Abstracts

SESSION 7 – Combustion and Homogeneous Charge Compression Ignition Regimes

Chair: **Gurpreet Singh, U.S. Department of Energy**

Are There Practical Approaches For Achieving the Theoretical Maximum Engine Efficiency?

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It is generally understood that the maximum theoretical work that can be obtained from an internal combustion engine is equal to the Gibbs free energy of the fuel being used as the energy carrier. For typical hydrocarbon fuels, like gasoline or Diesel, the Gibbs free energy is approximately equal to the heating value of the fuel. Therefore, the maximum theoretical efficiency of an internal combustion engine burning typical hydrocarbon fuels is 100 percent. This is the same theoretical limit as the fuel cell. Considering that the efficiencies of current internal combustion engines are no where near 100 percent, the question naturally arises as to where the losses occur and what can be done to reduce them?

The losses fall into many categories, which can be referred to as irreversibilities. Examples of the irreversibilites include, but are not limited to, heat transfer between the engine cylinder and the coolant and engine compartment, available energy contained within the exhaust which is thrown away during the exhaust process, and friction. Thermodynamic analysis of the combustion process within the engine indicates that typically 20 percent of the fuel availability is lost during combustion. The question being addressed in this presentation is can the energy release of combustion be affected in a different way such that this availability destruction can be reduced? And, if methods of reducing the irreversibility of combustion can be developed, can they be accomplished without undo loss in power density?

The mechanisms of loss of useful work during combustion (availability destruction) can be determined through second law analysis and explained in general as follows:

1. The availability destruction is directly proportional to the rate at which the chemical reactions are taking place.
2. The availability destruction is directly related to the affinity of the reactions that are occurring.
3. The availability destruction is inversely related to the temperature at which the reactions are taking place.

The analysis also allows one to postulate possible avenues by which irreversibilities of combustion can be reduced. The availability destruction within the combustion process potentially could be reduced by:

1. Slowing down the chemical reactions
2. Choosing fuels or establishing stoichiometries such that the chemical reactions have lower affinity
3. Raising the temperature at which the reactions occur.

Unfortunately some of these approaches conflict with one another, or the desire to obtain maximum power. For example, if one raises the temperature at which the reaction occurs two things will happen. The increased temperature will reduce the impact of the affinity on the availability destruction, which will tend to decrease the availability destruction rate. However, the chemical reaction rate is also a function of temperature, and typically an increase in temperature results in an exponential increase in reaction rate. The increased reaction rate will tend to increase the availability destruction rate. So, it is apparent that the approach of raising the temperature, which is motivated by heat engine thinking, results in conflicting drivers in terms of availability destruction.

In this presentation the fundamentals of combustion irreversibilities will be reviewed and cast in a form which highlights the processes responsible for the availability destruction during combustion. Then a philosophy will be postulated for carrying our combustion processes that will reduce availability destruction in combustion. Questions will then be raised as to whether this combustion philosophy can be carried out without loss in power density and what the critical issues will be of such an approach to energy transformation.

Factors Affecting HCCI Combustion Phasing for Fuels with Single- and Dual-Stage Chemistry

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Controlling combustion phasing is an important issue that must be addressed for the successful implementation of Homogeneous Charge Compression Ignition (HCCI) engines. As the engine load (fueling rate) is varied, the combustion phasing will shift unless some compensation is applied. Adjusting the intake temperature is a straightforward method for compensating so that the charge mixture auto-ignites at the desired crank angle. For a variety of fuels, including those with both single and dual-stage auto-ignition chemistry, the intake temperature must be reduced to maintain combustion phasing as the fueling rate is increased. This can give the appearance that for all fuels, richer fuel/air equivalence ratios (ϕ), auto-ignite more easily (*i.e.*, at lower temperatures) under HCCI conditions. However, more careful examination reveals that changes in ϕ affect several factors, each of which contributes to the change in required intake temperature. These factors include: combustion duration, wall temperatures, residuals, heat/cooling during induction, and fuel auto-ignition chemistry and thermodynamic properties (referred to as fuel chemistry). In order to understand the relative importance of these factors and to isolate the effects of fuel chemistry, a systematic study has been conducted. In this study, the experiment was altered in a series of steps to remove changes due to each of these factors, leaving only the changes due to fuel chemistry. This approach allowed the relative magnitude of these factors to be determined and the isolated fuel-chemistry effect to be evaluated for various fuels.

Heating/cooling during induction is a particularly important factor, and it can be affected by heat-transfer during induction, dynamic flow effects (whose magnitude depends on the engine speed and port configuration), and cooling by fuel vaporization if direct injection is used. As a result, the effective temperature of the fresh gases in the cylinder at the end of the intake stroke can be quite different from the temperature measured in the runner. These fresh gases then mix with residuals, further changing the in-cylinder temperature. A straightforward procedure is presented for estimating the charge mixture temperature at the end of the intake stroke. This procedure accounts for both heating/cooling during induction and for the effect of residuals.

The experiments were conducted in a single-cylinder HCCI engine (0.98 liters/cylinder). Three fuels were examined: iso-octane and gasoline, which are single-stage ignition fuels, and PRF80, which has significant two-stage ignition chemistry at the conditions studied. The results showed that iso-octane exhibits only a small change in auto-ignition chemistry with fueling rate (ϕ), and that gasoline had a change just slightly larger than iso-octane. In contrast, PRF80 had a large change, due to its significant cool-flame chemistry. As a result, sudden changes in fueling are shown to have little effect on combustion phasing for single-stage ignition fuels (iso-octane and gasoline), whereas two-stage ignition fuels (PRF80, or by inference Diesel fuel) can require significant compensation immediately with changes in fueling rate. However, because ignition is sensitive to ϕ for two-stage fuels, they offer the potential for controlling combustion phasing with stratification of the charge mixture. This was investigated, and the data showed that stratification can significantly and rapidly shift combustion phasing with PRF80, but not with iso-octane.

HCCI Fuel Selection: An Engine Heat Release Based Approach

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A study was performed to examine the effects of engine operating parameters on Homogenous Charge Compression Ignition (HCCI) combustion using multiple fuels. The parameters studied include compression ratio, inlet air temperature and pressure, and EGR level. Extensive experiments were performed using Diesel fuel, gasoline, blends of gasoline and Diesel fuel, and Fischer Tropsch Naphtha. Experiments were performed on a single-cylinder variable compression ratio research engine. The independent variables included compression ratio, exhaust gas recirculation level, intake manifold conditions, and the fuel composition.

A detailed heat release rate analysis was used to examine the effects of various characteristics of the heat release process on the engine efficiency. The results of the heat release rate analysis and cycle simulation modeling results were used to develop simple regression models and rules for controlling the heat release rate to produce the maximum efficiency. These results are used to suggest an optimum fuel formulation using a blend of gasoline and Fischer-Tropsch Naphtha.

Heavy Duty HCCI Development Activities

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Implementing a practical homogeneous charge compression ignition (HCCI) engine has numerous technical challenges. Among these are ensuring a proper mixture preparation, controlling combustion phasing and cylinder pressure rise rates, and expanding the operating range both to higher loads and idle/light loads. Methods to control combustion phasing include inlet manifold temperature and pressure, injection timing, valve timing, and fuel properties. Caterpillar and a major oil company are working together to understand HCCI using advanced engines, fuel combustion chemistry, and combustion models. Recent progress on part load HCCI operation in both single and multi-cylinder engines using Diesel fuels will be presented. Results from a single-cylinder engine have shown that HCCI technology can achieve very low particulate matter and nitrogen oxides emissions at light-medium load with a range of distillate fuel properties including U.S. market fuel. Three quarter load has been achieved using Diesel fuel with an in-cylinder injection strategy. Results from a multi-cylinder engine will also be reviewed.

Advanced Air Handling, Combustion, and Fuel Efficiency in Gasoline Engines

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Gasoline engines are likely to continue to be the power plant of choice for passenger cars in the U.S. market for the next decade. Improved fuel efficiency for these engines could result in significant energy savings. Techniques for improved part load efficiency include reducing pumping losses through variable valve timing strategies, increased or variable compression ratio, and homogeneous compression combustion ignition (HCCI) combustion.

Data showing efficiency benefits of these operating strategies and showing how these tools can be used to transition between conventional and HCCI combustion will be presented. HCCI combustion produces about 12 percent better fuel efficiency compared to conventional spark ignited combustion while reducing nitrogen oxides emissions by about 95 percent. The transition from conventional to HCCI combustion is made possible with a spark assist, which can then remain on or be shut off in HCCI mode. Reduced pumping losses through late intake valve closing and internal exhaust gas recirculation when combined with variable compression ratio also improve part load engine efficiency.

Fuel composition and chemistry also affects the transition to HCCI and HCCI combustion characteristics. Fuels with lower octane appear to enhance HCCI ignitability and ease the transition from conventional to HCCI combustion. Fuel properties such as octane, composition, and pre-flame chemistry correlate to the heat release characteristics in HCCI combustion.

Mixed-Mode Diesel HCCI/DI with External Mixture Preparation

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Diesel HCCI (Homogenous Charge Compression Injection) is a combustion technology showing great promise for the reduction of oxides of nitrogen and particulate matter from Diesel engines. Our implementation is a mixed-mode concept which relies on the use of an essentially unmodified common-rail CIDI (Compression Ignition Direct Injection) engine, coupled with a highly effective atomizer (patent pending) for external mixture formation. With this concept, the engine can operate in HCCI mode, HCCI/DI mixed mode, or DI (Direct Injection) mode depending on the load and with seamless, progressive mode transition.

The external mixture preparation for the HCCI mode offers a number of advantages over techniques that utilize only the DI system to perform HCCI mixture preparation. External mixture formation, with the additional residence time and very active mixing through the intake stroke, allows for better HCCI operation due to the very effective mixing and charge homogeneity when compared to direct injection HCCI. The traditional problems of external mixture formation (wall wetting, poor cold start, etc.) are eliminated by a novel fuel atomizer capable of ultra-fine, sub-micron atomization. Furthermore, when used in a mixed combustion mode or in pure DI mode at higher loads, the DI injectors can be optimized strictly for DI operation with respect to number, orientation, or size of injector holes without compromise for HCCI operation.

This mixed-mode operation has been recently demonstrated on a single cylinder engine (1/4 of a recent production 2 L engine, CR = 18) in collaboration between Ohio State University and the University of Stuttgart, Germany. The concept has demonstrated extremely low levels of nitrogen oxides (below 3 ppm) and negligible smoke (FSN < 0.01) in pure HCCI operation up to an Indicated Mean Effective Pressure (IMEP) of 4.7 bar. Operation at various conditions (engine speeds, loads, boost pressures, intake temperature, exhaust gas recirculation rates from 0 - 60 percent, etc.) have shown that this technique enables HCCI operation over a wide range of engine conditions with relative insensitivity of the combustion phasing process to operating conditions. This is probably due to the high level of charge homogeneity achieved by this technique. Furthermore, experiments in mixed mode (*i.e.*, part of the fuel supplied externally in homogeneous mixture plus fuel directly injected internally) demonstrated that the transition from HCCI to mixed HCCI/DI to DI combustion mode is seamless (superposable within a sizable finite region of overlap), significantly enabling the controllability of such a combustion system over the entire engine operating map.

Finally, recent experiments with the same technology for external mixture formation in a 2.4 L, 4-cylinder engine have confirmed the results obtained for HCCI operation in terms of load limits and emissions. Furthermore, the elevated levels of hydrocarbons and carbon monoxide in HCCI operation can be easily reduced through a simple Diesel oxidation catalyst despite the lower exhaust temperatures to their respective post-catalyst levels in DI operation at the same load points.

Achieving High Efficiency Clean Combustion in Diesel Engines

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We have been exploring the potential of Diesel combustion regimes that exhibit simultaneous low engine-out nitrogen oxides (NO_X) and particulate matter (PM) emissions. Through proper combustion management, we have achieved significant reductions in NO_X (90 percent) and PM (30 percent) emissions without the decrease in efficiency typically associated with operating in these regimes. This type of operation is commonly referred to as High Efficiency Clean Combustion (HECC) and was achieved on a multi-cylinder engine using only production-like hardware. The combustion process was characterized using in-cylinder pressure transducers as well as by applying powerful analytical methods to the exhaust constituents. The combination of thermodynamic and exhaust chemistry information results in a more complete description of the combustion process than is usually available. Another important aspect of operating Diesel engines in advanced combustion modes is the ability to transition in and out of these modes with minimal adverse effects on emissions or performance. We were able to demonstrate seamless transitions in and out of Diesel HECC operation with no significant emission spikes or effects on performance.

New Methodologies for Analysis of Premixed Charge Compression Ignition Engines

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Temperature gradients present in an engine cylinder due to heat transfer to the cylinder walls have a great deal of impact on the combustion process in the Homogeneous Charge Compression Ignition (HCCI) class of engines. Numerical models have been able to accurately capture these temperature effects on the combustion process for homogeneous mixtures. However, to facilitate control and higher power density, some researchers have deviated from truly homogeneous mixtures and looked to more elaborate ways of mixture formation, such as Variable Valve Actuation (VVA) or Direct Injection. These techniques introduce composition stratification in addition to temperature stratification in these engines, which we will call Premixed Charge Compression Ignition (PCCI) to differentiate from HCCI engines. Modeling of this process becomes much more complicated because both mixing and chemistry must be handled in a computationally efficient way.

We have developed a multiple modeling approach that fully integrates a computational fluid dynamics code (KIVA-3V) with a multi-zone model with detailed chemical kinetics. These methodologies are an extension of the authors' previous work in that they can now account for both temperature and equivalence ratio (composition) gradients in the cylinder. In this direction, a method of tracking down the equivalence ratio in each cell during combustion is introduced. One important consideration is how to actually define equivalence ratio to adequately capture the spatial composition field throughout the cycle.

Validation cases were developed by solving the detailed chemistry in every cell of a KIVA-3V grid. This allowed the validation of the chemistry model alone, isolating the chemistry model from depending on other KIVA-3V sub-models. The methodology was tested for several cases with varying initial temperature and equivalence ratio distributions, showing good agreement with the detailed solutions, while providing further insight into the effect of equivalence ratio distribution on ignition, burn duration and emissions in a PCCI engine.

High-Energy, Pulsed-Laser Diagnostics for the Measurement of Diesel Particulate Matter

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With stricter particulate matter (PM) emission regulations looming ahead in 2007, there is a need for new instrumentation capable of real-time measurements with high sensitivity. We foresee applications for both extractive sampling and *in situ* measurements, where the former is the simplest approach to implement, and the latter is needed to characterize engine-out/aftertreatment-in conditions for design optimization and life-cycle simulation. High-energy, pulsed-laser diagnostics are well suited for these tasks, and offer a wide range of measurement capabilities that include the following:

LII: Laser-Induced Incandescence directly measures soot volume fraction (elemental carbon only) and the diameter of the primary particles that make up soot aggregates. Primary particle size is important because it represents the smallest size of carbonaceous particles in the exhaust, and because it can be used to estimate aggregate particle surface area, which has significant health implications.

ELS: Elastic Laser Scattering measures particle size. The most simple application, Rayleigh scattering, yields an estimate of the mean equivalent-sphere diameter of polydisperse aerosols. A more complex application, Rayleigh-Debye-Gans polydisperse aggregate (RDG/PDA) analysis, provides additional information such as the radius of gyration and fractal dimension of aggregates. While it is possible to estimate a size distribution based on an assumed shape (i.e., log-normal), ELS cannot measure size distributions directly.

LIDELS: Laser-Induced Desorption with Elastic Laser Scattering measures the volatile organic fraction (VOF) of PM. Measurements at low laser energy give the mean equivalent-sphere diameter of the total PM; measurements at high laser energy vaporize the VOF, yielding the mean equivalent-sphere diameter of the remaining soot.

LIBS: Laser-Induced Breakdown Spectroscopy identifies elemental species and measures their concentration, and is well-suited to investigate the metallic ash in Diesel PM. These include sulphates; phosphates; oxides of calcium, zinc, magnesium, and other metals that are formed from fuel and lubricant additives; metal oxides of iron, copper, chromium and aluminum that result from engine wear; and iron oxides that result from corrosion of exhaust system components.

3D-Combustion Simulation Strategy Status, Future Potentials and Applications Issues

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Concerning the development of future internal combustion engines, the automotive industry is searching for new approaches to shorten the classical procedure of trail and error. The rapid increase of computing power enables the 3D simulation of reactive in-cylinder flow dynamics as an increasingly valuable tool for combustion designers. In this paper, a computational fluid dynamics concept for the simulation of direct injection - Diesel engine combustion is introduced, complying with industrial requirements, such as a high degree of predictability and economical computational costs. The proposed approach allows the incorporation of complex chemistry into a detailed turbulent flow prediction.

In order to overcome the well-known drawbacks of conventional stochastic spray models in the near nozzle region, an Eulerian approach in combination with orifice resolving meshes is applied to improve predictability. For the numerical simulation of the Diesel combustion process, a limited number of appropriate progress variables are defined to describe the reactive phases of self-ignition, premixed, and diffusion combustion. For each progress variable, a transport equation is solved in the CFD code. The mixture field in physical space is characterized by the mixture fraction and its variance. By weighting the chemical solution in mixture fraction space with a presumed probability density function, the transport equations for each progress variable in physical space are closed. The introduced progress variable approach offers a way of separating the numerical effort associated with the solution of the turbulent flow field from that of solving the chemistry. Thereby, arbitrarily complex chemistry can be used to simulate the reactive processes.

In order to evaluate the models developed in this study, various Diesel engines were simulated, including a passenger car, heavy-duty truck, and marine engine. Both, the passenger car and the marine engine are equipped with a Common-Rail injection system, whereas the heavy-duty truck engine is set up with a Pump-Line-Nozzle system. Several operating conditions have been investigated. For the validation of the combustion models, the measured cylinder pressures are used. The pressure data were obtained with single-cylinder engines. Additionally, heat release curves are compared which results from zero-dimensional heat release calculations based on the pressure traces. For the spatial characterization of mixture formation and combustion of the heavy-duty truck engine, at DaimlerChrysler a single cylinder optical engine has been set up, allowing full optical access to the combustion chamber, for e.g. high speed photography. Photographic sequences of combustion processes are used to compare the flame front propagation between simulation and experiment. The results show good agreement. The computational costs fulfill industrial demands.

New Developments of the NADI™ Concept to Improve Operating Range, Exhaust Emissions, and Noise

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Due to their high thermal efficiency coupled with low carbon dioxide (CO_2) emissions, Diesel engines are promised to be an increasing part of the transportation market if their oxides of nitrogen (NO_X) and particulate (PM) emissions are reduced. Today, Diesel PM traps seem to be the industrial solution for reducing PM emissions. On the other side, adequate deNO_X after-treatments are underdevelopment with concerns about fuel economy, robustness, sensitivity to sulfur fuel content, and cost because of their complex and sophisticated strategies.

New combustion processes, such as Homogeneous Charge Compression Ignition (HCCI) or heavy premixed combustion, are being investigated for their potential to achieve near zero PM and NO_X emissions. Their main drawbacks are high hydrocarbon (HC) and carbon monoxide (CO) emissions and combustion control (timing and noise) at high load as a consequence of the limited operating range and power output.

As a result of the challenges facing the Diesel engine, the Institut Français du Pétrole has developed a combustion system able to achieve near zero PM and NO_X emissions while maintaining performance standards of the direct injection Diesel engine. This "dual mode" engine application called NADI™ (Narrow Angle Direct Injection) applies HCCI at part load and switches to conventional Diesel combustion to reach high and full load requirements.

This presentation will cover the latest development regarding power density, operating range, CO and HC emissions, and combustion noise for this concept obtained on a single cylinder engine. At full load, the NADI™ system is consistent with the future Diesel engine power density standard (60 kW/l has been reached). In HCCI combustion mode, above 1500 RPM, 9 bar of Brake Mean Effective Pressure (BMEP) has been achieved with NO_X emissions under 0.05 g/kWh, which is 100 times lower than a conventional Diesel engine. CO and HC emissions have been deeply improved, especially at low engine load. To be fully compatible with the future stringent standard levels and thanks to an appropriate multiple staged injections strategy, a large reduction of combustion noise was reached at high load. Except for the highest load, these results have been obtained without any fuel penalty when compared to a conventional Diesel engine.

This presentation will also cover the preliminary results obtained on a 2.2L multi-cylinder engine. The associated new technologies in fuel injection system, air loop control, supercharging, exhaust after-treatment, and engine management system fields are covered and discussed. The results show a large potential to reach the future Euro V emissions standard proposed by the UBA (German EPA), 0.08 g/km of NO_X, on an 1810 kg class vehicle.