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Modeling HCCI using CFD and Detailed Chemistry with Experimental Validation and a Focus on CO Emissions

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Multi-zone CFD simulations with detailed kinetics were used to model engine experiments performed on a diesel engine that was converted for single cylinder, HCCI operation, here using iso-octane as the fuel. The modeling goals were to validate the method (multi-zone combustion modeling) and the reaction mechanism (LLNL 857 species iso-octane), both of which performed very well. The purpose of this paper is to document the validation findings and to set the ground work for further analysis of the results by first looking at CO emissions characteristics with varying equivalence ratio.

Experimental Setup

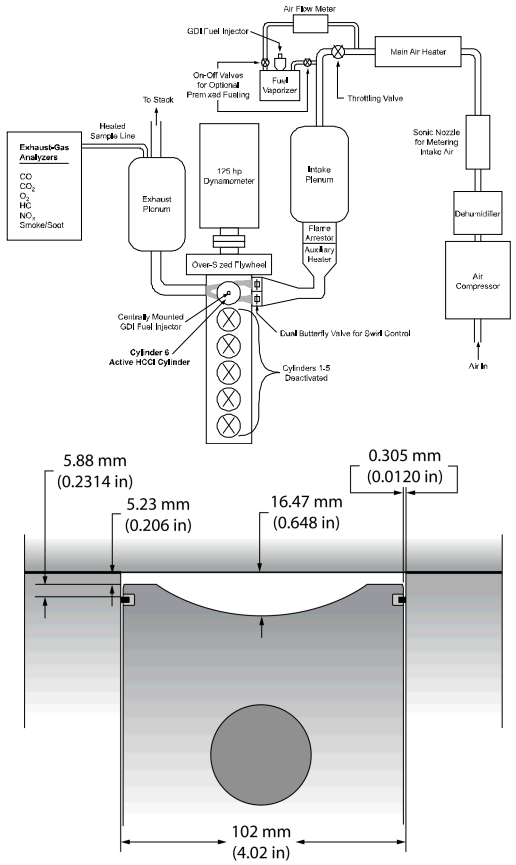

Figure 1. Schematics of engine (top) and combustion chamber (bottom).

Experiments were carried out on a Sandia National Laboratories research engine, which is based on a Cummins B-series diesel engine, a typical medium-duty diesel engine with a displacement of 0.98 liters/cylinder. Figure 1 (top) shows a schematic of the engine, which has been converted for single cylinder HCCI operation. The engine specifications are listed in Table 1 [1].

Figure 1 (bottom) is a schematic of the combustion chamber and includes representations of the liner, head (no valves), piston with a shallow dish, the top ring and ring groove. The air compressor (figure 1 top) was used to boost the intake charge (table 1) so that the currently used 13.8 compression ratio piston would be representative of previous work done on this engine, but performed naturally aspirated, with a 18:1 compression ratio piston. Intake temperature (table 1) was varied with the Main Air Heater (figure 1) to maintain the 50% heat release point at top dead center as equivalence ratio was varied from 0.08 to 0.28 in steps of 0.02. Iso-octane was injected into the Fuel Vaporizer (figure 1 top, top-center) to provide a pre-mixed charge to the cylinder.

Table 1. Engine and model specifications. Equivalence ratio increment was 0.02.

	Engine	Model
Fueling mode	Fully pre-mixed	Fully pre-mixed
Combustion mode	HCCI	HCCI
Fuel	Iso-octane	Iso-octane
Engine speed, RPM	1200	1200
Compression ratio (CR)	13.8 *	13.5 *
Bore x Stroke, mm	102 x 120	102 x 120
Cycle	4 stroke	IVC - EVO
Equivalence ratio sweep	0.08,0.10,… 0.28	0.08,0.10,… 0.28
Intake(engine),IVC(model) pres, bar	1.35	1.35
Intake(engine),IVC(model) temp, K	454 – 482	468 - 478
Swirl ratio	0.9	0.9

*CR was measured on engine and was adjusted to match motored pressure traces in the model.

Model Setup

KIVA3V from Los Alamos National Lab [2] with additional subroutines and model improvements from UW-Madison's Engine Research Center (ERC) was the foundation on which a multi-zone version of KIVA3V, KIVA3V-MZ [3], was built. Like KIVA3V, at each time step KIVA3V-MZ solves for mass, momentum, energy, turbulence, wall heat transfer, chemical reactions, etc. What sets KIVA3V-MZ apart is how it solves the chemical reaction mechanism, i.e., how KIVA3V-MZ uses CHEMKIN to estimate the evolution of in-cylinder species resulting from combustion. All simulations used the LLNL 857 species/3605 reactions iso-octane mechanism [4].

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 gathers the species of cells, 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 were used for each simulation. More detailed information about KIVA3V-MZ can be found in [3].

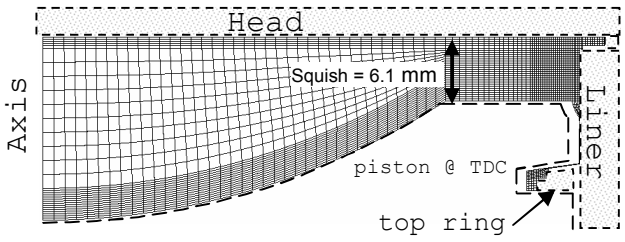

Fig. 2 Mesh at TDC, 2D axi-symmetric.

Figure 2 shows the mesh at TDC that was used for modeling the Sandia engine. The mesh is 2D and axi-symmetric and going around it in the clockwise direction, the left side represents the cylinder axis, the top a flat head (no valves represented) extending to the head gasket (gasket hole is larger than the bore), then over and down along the liner to the top of the top ring, following the top ring inward and down to where the ring rests on the piston's ring groove. The remainder of the grid boundary represents piston surfaces.

Model gases flow freely between the main chamber and the crevices, but no gas leaves the grid, i.e., mass is constant. The engine exhibits only a small fraction of blowby, so the constant mass assumption should not contribute significantly to inaccuracies. Model specifications are given in table 1. Equivalence ratio was increased primarily by homogenously adding more fuel at IVC. Other species initialized at IVC included CO2, H2O, CO, and IC8H18 and CH2O as the primary residual unburned hydrocarbon and oxygenated hydrocarbon species.

Results

Measured and calculated pressure traces are shown in figure 3. The figure's top row shows that the model captures pressure trends with varying equivalence ratio (phi). The bottom row shows particular case comparisons and demonstrates that pressure magnitudes are also captured very well, although slightly under-predicting at the lower phi values.

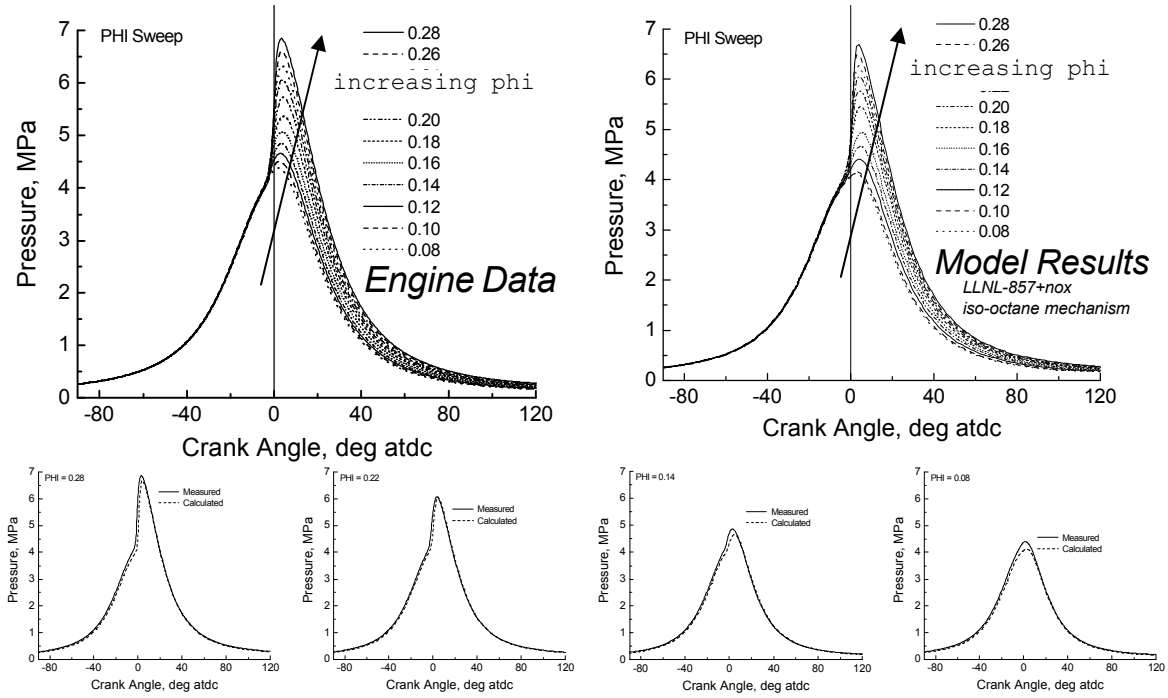

Figure 3. (Top) Pressure traces with varying equivalence ratio, engine data (left) and model results (right). (Bottom) Pressure trace comparisons for (left to right) equivalence ratio=0.28, 0.22, 0.14, 0.08.

Figure 4 compares CO, CO2, unburned hydrocarbons (HC) and oxygenated hydrocarbons (OHC). Measured values were sampled downstream of the exhaust tank, while "Calculated" were in-cylinder values at exhaust valve opening. Units for figure 4 are grams of species in the exhaust gas (measured), or at EVO (calculated) per kg of fuel.

CO and CO2 trends and magnitudes are considered well characterized by the model, as are HC and OHC considering the following. Measured HC is an estimate of H-C bonds of all unburned hydrocarbons in the exhaust, while the calculated curve only accounts for unburned iso-octane. Therefore, measured vales are, as expected, larger, due to the presence of smaller HC's, but trends are the same. Measured OHC are estimates of all OHC in the exhaust stream and the values result from carbon balance calculations. The measured OHC values reflect uncertainties in the measurements of all other carbon atoms, i.e., uncertainties in fuel flow, CO, CO2 and HC measurements, resulting in rather sharp changes in slope. The calculated values only account for three of the more prevalent OHC species, and therefore are, as expected, lower than measured, but with the same general trend.

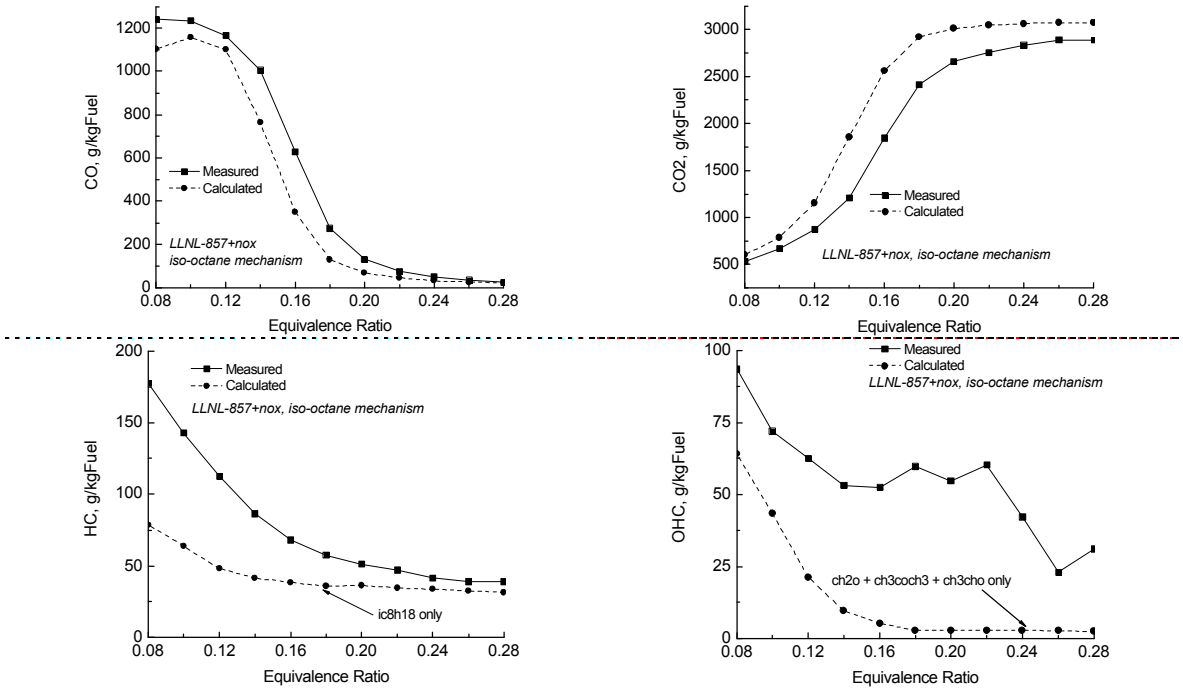

Figure 4. Emissions comparisons CO, CO2 HC and OHC. Measured values (solid lines) are from exhaust stream, calculated values (dashed lines) are in-cylinder averages at EVO.

Results from a similar study [5] using the same engine and engine speed, but using an 18:1 compression ratio piston with atmospheric pressure intake charge, concluded that a peak temperature of "1500 K was needed for the CO-to-CO2 reactions to go to completion before combustion is quenched by piston expansion." Their conclusion was based on analysis of measured data and single zone modeling. The "peak temperature" referred to was the maximum in-cylinder temperature during the closed portion of the cycle and since the analysis used a single zone model, the average in-cylinder and peak temperatures at any given crank angle were the same number. Figures 5 through 7 give a multi-zone twist to this conclusion.

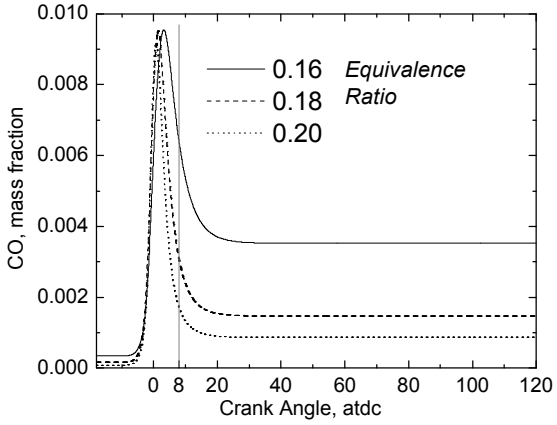

Figure 5. CO mass fraction vs. crank angle for three phi cases.

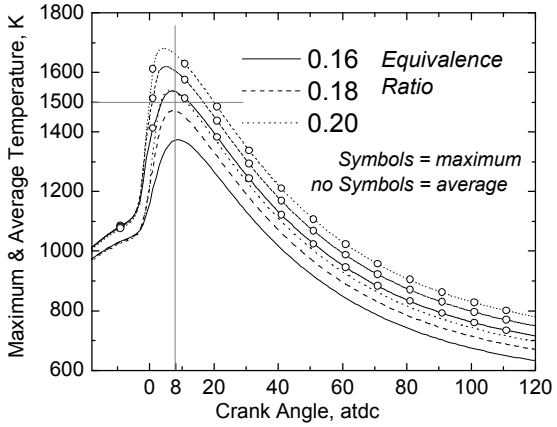

Figure 6. Maximum and average temperature for three phi cases.

The CO graph of figure 4 shows a substantial CO increase over the equivalence ratios (phi) 0.20 - 0.18 - 0.16. For this discussion, as in [5], the CO-to-CO2 reactions are considered as going to completion for the phi=0.20 case (CO is relatively low). Figure 5 shows how the in-cylinder average CO varies with crank angle for these three cases (the values at 120 atdc are the same values as those plotted in figure 4). It is

interesting that all cases have almost the same maximum in-cylinder CO value and at almost the same crank angle, then come to equilibrium in a similar manner.

Figure 6 shows the average and maximum temperatures vs. crank angle for the same cases as figure 5. The maximum temperatures all surpass the 1500 K 'threshold' for the CO-to-CO2 reactions to go to completion, but the average temperatures do not. Thus, this finding is in agreement with [5], with the stipulation that it is the average temperature that must reach 1500 K.

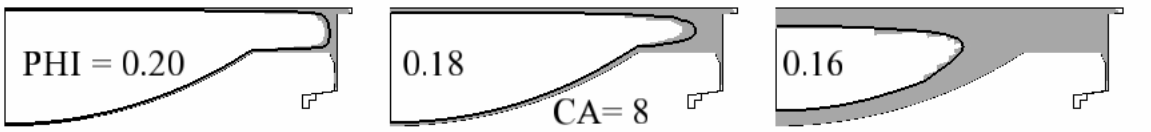

Figure 7. Shaded regions indicate relatively high CO concentration. The black line is the 1500 K iso-surface.

Figure 7 goes into one more level of detail. The gray shaded regions highlight where CO mass fractions are the highest (greater than or equal to 0.002) at 8 degrees after TDC (atdc). Concentrations below 0.002 are invisible. The black line is the 1500 K iso-surface at 8 atdc. All temperatures encompassed by the iso-surface are greater than 1500 K and all temperatures outside are below 1500 K. This crank angle was chosen because it is the crank angle where the average temperature reaches its maximum value (figure 6). What this means in terms of the 1500 K line is that prior to 8 atdc the line is moving outward, toward the surfaces and engulfing more mass into the >1500 K zone. After 8 atdc the line is moving inward, away from the surfaces and no, or little new mass is being subjected to temperatures greater than 1500 K.

Figure 8. CO distribution for the phi=0.08 case @ EVO. Dark=high, light=low concentration.

Figure 7 supports the claim from [5] and previously supported by Aceves et al. [6], that in this engine, "The progressive spread of incomplete combustion from the top ring land crevice (and the head gasket volume) to the boundary layer and finally throughout the bulk of the charge as the fueling is reduced causes the more gradual rise of CO (as compared to a single zone model in this phi range)."

Finally it is worth mentioning that as phi is further reduced, most of the CO forms in the bulk gas, as iso-octane in the boundary layer only breaks down to the intermediate HC stage, not down to the CO forming stage (figure 8).

Summary/Conclusions/Future Work

Using a multi-zone version of KIVA3V combined with the LLNL 857-species mechanism for iso-octane, we have demonstrated the ability to capture observed combustion and emissions characteristics of these HCCI experiments.

Model results suggest that:

- At the higher phi values, most CO comes from the relatively cold crevice gases and the gases that leave the crevices during the expansion stroke and form near crevice boundary layers.
- At intermediate phi values, most of the CO comes from the same source as just mentioned, but also includes non-crevice related boundary layers that are again, relatively cold.

- At lower phi values most of the CO comes from bulk gases, as they are hot enough to form CO, but are not hot enough for long enough to form CO2. At these conditions, the near-surface gas does not get hot enough to form CO, and it produces OHC and HC emissions.
- The 1500 K average temperature looks to be a good indicator for the measure of completion of the CO-to-CO2 reactions for this engine. Visualization shows that as the maximum average temperature falls below 1500 K, the mass of charge that remains cold, and hence does not burn to completion, increases rapidly.

Future work:
- Investigate the model results more fully.
- Compare model results to speciation data that was taken for the 14:1 compression ratio experiments.

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References

1. Sjoberg, M., Dec, J.E., "An Investigation of the Relationship between Measured Intake Temperature, BDC Temperature, and Combustion Phasing for Premixed and DI HCCI Engines", SAE Paper 2004-01-1900, 2004.
2. Amsden, A. A., "KIVA-3V: A Block-Structured KIVA Program for Engines with Vertical or Canted Valves", Los Alamos National Laboratory Report No. LA-13313-MS, 1997.
3. Babajimopoulos, A., Assanis, D.N., Flowers, D L, Aceves, S.M. and Hessel, R.P., "A fully coupled computational fluid dynamics and multi-zone model with detailed chemical kinetics for the simulation of premixed charge compression ignition engines", IJER, Vol. 6, No. 5, p. 497, 2005.
4. Curran, H.J., Gafurri, P., Pitz, W.J. and Westbrook, C.K., "A Comprehensive Modeling Study of iso-Octane Oxidation", Combustion & Flame 129:253-280, 2002.
5. Sjoberg, M., Dec, J.E., "An Investigation into Lowest Acceptable Combustion Temperatures for Hydrocarbon Fuels in HCCI Engines", Combustion Symposium, 2005.
6. Aceves, S.M., Flowers, D.L., Francisco Espinosa-Loza, J.M., Dec, J.E., Magnus, S., Dibble, R.W., Hessel, R.P., "Spatial Analysis of Emissions Sources for HCCI Combustion at Low Loads Using a Multi-Zone Model", SAE Paper 2004-01-1910, 2004.