David Rothamer Joins the Engine Research Center

This January Professor David A. Rothamer joined the Engine Research Center as a Principal Investigator. Professor Rothamer recently graduated with his PhD from the High Temperature Gas Dynamics Laboratory at Stanford University and is a former graduate student member of the Engine Research Center, where he received his M.S. degree. His PhD work focused on the development and optimization of planar laser-induced fluorescence diagnostics for simultaneous measurement of temperature and EGR in IC engines. The developed diagnostic technique was applied in an optical engine at Sandia National Laboratories Combustion Research Facility to study in-cylinder stratification in temperature and EGR during HCCI operation and HCCI operation with large NVO.

Professor Rothamer will be setting up research laboratories in the ERC and will be directing graduate students in research. His research interests include the optimization of alternative fuels combustion in IC engines and studying the formation mechanisms and in-cylinder minimization of soot and other pollutants.

Mike Andrie Joins the Engine Research Center

This fall Michael J. Andrie joined the Engine Research Center as an Associate Researcher. He coordinates and mentors ERC graduate students in their experimental internal combustion engine lab research activities. He will also serve as Program Manager for DERC. Mike has 26 years of industry performance and mechanical development experience on advanced compression ignition engines for commercial automotive and off-road applications. During this time, he developed and patented two different heat exchanger systems and led multiple project teams who delivered very successful products to the market place. His wealth of experience and understanding of combustion, emissions, and fuel systems in compression ignition engines as related to practical constraints provides valuable direction for ERC research. He received his BS and MS degrees from the University of Minnesota and worked for John Deere, and Cummins on diesel engine development.
ERC Student Seminars
Begin in Collaboration with
EPD’s MEES Students

ERC has launched a student seminar series to provide a venue for wider com-
communication on the various research projects being conducted at the ERC. The
seminars are also intended to foster communication, knowledge transfer, and
networking between the MEES (Masters in Engineering of Engine Systems, http://mees.engr.wisc.edu) students in
industry and ERC students on campus. In addition, these seminars allow speakers
an opportunity to receive constructive feedback on their projects from the audi-
ence. DERC members are encouraged to review any of the seminars that are of
interest.

The Spring 2008 seminars schedule is
listed below:
Place: 1106 ME
Time: 4:15 – 4:45 PM on
Tuesdays
Start date: January 22nd (1st
week of classes)
End date: May 6th (last week of
classes)
Skipped dates: March 18th (Spring
break); April 15th (SAE week)
Taped Sessions*: http://mediasite.engr.wisc.edu

*Note that there is no ‘www.’ Use the scrollbar on the left to find the ‘ERC Student Seminar’ link which can be viewed
anytime.
The presentations should be about 30
minutes long, which includes time for
questions. Questions can be asked at
anytime during the presentation (when a
live feed is available). The seminars will
include the following information:
• Sufficient background for a general
  audience,
• The goals and objectives of the pro-
  ject.
• How the project ties in with other
  ERC projects.
• How the project fits into the big pic-
  ture view of research area.
• Acknowledgments.
• Technical content.
• Contact information

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T-25 Breakfast

Once again we invite all of the ERC alumni to the T-25 breakfast. The breakfast oc-
curs from 7:00 am–10:00 am, Wednesday morning during the week of the SAE
International Congress. A continental breakfast will be available in the atrium at the
Marriott Courtyard in Downtown Detroit on April 16th. We are very pleased that Gen-
eral Motors Research and Development Center is sponsoring the event.

DERC Sets Annual Meeting

Progress on the four Diesel Emissions Research Consortium (DERC) research projects
during the fourth quarter of 2007 was good. Please mark your calendars, the DERC
Annual Meeting will be June 3rd, 2008. Several new graduate students are now supported
under DERC projects and are making good progress. The current projects and
students include:

• Project #1: Examination of the characteristics of stoichiometric diesel combustion.
The engine has been moved to its new location, upgraded and is under-
going initial tests, as performed by DERC PhD student Junghwan
Kim. In addition, a post-doctoral student, Dr. Kian Sung is participat-
ing in the lab development.

• Project #2: The transient engine test cell for the new engine is being benchmarked
by DERC student Jon Burton.

• Project #3: System level tools are being extended and applied to analyze the tran-
sient test cell data by DERC student James Popp.

• Project #4: DERC student Sage Kokjohn is exploring injection strategies for two-
stage combustion, as applied to high load HCCI operation in heavy-
and light-duty diesel engines.

• Project #5: A new project has been initiated on the transient engine used in project
#2. This project is co-sponsored by the Myers fund, and is being conducted
by new student Will Glewen.

If you have any comments about the projects in this Newsletter, please feel free to
contact the relevant student or contact Mike Andrie (mandrie@wisc.edu - DERC Pro-
gram Manager) or me (reitz@engr.wisc.edu). We will be pleased to consider any sug-
gestions you may have for project improvements in our project planning.
In the present study a reduced chemical reaction mechanism for biodiesel surrogate fuel was developed and validated for multi-dimensional engine combustion simulations. An existing detailed methyl butanoate mechanism that contained 264 species and 1219 reactions was chosen to represent the oxygenated portion of the fuel. The reduction process included flux analysis, ignition sensitivity analysis, and optimization of reaction rate constants under constant volume conditions. The current reduced mechanism consists of 41 species and 150 reactions and gives predictions in excellent agreement with those of the comprehensive mechanism. In order to validate the mechanism under biodiesel-fueled engine conditions, it was combined with another skeletal mechanism for n-heptane oxidation. This combined reaction mechanism can be used to adjust the energy content of the fuel, and account for diesel/biodiesel blend engine simulations. The combined mechanism, ERC-bio, contains 53 species and 156 reactions. Biodiesel-fueled engine operation was successfully simulated using the ERC-bio mechanism.

In these studies, the swirl center was initialized at different positions in the chamber for different cases to simulate the effects of different intake flow arrangements. To aid the comparisons, the angular momentum referred to the swirl center was kept constant in each case. Numerical results of off-centered swirl cases were compared with the centered swirl case, as well as with available experimental images obtained using laser induced fluorescence (LIF), laser induced incandescence (LII), and particle image velocimetry (PIV). Eccentric phenomena observed in the experiments were well predicted by the present method. The off-centered swirl was found to have higher turbulence intensities and effective diffusivities, which enhance the mixing process. Soot formation is strongly correlated with the turbulent viscosity. Off-centered swirl flow results in an asymmetric distribution of turbulent viscosity and consequently an asymmetric distribution of soot emissions. Analysis of the mass distributions of temperature showed that the resulting mixture is a little more homogeneous with larger off-centered swirl flows, which leads to a slight reduction in NOx emissions. The off-centered swirl delays the formation of acetylene, which changes the phasing of soot formation.

The lift-off length plays a significant role in spray combustion as it influences the air entrainment upstream of the lift-off location and hence the soot formation. Accurate prediction of lift-off length thus becomes a prerequisite for accurate soot prediction in lifted flames. In the present study, KIVA-3v coupled with CHEM/KIN, as developed at the Engine Research Center (ERC), is used as the CFD model. Experimental data from the Sandia National Labs. is used for validating the model predictions of n-heptane lift-off lengths and soot formation details in a constant volume combustion chamber. It is seen that the model predictions, in terms of lift-off length and soot mass, agree well with the experimental results for low ambient density (14.8 kg/m3) cases with different EGR rates (21% O2 - 8% O2). However, for high density cases (30 kg/m3) with different EGR rates (15% O2 - 8% O2) disagreements were found. Accordingly, the reduced chemistry mechanism was updated to include intermediate cool flame reactions involving ketohydroperoxide and formaldehyde radicals for improving the lift-off length predictions. Also, a comparison of the predictive capabilities of a two-step and a detailed nine-step phenomenological soot model was done. Overall, the present CFD model is able to replicate the qualitative trends of lift-off and soot formation at different EGR rates for both ambient densities.
Engine design is a time consuming process in which many costly experimental tests are usually conducted. With increasing prediction ability of engine simulation tools, engine design aided by CFD software is being given more attention by both industry and academia. It is also of much interest to be able to use design information gained from an existing engine design of one size in the design of engines of other sizes to reduce design time and costs. Therefore it is important to study size-scaling relationships for engines operating in different regimes and will benefit the engine design process and provide guidelines for meeting future emission regulations.

Homogeneous Charge Compression Ignition (HCCI) combustion is being considered as a practical solution for diesel engines due to its high efficiency and low NOx and PM emissions. However, for diesel HCCI operation, there are still several problems that need to be solved. One is the spray-wall impingement issue associated with early injection, and a further problem is the extension of HCCI operation from low load to higher engine loads. In this study, a combination of Adaptive Injection Strategies (AIS) and a Two-Stage Combustion (TSC) strategy are proposed to solve the aforementioned problems.

A multi-dimensional Computational Fluid Dynamics (CFD) code with detailed chemistry, the KIVA-CHEMKIN-GA code, was employed in this study, where Genetic Algorithms (GA) were used to optimize heavy-duty diesel engine operating parameters. The TSC concept was applied to optimize the combustion process at high speed (1737 rev/min) and medium load (57% load). Two combustion modes are combined in this concept. The first stage is ideally HCCI combustion and the second stage is diffusion combustion under high temperature and low oxygen concentration conditions. AIS were proposed to achieve and optimize the TSC. AIS incorporates the use of multiple injections with different spray geometries and injection pressures. Part of the fuel is injected into the cylinder at a low injection pressure (10MPa) and a narrow spray angle (90°) to avoid spray-wall impingement and to prepare a homogeneous mixture for the HCCI combustion. The remaining fuel is injected into the cylinder at a high injection pressure (150MPa) and a wide spray angle (127°) to experience diffusion combustion and to provide extended load capability. An Adaptive Injection Strategy, which uses one injector with single included angle but two different injection pressure levels, was also evaluated in this study.

Several engine operating parameters were optimized: Intake Valve Closure (IVC) timing, Exhaust Gas Recirculation (EGR) ratio, start of low-pressure and high-pressure injection timings and the fraction of fuel participating in the HCCI combustion (HCCI ratio). The results show that by combining the AIS with a late IVC timing, a medium EGR level, and a high HCCI ratio, TSC is able to achieve low engine-out emissions with spray-wall impingement avoided at a medium engine load. The TSC concept shows great potential to meet future ultra-low emission standards.
Homogeneous charge compression ignition (HCCI) combustion is considered to be an attractive alternative to traditional internal combustion engine operation because of its extremely low levels of pollutant emissions. However, there are several difficulties that must be overcome for HCCI practical use, such as difficult ignition timing controllability. Indeed, too early or too late ignition can occur with obvious drawbacks. In addition, the increase in cyclic variation caused by the ignition timing uncertainty can lead to uneven engine operation. As a way to solve the combustion phasing control problem, dual-fuel combustion has been proposed. It consists of a diesel pilot injection used to ignite a pre-mixture of gasoline (or other high octane fuel) and air. Although dual-fuel combustion is an attractive way to achieve controllable HCCI operation, few studies are available to help the understanding of its in-cylinder combustion behavior. In this paper, numerical simulations of dual-fuel combustion processes are presented. An implemented version of the multidimensional CFD KIVA3V code was used for the study. This version incorporates various advanced sub-models, including the G-equation flame propagation model coupled with CHEMKIN. The influence of injection timing and mixture composition on emission production, as well as on combustion pressure and on heat release rate has been analyzed with two different multi-hole injectors (six and eight holes). Four combustion strategies were compared, and pressure, heat release rate, temperature and emissions results are provided. As expected, decreasing the amount of diesel fuel injected, combustion behavior becomes closer to HCCI combustion, especially with the eight-hole injector. An effective ignition controllability has been obtained with very low percentages of injected diesel fuel for the whole set of considered injection timings.


Lagrangian-Droplet and Eulerian-Fluid (LDEF) based spray models are widely used in engine and combustion system computations. Numerical grid and time-step dependencies of Discrete Droplet Lagrangian spray models have been identified by previous researchers [1, 2]. The two main sources of grid-dependency are due to errors in predicting the droplet-gas relative velocity, and errors in describing droplet-droplet collision and coalescence processes. For reducing grid-dependency due to the relative velocity effects, results from gas jet theory are introduced along with a Lagrangian collision model [1, 3] and applied to model diesel sprays. The improved spray model is implemented in the engine simulation code KIVA-3V [4] and is tested under various conditions, including constant volume chambers and various engine geometries with vaporizing and combusting sprays with detailed chemistry. The results with the improved model show greater meshindependency as compared to the conventional LDEF methodology.


A computational study using multi-dimensional CFD modeling was performed to investigate the effects of physical properties on diesel engine combustion characteristics with bio-diesel fuels. Properties of typical bio-diesel fuels that were either calculated or measured are used in the study and the simulation results are compared with those of conventional diesel fuels. The sensitivity of the computational results to individual physical properties is also investigated, and the results provide information about the desirable characteristics of the blended fuels. The properties considered in the study include liquid density, vapor pressure, surface tension, liquid viscosity, liquid thermal conductivity, liquid specific heat, latent heat, vapor specific heat, vapor diffusion coefficient, vapor viscosity and vapor thermal conductivity. The results show significant effects of the fuel physical properties on ignition delay and burning rates at various engine operating conditions. It is seen that there is no single physical property that dominates differences of ignition delay between diesel and biodiesel fuels. However, among the 11 properties considered in the study, the simulation results were found to be most sensitive to the liquid fuel density, vapor pressure and surface tension through their effects on the mixture preparation processes.
A three-dimensional homogeneous equilibrium model (HEM) has been developed and implemented into an engine computational fluid dynamics (CFD) code KIVA3V. The model was applied to simulate cavitating flow within injector nozzle passages. The effects of nozzle passage geometry and injection conditions on the development of cavitation zones and the nozzle discharge coefficient were investigated. Specifically, the effects of nozzle length (L/D ratio), nozzle inlet radius (R/D ratio) and K or KS factor (nozzle passage convergence) were simulated, and the effects of injection and chamber pressures, and time-varying injection pressure were also investigated. These effects are well captured by the nozzle flow model, and the predicted trends are consistent with those from experimental observations and theoretical analyses. The flow distributions (density, velocity, etc.) at the nozzle exit obtained from the nozzle flow simulations were further coupled with an Eulerian-Lagrangian Spray and Atomization (ELSA) model to investigate the effects of nozzle flow physics on the downstream spray atomization process. Both non-vaporizing and vaporizing sprays were investigated in this study.

Low-temperature combustion (LTC) strategies for diesel engines are of increasing interest because of their potential to significantly reduce particulate matter (PM) and nitrogen oxide (NOx) emissions. LTC with late fuel injection further offers the benefit of combustion phasing control because ignition is closely coupled to the fuel injection event. But with a short ignition-delay, fuel jet mixing processes must be rapid to achieve adequate premixing before ignition. In the current study, mixing and pollutant formation of late-injection LTC are studied in a single-cylinder, direct-injection, optically accessible heavy-duty diesel engine using three laser-based imaging diagnostics. Simultaneous planar laser-induced fluorescence of the hydroxyl radical (OH) and combined formaldehyde (H2CO) and polycyclic aromatic hydrocarbons (PAH) are compared with vapor-fuel concentration measurements from a non-combusting condition. Through comparative analysis of OH, H2CO, and PAH fluorescence, mixtures are identified as either fuel-lean, fuel-rich, or of intermediate stoichiometries. The impacts of combustion chamber design on in-cylinder mixing processes are explored by comparing three piston bowl diameters of 60%, 70%, and 80% of the cylinder bore. The data show that piston-bowl diameter influences in-cylinder mixing and pollutant formation processes by altering jet-jet and jet-wall interactions. When the fuel jets impinge on the bowl wall prior to ignition, adjacent jets merge, forming fuel-rich regions where soot formation occurs. By using a larger diameter bowl, wall impingement prior to ignition is reduced and delayed, and mixtures are leaner throughout the jet. However, a greater fraction of the jet becomes too lean for complete combustion. By using a smaller diameter bowl, a strong jet-wall interaction pushes the fuel-rich jet-jet interaction regions into the center of the chamber, where mixtures are predominantly lean. This reduces net soot formation and displaces fuel-lean regions of otherwise incomplete combustion into the combusting regions near the bowl wall.

In-cylinder flow and combustion processes simulated with the standard k-ε turbulence model and with an alternative model—employing a non-linear, quadratic equation for the turbulent stresses—are contrasted for both motored and fired engine operation at two loads. For motored operation, the differences observed in the predictions of mean flow development are small and do not emerge until expansion. Larger differences are found in the spatial distribution and magnitude of turbulent kinetic energy. The non-linear model generally predicts lower energy levels and larger turbulent time scales. With fuel injection and combustion, significant differences in flow structure and in the spatial distribution of soot are predicted by the two models. The models also predict considerably different combustion efficiencies and NOx emissions. The turbulence model impacts entrainment and jet velocity; this is believed to be the major factor influencing the flow structure development and the formation of NOx emissions. Like the motored simulations, major differences in the distribution and magnitude of turbulent kinetic energy and time scale are seen—differences which are likely to impact the modeled combustion behavior.
In this study we identify components of a typical biodiesel fuel and estimate both their individual and mixed thermo-physical and transport properties. We then use the estimated mixture properties in computational simulations to gauge the extent to which combustion is modified when biodiesel is substituted for conventional diesel fuel. Our simulation studies included both conventional diesel combustion (DI) and premixed charge compression ignition (PCCI). Preliminary results indicate that biodiesel ignition is significantly delayed due to slower liquid evaporation, with the effects being more pronounced for DI than PCCI. The lower vapor pressure and higher liquid heat capacity of biodiesel are two key contributors to this slower rate of evaporation. Other physical properties are more similar between the two fuels, and their impacts are not clearly evident in the present study. Future studies of diesel combustion sensitivity to both physical and chemical properties of biodiesel are suggested.
A new predictive model for collisional interactions between liquid droplets, which is valid for moderate to high Weber numbers (>40), has been developed and validated. Four possible collision outcomes, viz., bouncing, coalescence, reflexive separation and stretching separation, are considered. Fragmentations in stretching and reflexive separations are modeled by assuming that the interacting droplets form an elongating ligament that either breaks up by capillary wave instability, or retracts to form a single satellite droplet. The outcome of a collision, number of satellites formed from separation processes and the post-collision characteristics such as velocity and drop-size are compared with available experimental data. The comparisons include colliding mono- and poly-disperse streams of droplets of different fuels under atmospheric conditions, and the results agree reasonably well.

A highly diluted, low-flame-temperature diesel engine combustion strategy with two separate fuel-injections per cycle was investigated using simultaneous optical diagnostics at a low-load operating condition. In-cylinder processes were visualized with a suite of laser-imaging diagnostics. The cool flame first-stage ignition reactions occur along the entire length of the jet for the first combustion event. For both injections, the second-stage ignition reactions occur after the end of injection, primarily in the downstream regions of the jet. OH is found throughout the cross-section of the jet, indicating greater mixing and leaner mixtures than observed for conventional diesel combustion. For the first combustion event, very little soot is formed and it is found in small pockets near the tip of the jet. For the second combustion event, much more soot is formed throughout the downstream jet cross-section. Finally, Sandia’s conceptual model of diesel combustion has been extended to describe this operating condition.

Two-color soot optical pyrometry is a widely used technique for measuring soot temperature and volume fraction in many practical combustion devices, but line-of-sight soot temperature and volume fraction gradients can introduce significant uncertainties in the measurements. For diesel engines, these uncertainties usually can only be estimated based on assumptions about the soot property gradients along the line of sight, because full three dimensional transient diesel soot distribution data are not available. Such information is available, however, from multidimensional computer model simulations, which are phenomenologically based, and have been validated against available in-cylinder soot measurements and diesel engine exhaust soot emissions. Using the model predicted in-cylinder soot distributions, uncertainties in diesel two-color pyrometry data are assessed, both for a conventional high-sooting, high-temperature combustion (HTC) operating condition, and for a low-sooting, low temperature combustion (LTC) condition. The simulation results confirm that the two-color soot measurements are strongly biased toward the properties of the hot soot. For the HTC condition, line-of-sight gradients in soot temperature span 600 K, causing relatively large errors. The two-color temperature is 200 K higher than the sootmass-averaged value, while the two-color volume fraction is 50% lower. For the LTC condition, the two-color measurement errors are half as large as for the HTC condition, because the model-predicted soot temperature gradients along the line of sight are half as large. By contrast, soot temperature and volume fraction gradients across the field of view introduce much smaller errors of less than 50 K in temperature and 20% in volume fraction.
Fundamental simulations in a quiescent cell under adiabatic conditions were made to understand the effect of temperature, equivalence ratio and the components of the recirculated exhaust gas, viz., CO₂ and H₂O, on the combustion of n-Heptane. Simulations were made in single phase in which evaporated n-Heptane was uniformly distributed in the domain. Computations were made for two different temperatures and four different EGR levels. CO₂ or H₂O or N₂ was used as EGR.

It was found that the initiation of the main combustion process was primarily determined by two competing factors, i.e., the amount of initial OH concentration in the domain and the specific heat of the mixture. Further, initial OH concentration can be controlled by the manipulating the ambient temperature in the domain, and the specific heat capacity of the mixture via the mixture composition. In addition to these, the pre combustion and the subsequent post combustion can also be controlled via the equivalence ratio.

In order to verify these findings in a two phase scenario, Direct Numerical Simulation (DNS) type procedures were applied to a two-dimensional domain in which liquid n-Heptane droplets were pre-distributed. Simulations were performed using an enhanced version of the parallel code for turbulent reacting flows, called S3D, which was developed at Sandia National Laboratories at Livermore. The code comprises a DNS quality Eulerian method to solve the carrier gas flow field, while the Lagrangian method is used to track the liquid fuel droplets. Two-way coupling between the liquid and the gas phases were established via the mass, momentum and energy equations. A detailed chemistry mechanism involving 33 species and 64 reactions was used to describe the chemical reactions.

A general combustion model, in the context of large eddy simulations, was developed to simulate the full range of combustion in conventional diesel-type and HCCI-type diesels. The combustion model consisted of a Chemkin sub-model and an Extended Flamelet Time Scale (EFTS) sub-model. Specifically, Chemkin was used to simulate auto-ignition process. In the post-ignition phase, the combustion model was switched to EFTS. In the EFTS sub-model, combustion was assumed to be a combination of two elementary combustion modes: homogeneous combustion and flamelet combustion. The combustion index acted as a weighting factor blending the contributions from these two modes. The Chemkin sub-model neglected the subgrid scale turbulence-chemistry interactions whereas the EFTS model took them into account through a presumed PDF approach. The model was used to simulate an early injection mode of a Cummins DI diesel engine and a mode of a Caterpillar DI diesel engine. These engine modes are representatives of HCCI-type and conventional diesel-type combustion, respectively. The comparison with experiments shows that the model can predict both types of diesel combustion without the need of ad-hoc adjustments.

An integrated system model containing sub-models for diesel engine, emissions, and aftertreatment devices has been developed. The objective is to study engine-device and device-device interactions. The emissions sub-models used are for NOx and PM (particulate matter) prediction. The aftertreatment sub-models used include a diesel oxidation catalyst (DOC) and a diesel particulate filter (DPF). Controllers have also been developed to allow for transient simulations, active DPF regeneration, and prevention/control of runaway DPF regenerations. The integrated system-level model has been used to simulate DPF regeneration via exhaust fuel injection ahead of the DOC. In addition, the controller model can use intake throttling to assist in active DPF regeneration if needed. Regeneration studies have been done for both steady engine load and with load transients. High to low engine load transients are of particular interest because they can lead to runaway DPF regeneration. Therefore, the integrated model has been used to simulate methods to prevent and control runaway regenerations. The simulation results are consistent with experimental observations, thus confirming the utility of the developed integrated model.
A-priori tests of subgrid-scale (SGS) models are performed using results of 1283 direct numerical simulations for forced isotropic (Re = 100) and rotating turbulence (0.1 < Ro < 0.4). A range of SGS models are tested varying from algebraic, gradient, and scale similarity, to one-equation viscosity and non-viscosity dynamic structure models. Anisotropy and Material Frame Invariance (MFI) requirements for SGS models in rotating systems are reviewed and used to help construct new models based on the dynamic structure approach. The models are evaluated primarily using correlation and regression coefficients of individual components of the SGS tensor, components of the divergence of the SGS stresses, and the kinetic energy transfer term between large and small scales. For all measures examined, the MFI-consistent dynamic structure models perform significantly better, especially for rotating turbulence.


Direct numerical simulation was used for fundamental studies of the ignition process of turbulent n-heptane liquid fuel spray jets. A chemistry mechanism with 33 species and 64 reactions was adopted to describe the chemical reactions. The Eulerian method is employed to solve the carrier gas flow field and the Lagrangian method is used to track the liquid fuel droplets. Two-way coupling interaction is considered through the exchange of mass, momentum and energy between the carrier gas fluid and the liquid fuel spray. The initial carrier gas temperature was 1500 K. Six cases were simulated with different droplet radii (from 10 microns to 30 microns) and two initial velocities (100 m/s and 150 m/s). From the simulations, it was found that evaporative cooling and turbulence mixing play important roles in the ignition process of liquid fuel spray jets. Ignition first occurs at the edges of the jets where the fuel mixture is lean, and the scalar dissipation rate and the vorticity magnitude are very low. For smaller droplets, ignition occurs later than larger droplets due to increased evaporative cooling. Higher initial droplet velocity enhances turbulence mixing and evaporative cooling. For smaller droplets, higher initial droplet velocity causes the ignition to occur earlier, whereas for larger droplets, higher initial droplet velocity delays the ignition time.


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Multi-zone CFD simulations with detailed kinetics were used to model iso-octane HCCI experiments performed on a single-cylinder research engine. The modeling goals were to validate the method (multi-zone combustion modeling) and the reaction mechanism (LLNL 857 species iso-octane) by comparing model results to detailed exhaust speciation data, which was obtained with gas chromatography. The model is compared to experiments run at 1200 RPM and 1.35 bar boost pressure over an equivalence ratio range from 0.08 to 0.28. Fuel was introduced far upstream to ensure fuel and air homogeneity prior to entering the 13.8:1 compression ratio, shallow-bowl combustion chamber of this 4-stroke engine. The CFD grid incorporated a very detailed representation of the crevices, including the top-land ring crevice and head-gasket crevice. The ring crevice is resolved all the way into the ring pocket volume. The detailed grid was required to capture regions where emission species are formed and retained. Results show that combustion is well characterized, as demonstrated by good agreement between calculated and measured pressure traces. In addition, excellent quantitative agreement between the model and experiment is achieved for specific exhaust species components, such as unburned fuel, formaldehyde, and many other intermediate hydrocarbon species. Some calculated trace intermediate hydrocarbon species do not agree as well with measurements, highlighting areas needing further investigation for understanding fundamental chemistry processes in HCCI engines.
SAE 2008-01-1070

Data Normalization Schemes for Assessing Mixture Stratification from PLIF Data
R.E. Herold, J.B. Ghandhi

Planar laser-induced fluorescence (PLIF) has become a useful diagnostic for the quantification of in-cylinder flowfield conditions, and in many applications determining the homogeneity of the in-cylinder flowfield is of primary importance. In some cases, noise associated with this imaging technique (i.e., camera noise, shot-to-shot laser energy variation, and laser sheet profile variations) can dominate the flowfield inhomogeneities, leading to biased mixture stratification statistics. Presented herein are three data normalization schemes (global-, image-, and ray-mean) that can be used to correct for these noise sources when assessing mixture stratification from PLIF data. The normalization schemes are applied to in-cylinder PLIF data obtained over a wide range of inhomogeneity levels, and the conditions over which the use of each normalization scheme is appropriate are discussed.

SAE 2008-01-0047; Modeling Iso-octane HCCI using CFD with Multi-Zone Detailed Chemistry; Comparison to Detailed Speciation Data
Randy P. Hessel, David E. Foster, University of Wisconsin-Madison, Salvador M. Aceves, M. Lee Davisson, Francisco Espinosa-Loza, Daniel L. Flowers and William J. Pitz, Lawrence Livermore National Laboratory, John E. Dec, Magnus Sjoberg, Sandia National Laboratories, Aristotelis Babajimopoulos, University of Michigan

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Results show that combustion is well characterized, as demonstrated by good agreement between calculated and measured pressure traces. In addition, excellent quantitative agreement between the model and experiment is achieved for specific exhaust species components, such as unburned fuel, formaldehyde, and many other intermediate hydrocarbon species. Some calculated trace intermediate hydrocarbon species do not agree as well with measurements, highlighting areas needing further investigation for understanding fundamental chemistry processes in HCCI engines.


We have adapted a standard Fourier-transform infrared (FTIR) spectrometer (Thermo-Scientific Nexus 670) for in-cylinder measurements of gas spectra. During engine operation, the engine shaft encoder signal is logged continuously along with the FTIR’s He-Ne laser signal and infrared interferogram signal. The engine piston and FTIR mirror move in an uncorrelated fashion, so that after many minutes of engine operation, a complete interferogram is populated at each piston position. Afterward, the data is compiled into a series of spectra versus crank-angle-degree. Here we present a near-infrared H2O thermal emission spectrum measured through a fiber-optic spark plug connected to an engine (Briggs 128603-OHV).
Initial estimation of the piston ring pack contribution to hydrocarbon emissions from a small engine

Salazar, V.M., and Ghandhi, J.B.

The contribution to the engine-out hydrocarbon (HC) emissions from fuel that escapes the main combustion event in piston ring crevices was estimated for an air-cooled, V-twin utility engine. The engine was run with a homogeneous pre-vaporized mixture system that avoids the presence of liquid films in the cylinder, and their resulting contribution to the HC emissions. A simplified ring pack gas flow model was used to estimate the ring pack contribution to HC emissions; the model was tested against the experimentally measured blowby. At high load conditions the model shows that the ring pack returns to the cylinder a mass of HC that exceeds that observed in the exhaust, and thus, is the dominant contributor to HC emissions. At light loads, however, the model predicts less HC mass returned from the ring pack than is observed in the exhaust. Time-resolved HC measurements were performed and used to assess the effect of combustion quality on HC emissions. It was shown that the both the HC concentration and the HC mass emitted per cycle, from a single-cycle gas flow model, correlated with low IMEP and late combustion phasing. A statistical analysis showed that the correlation was significant. Thus, at light load incomplete combustion was found to be a significant contributor to engine-out emissions.

A detailed comparison of emissions and combustion performance between Optical and Metal Single-Cylinder Diesel Engines at Low Temperature Combustion Conditions; Will F. Colban, Duksang Kim, Paul C. Miles, Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA, Seungmook Oh, Korea Institute of Machinery and Materials, Daejeon, S. Korea, Richard Opat, Roger Krieger, David Foster, University of Wisconsin – Madison, Engine Research Center, Madison, WI, USA, Russell P. Durrett, Powertrain Systems Research Laboratory, General Motors Research and Development Center, Warren, MI, USA, Manuel A. Gonzalez D., Advanced Diesel, General Motors Powertrain, Pontiac, MI, USA

A detailed comparison of cylinder pressure derived combustion performance and engine-out emissions is made between an all-metal single-cylinder light-duty diesel engine and a geometrically equivalent engine designed for optical accessibility. The metal and optically accessible single-cylinder engines have the same nominal geometry, including cylinder head, piston bowl shape and valve cutouts, bore, stroke, valve lift profiles, and fuel injection system. The bulk gas thermodynamic state near TDC and load of the two engines are closely matched by adjusting the optical engine intake mass flow and composition, intake temperature, and fueling rate for a highly dilute, low temperature combustion (LTC) operating condition with an intake O2 concentration of 9%.

Subsequent start of injection (SOI) sweeps compare the emissions trends of UHC, CO, NOx, and soot, as well as ignition delay and fuel consumption. The effect of EGR composition is also investigated to determine the level of chemical equivalency required for adequate EGR simulation in an optical engine. Five simulated EGR conditions are compared to evaluate the influence of water vapor, CO, and UHC.

Results show that the optical engine pressure and heat release characteristics are influenced by the larger crevice volumes and the compliance of the extended optical piston. Greater fueling rates are also needed in the optical engine to achieve an equivalent load. The same general trends in emissions behavior are found in both engines, capturing the location of minimum UHC and CO emissions with changes in SOI. In addition, quantitative emissions levels agree well. Simulated EGR composition is found to have a minor influence on combustion behavior and emissions levels, but does not affect the general emissions trends.
A computational, three-dimensional approach to investigate the behavior of diesel soot particles in the microchannels of wall-flow Diesel Particulate Filters is presented. The KIVA3V CFD code, already extended to solve the 2D conservation equations for porous media materials [1], has been enhanced to solve in 2-D and 3-D the governing equations for reacting and compressible flows through porous media in non axisymmetric geometries.

With respect to previous work [1], a different mathematical approach has been followed in the implementation of the numerical solver for porous media, in order to achieve a faster convergence as source terms were added to the governing equations. The Darcy pressure drop has been included in the Navier-Stokes equations and the energy equation has been extended to account for the thermal exchange between the gas flow and the porous wall. The mesh generator K3PREP and the code have been extended to define geometries having an arbitrary number of symmetry axis, in order to perform simulations of 3D sectors of the filter, where a sector represents a group of DPF channels.

Also, Lagrangian particles in the flow were used to represent the diesel soot particles. The increase of the soot cake layer thickness on the porous wall and its spatial distribution as a function of time have been determined by the fully coupled particle-hydrodynamics in the gaseous flow, since KIVA3V calculates in the computational domain the rates of mass, momentum, and energy exchange between the gas and particles. The influence of gas molecules-particle interaction on overall particle behavior is examined by including Brownian motion and partial slip in particle equation of motion. Simulations help to highlight three-dimensional non-uniform particle deposition, mainly due to flow distribution in the micro-channel; the soot packing density and thickness on each face of the computational porous cells are calculated.

A set of unsteady simulations was run to steady state for wall-flow Diesel Particulate Filters having substrates with different geometrical and physical properties. Distinct types of diesel particulate matter (PM) in terms of chemical composition, concentration, and size distribution, known by the experiments carried out on a single cylinder 2.3-liter D.I. heavy-duty diesel engine, were used in the simulations. The experimental distribution of particle sizes and density was injected through the inlet boundary of the computational domain and its deposition along the filter porous surface was monitored. A validation of the code has been carried out by the comparison with pressure drop measurements across the different DPF's studied.

The development of the Diesel Exhaust Filtration Analysis system (DEFA), which utilizes a rectangular wafer of the same substrate material as used in a fullscale Diesel Particulate Filter (DPF), is presented in this paper. Washcoat variations of the wafer substrate (bare, washcoat, and catalyzed washcoat) were available for testing. With this setup, the complications of flow and temperature distribution that arise in the fullscale DPF can be significantly minimized while critical parameters that affect the filtration performance can be fully controlled.

Cold flow experiments were performed to test the system’s reliability, and determine the permeability of each wafer type. A Computational Fluid Dynamics (CFD) package was utilized to ensure the flow uniformity inside the filter holder during the cold flow test. The system was then exposed to several engine exhaust flow rates drawn by a sampling probe in the exhaust line to test the consistency of emissions measurements with other standardized techniques.

Particulate Matter (PM) size distribution measurements from this new sampling system were found nearly identical to the measurements found with a commercial dilution system. Finally, the system was tested in a PM filtration condition. The DEFA proved to have the capability for performing PM filtration experiments at various filtration velocities.
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

Flow is modeled with KIVA3V-MZ-MPI, which is a multizone 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.

Two engine operating conditions of the same engine speed and torque but distinct PM characteristics were selected for this study. Diesel exhaust has been sampled though the newly developed Diesel Exhaust Filtration Analysis system (DEFA) holding a wafer disk made of the same substrate material as a full-scale DPF. The wafer disk also has similar wall thickness and pore geometry to the full-scale DPF substrate. Washcoat variations on the wafer (washcoat and catalyzed washcoat) were also investigated available. Previous research has shown that the pressure drop and filtration efficiency measured from the DEFA are similar to the full-scale DPF. The PM loaded wafers were analyzed in a thermal mass analyzer that measured the semi-volatile organic fraction (SOF) as well as soot and sulfate fractions of PM. Two exhaust flow rates have been investigated for their impact on PM wall filtration. Data have been analyzed for differences in wall loading and transition to soot cake layer build up.

Results indicate that PM partitioning on the wafer disk are similar to those found using gravitational analysis. Relative SOF magnitudes are seen to increase but only to a limit of wall loading capacity. Filling the wafer disks with PM laden exhaust from the same engine mode but using different filtration velocities affects the wafer filtration performance. This in turn changes the amount of PM trapped in the wall and soot cake as well as soot/SOF partitioning. Filling wafer disks with same exhaust flow rate but different PM characteristics also affects wall loading performance and soot/SOF partitioning.

Submitted to COMODIA 2008; Impact of Filtration Velocities and Particulate Matter Characteristics on Diesel Particulate Filter Wall Loading Performance; Ekathai Wirojsakunchai, Renato Yapaulo, and David E. Foster, Department of Mechanical Engineering, University of Wisconsin – Madison

The catalytic oxidation (low temperature oxidation) of Particulate Matter (PM) deposited on a catalyst coated Diesel Particulate Filter (DPF) is important to DPF regeneration processes. It was found that PM/catalyst contact plays a crucial role in catalytic oxidation effectiveness. Despite extensive DPF development in recent years, there is still a lack of fundamental understanding of the nature of the contact between PM and the DPF substrate, and its correlation with engine exhaust flow rates and PM characteristics. The goal of this study is to gain more understanding of PM deposition characteristics within the DPF and how engine exhaust flow rates impact DPF wall loading performance.

Two engine operating conditions of the same engine speed and torque but distinct PM characteristics were selected for this study. Diesel exhaust has been sampled though the newly developed Diesel Exhaust Filtration Analysis system (DEFA) holding a wafer disk made of the same substrate material as a full-scale DPF. The wafer disk also has similar wall thickness and pore geometry to the full-scale DPF substrate. Washcoat variations on the wafer (washcoat and catalyzed washcoat) were also investigated available. Previous research has shown that the pressure drop and filtration efficiency measured from the DEFA are similar to the full-scale DPF. The PM loaded wafers were analyzed in a thermal mass analyzer that measured the semi-volatile organic fraction (SOF) as well as soot and sulfate fractions of PM. Two exhaust flow rates have been investigated for their impact on PM wall filtration. Data have been analyzed for differences in wall loading and transition to soot cake layer build up.

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We present a novel multiwavelength, time-division multiplexed laser design that continuously cycles through N spectrally narrow wavelengths, spending a specified, fixed time on each one. The design is based on a matched compressor/stretcher and a custom waveform generator applying modulation preferably to the gain medium. The realization discussed here utilizes a pulsed semiconductor optical amplifier in an all-fiber cavity containing fiber Bragg gratings. The laser cycles through 19 wavelengths in a 44-nm-wide spectral band (1333–1377 nm) every 15 µs. The source contains no moving parts, offers high repetition rates, narrow spectral linewidths and custom spectral profiling of the output.

Optics Letters; Simple Multiwavelength Time-Division Multiplexed Light Source for Sensing Applications; Thilo Kraetschmer, Daryl Dagel and Scott T. Sanders
Seminar Schedule is as follows:

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Three years has passed since Professor Rutland stepped into the role of ERC Director and the mantle of Director has been passed on again. This time it was passed back to me.

The ERC continues to be a dynamic and broad spectrum laboratory. This is evident by looking at the array of papers, for which the abstracts are included in this newsletter, that will be presented at the 2008 SAE Congress and other venues.

We are pleased to welcome Professor Dave Rothamer as a new faculty member. Dave received his Master’s Degree from Professor Ghandhi and then went to Stanford where he has just completed his Ph.D. under Professor Ron Hanson. Perhaps you have seen Dave’s picture in the recent Sandia CRF Newsletter. Dave joined us in January and is already involved in experimental projects.

We also welcomed a new Research Associate, Michael Andrie. Mike started in September 2007. Mike hails from Minnesota and brings a wealth of experience to the ERC. He has engine research experience from John Deere, Cummins and Adiabatics Inc. His time is being partitioned between helping students working within the GM-ERC-CRL and DERC. Those of you connected with our Diesel Emission Reduction Consortia have already been introduced to Mike through the DERC Newsletter.

Congratulations go to Professor Sanders. Scott’s promotion to Associate Professor with Tenure was conferred by the UW Board of Regents this summer. There was never any doubt in our minds, but it was nice to get the official confirmation of what we already knew, validated by Scott’s recent recognition in receiving the Publishers Choice in the journal Measurement Science and Technology for his paper “Fourier-transform Infrared Spectroscopy.”

(Continued on page 15)