.

Another important consideration is pathline termination. In EnSight, pathlines terminate for any of the following reasons: [10]

1. The pathline moves outside the space in which the vector field is defined (*the user may choose to define only a portion of the flow domain for pathline creation*),
2. A user-specified time limit is reached,
3. The particle becomes stationary in a place where the vector field is zero, or
4. The last transient-data time step is reached.

Therefore, a pathline created at the first available time step may not survive until the last available time step, it