Zhiqin Jia

Dual-Fuel Combustion in a Heavy-Duty Engine

PhD Thesis, 2018

The need to control climate change and improve the fuel efficiency of internal combustion engines has prompted global efforts to develop alternative fuels in order to reduce dependence on conventional petroleum derivatives. This thesis deals with three such alternative fuels: compressed natural gas (CNG), pure methane (used to mimic biogas), and methanol. The first parts of the thesis discuss experimental investigations into conventional gas-Diesel dual-fuel combustion.

The effect of the CNG/methane supplement ratio on engine performance and emissions was explored at two different load points. The results indicated improved performance and emissions at intermediate load more than at low load. In addition, a 3D dual-fuel combustion model developed at Chalmers was validated against experimental data generated during these studies. Reasonably good agreement was achieved between experiment and simulation for most aspects of engine performance, but there were some discrepancies regarding the onset of ignition delay and emissions.

The later parts of the thesis deal with studies on a low temperature combustion concept, Reactivity Controlled Compression Ignition (RCCI), using two alternative fuels: CNG and methanol. Engine performance and emissions were studied for both CNG-Diesel and methanol-Diesel RCCI combustion. Experiments on CNG-Diesel RCCI combustion were performed to explore the effects of different engine parameters on engine performance and emissions, revealing that high indicated thermal efficiencies (over 50%) could be achieved. However, this combustion strategy presented difficulties when operating at high load and high compression ratios due to the peak in-cylinder pressure limitation. Another CNG-Diesel RCCI combustion study was therefore conducted, focused on extending the operational load range for this combustion strategy and improving combustion phasing by using late inlet valve closing (IVC). This approach increased the maximum load for CNG-Diesel RCCI combustion by 40% compared to the first CNG-Diesel RCCI study. Finally, experiments on methanol-Diesel RCCI combustion showed that port injection of methanol offered better performance than direct injection of methanol during either the intake stroke or the compression stroke in terms of net indicated thermal efficiency and emissions of HC and CO.

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Chengjun Du

Studies on Diesel sprays under non-reacting and reacting conditions

PhD Thesis, 2017

Methods for reducing engine-out emissions are urgently needed to mitigate climate change and air pollution. In diesel engines, the quality of fuel-air mixing and the subsequent combustion process strongly affect fuel efficiency and engine-out emissions. However, fuel-air mixing, the subsequent combustion processes, and their dependence on the operating conditions are not yet fully understood. This thesis aims to address this deficiency by analyzing the effects of various orifice geometries and high injection pressures on the characteristics of diesel sprays. The thesis briefly reviews the fundamental physics governing the flow of pressurized fuel through the internal nozzle of a diesel injector, the subsequent formation of the liquid and vapor spray, and the turbulent diffusion combustion processes. The experimental work presented in this thesis can be divided into three main parts. The first focuses on the effects of geometry-induced cavitation on the liquid/vapor phase spray and injection rate evaluation. To this end, a light absorption and scattering technique (LAS) was used to measure the distributions of liquid and vapor sprays formed using nozzles with various geometries. It was found that the vaporization of the diesel spray was controlled by turbulent air mixing. The effects of geometry-induced cavitation on the spray properties were mainly due to differences in the fuel mass flow rate, spray momentum and spreading angle. In addition, the injection rates of cavitating and non-cavitating nozzles were evaluated using the momentum flux measurement method. It was found that failure to account for cavitation caused the injection rate to be overestimated for the cavitating nozzle but not for the non-cavitating nozzle. The second part of the experimental campaign investigates the effect of the injection pressure and nozzle geometry on soot formation and oxidation. A two-dimensional laser extinction method was used to measure time-resolved soot concentrations and soot volume fractions; OH* chemiluminescence imaging was used to measure the lift-off length and measure the distributions of the OH radicals qualitatively; soot luminosity images were used to identify the sooting area in the soot shadowgraph images. It was found that the equivalence ratio in the jet center at the lift-off length (ϕ_{cl}), which is influenced by the operating conditions, played a critical role in soot formation. Reductions in ϕ_{cl} thickened the OH zone in the upstream region of the jet, reducing the volume corresponding to the maximum soot volume fraction. The expansion of the OH zone also helped reduce the sooting zone's width. However, under high sooting conditions (e.g. $\phi_{cl}>3.5$), the sooting zone width in the downstream jet was independent of ϕ_{cl}. The third part of the thesis investigates combusting and non-combusting sprays formed from different blends of ethanol with diesel fuel. Using 0%-20% ethanol blended with diesel fuels, liquid/vapor phase spray images were captured, the ignition delay was measured, the lift-off length was measured, and natural soot luminosity images were captured. It was found that the differences in the fuels' composition did not significantly affect the liquid/vapor phase sprays. However, as the ethanol content of the fuel was increased from 0% to 20%, the lift-off length increased and the detectable soot luminescence decreased. This indicates that soot formation declines as the fuel's ethanol content increases.

ISBN 978-91-7597-629-7

Tim Lackmann

A representative interactive linear-eddy-model (RILEM) for simulating spray combustion

PhD Thesis, 2017

Engine development aims at reducing pollutant emissions (e.g. NOx, soot, UHC) while maintaining high efficiencies. Detailed experimental results in combination with precise numerical predictions are of great importance in order to develop combustion systems for new clean and efficient internal combustion engines. Computational fluid dynamics (CFD) tools must be able to deal with multi-mode (premixed, partially premixed and non- premixed) and multi-regime (from kinetically controlled to mixing con- trolled) turbulent combustion under various conditions (low temperatures, high pressures, high EGR rates). Work on laboratory flames [1, 2] clearly demonstrates the strong need to account for the impact of unresolved turbulent fluctuations of temperature and composition on chemical reaction rates in Reynolds-averaged and large-eddy simulations (LES) of turbulent combustion. Combustion models that neglect this so called turbulence- chemistry interaction (TCI) cannot predict fundamental physical phenomena like local or global extinction and re-ignition, possibly leading to imprecise predictions of essential quantities including heat release rates, temperatures and emissions. In order to maximize volumetric combustion efficiency and minimize pollutant formation, it is desirable to maximize the rate of combustion subject to the limits of overall flame stability. These limits of flame stability are determined by the rate of local extinction. Especially in new combustion concepts for engines, including stratified charged compression ignition (SCCI), lean stratified premixed combustion, and the use of high levels of exhaust gas recirculation (EGR) the impact of the flow field on the chemistry plays an important role. This thesis is divided into two parts. The first part deals with the introduction of a new regime independent combustion model for engine applications, which is able to predict turbulent combustion under the before mentioned challenging conditions, while the second part deals with the extension of existing knowledge about extinction in non-premixed combustion.

ISBN 978-91-7597-611-2

Anders Johansson

Challenges and Advantages of Stratified Combustion in Gasoline Direct-Injected Engines

PhD Thesis, 2017

The modern world is based on an extensive transport network in which passenger vehicles play a major role. Although passenger vehicles have improved significantly in recent decades, they still contribute to the pollution of our environment and global warming. Consequently, new ways of reducing their emissions are needed. Moreover, most modern passenger vehicles are propelled by a combustion engine that operates on non-renewable fuels such as gasoline or diesel produced from crude oil. However, such fossil fuels are limited resources, so there is also a need to reduce the fuel consumption of passenger vehicles. As such, improvements in engine technology will play a central role in the development of more efficient and cleaner passenger vehicles. In recent years, alternatives to the internal combustion engine such as electric motors and fuel cells have attracted increasing attention. While these technologies are undergoing rapid development and electric vehicles in particular are gaining market share, the combustion engine remains the dominant power source for passenger vehicles. The most common type of combustion engine used in passenger vehicles is the gasoline engine. Several advanced combustion concepts have been developed to make gasoline engines cleaner and more efficient. One such concept is stratified combustion, which is discussed in this thesis. In gasoline engines, stratified combustion increases fuel efficiency. However, it also tends to produce high particulate emissions and can reduce combustion stability. These problems mainly occur because stratified combustion involves a complex mixing process that generates a heterogeneous air/fuel mixture with both rich and lean regions. This thesis describes work undertaken to minimize or eliminate these drawbacks, particularly the increased particulate emissions, while maintaining low fuel consumption. Most of the studies presented herein were performed with metal and optical single-cylinder engines, but a four-cylinder production engine was also used in some cases. Tests were performed in steady state mode at various engine operating points. All engines utilized in the studies were fitted with a Spray-Guided Direct-Injected (SGDI) system and multi-hole solenoid-actuated fuel injectors. Depending on scope of the study, the engines were equipped with different measurement devices such as instruments for measuring pressures and temperatures or emissions of HC, NOx, CO, CO2, O2 and particulates (both mass and number). The results obtained during this thesis work have been presented in five publications. The first of these publications describes a study on the relationship between particulate emissions during stratified combustion and generic combustion variables such as the fuel injection pressure, as well as injection and ignition timings. This was done to identify variables that could be manipulated to reduce particulate emissions. The later publications describe how measured particulate emissions are affected by forced induction, increased fuel injection pressure, the use of novel ignition systems, air movements, and the use of different sampling systems. Key objectives of these studies were to find ways of reducing particulate emissions and increasing combustion stability. It was found that stratified combustion in SGDI gasoline-fueled engines fitted with a solenoid multi-hole injector can increase fuel efficiency but does not alleviate the problem of high particulate emissions. In addition, a positive correlation between the extent of non-premixed flames and particulate mass and number emissions was identified. The use of novel ignition systems was shown to expand the ignition window, while boosting and increasing the fuel injection pressure were found to reduce soot levels. Finally, the internal relationship between the ignition and injection timings was found to strongly affect combustion stability and soot levels, primarily because it influenced the dilution of the air-fuel mixture and the risk of the fuel spray striking the piston top. The thesis concludes with some suggestions for ways of improving stratified combustion and directions for future research.

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Gunnar Latz

Waste Heat Recovery from Combustion Engines based on the Rankine Cycle

PhD Thesis, 2016

Most of the energy in the fuel burned in modern automotive internal combustion engines is lost as waste heat without contributing to the vehicle's propulsion. In principle some of this lost energy could be captured and used to increase the vehicle's fuel efficiency by fitting a waste heat recovery system to the engine. This thesis presents investigations into the design and functioning of waste heat recovery systems based on Rankine cycle technology for vehicular applications. To facilitate the design of such systems, the performance of different working fluids and expansion devices was investigated using a zero-dimensional model of the Rankine cycle. Simulations using this model indicated that water-based fluids should perform well when recovering waste heat from a high temperature source such as a combustion engine's exhaust gas. In addition, evaluations based on similarity parameters indicated that displacement expanders are optimal in systems having low flow rates and high expansion pressure ratios, both of which are to be expected in vehicular systems using water as the working fluid. Organic working fluids allow higher flow rates in the cycle, making the efficient use of turbines possible. Data from the simulations using the zero-dimensional model were used to guide the design and construction of a demonstrator test bench featuring a Rankine cycle-based recovery system that recovers waste heat from the exhaust gas recirculation system of a heavy duty Diesel engine. The test bench uses water as the working fluid and a piston expander as the expansion device. The Rankine cycle's thermal efficiency was 10%, corresponding to 1-2% of the engine's power output. To find ways of improving the system's performance, one-dimensional models of the expander and the system as a whole were created and then validated by comparing their output to experimental data obtained with the test bench. The expander model suggested that reducing the compression ratio would make it possible to reduce the steam inlet pressure by 30% without affecting the expander's power output. This hypothesis was then confirmed experimentally. The expander model was used to rank the relative influence of selected steam boundary conditions and expander geometry parameters on the performance of a piston expander. The inlet pressure, steam inlet cut-off timing, expander speed and outlet pressure were found to be the most significant main effects on expander performance. It was also shown that interaction effects between steam conditions and expander geometry had considerable influence on both power output and efficiency.

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Chen Huang

Numerical Modelling of Fuel Injection and Stratified Turbulent Combustion in a Direct-Injection Spark-Ignition Engine Using an Open Source Code

PhD Thesis, 2014

Stringent regulations on the emission of pollutants, especially carbon dioxide (CO2), necessitate the development of advanced combustion technologies. Gasoline direct injection (GDI) into the combustion chamber of a Spark Ignition (SI) engine is a combustion strategy that is widely recognized as having the potential to improve fuel efficiency of internal combustion engines for passenger cars. In particular, the CO2 emissions of GDI engines could be 20-26% lower than those of equivalent port-fuel injected (PFI) SI engines. Unfortunately, the development of combustion systems for GDI engines is very challenging because the creation of an appropriate combustion system is a major challenge because they require very precise formation of an ignitable fuel-air mixture with a steep stratification gradient right between the ignition electrodes to permit efficient operation under a wide range of operating conditions. CFD simulations are widely used to increase the efficiency of engine R&D. This thesis aimed at development of a tool for numerically modelling of working process in a GDI engine. The work had two main objectives. First, an available CFD code should be applied to multidimensional GDI engine simulations. Second, the code should be developed by implementing advanced models of stratified turbulent combustion, followed by validation against experimental data. As far as a code is concerned, although there are several mature commercial CFD packages on the market, there is also a need for less expensive software. Consequently, there is growing interests from both industry and academia in the OpenFOAM® open source CFD code, whose source code is freely available so that users can implement and test new models without paying license fees. However, it had not been used to simulate combustion in a GDI engine when the work reported herein was begun. This thesis presents an assessment of OpenFOAM® as a tool for the numerically modelling of fuel injection, spray breakup, evaporation, mixture formation, and stratified turbulent burning in the combustion chamber of a GDI engine. OpenFOAM® was used to simulate hollow-cone sprays of gasoline and ethanol discharged by a piezo-controlled pintle-type injector. The liquid properties of gasoline were implemented in the code to enable the simulation of gasoline sprays. In addition, the implementations of various spray breakup models such as LISA, TAB, Reitz-Diwakar, and KHRT into the standard OpenFOAM® package were checked and modified in order to more closely reflect their descriptions in the original papers. Liquid penetration and SMD calculated by simulations using the revised model implementations were compared to experimental data provided by my colleagues. These comparisons showed that the best agreement between the experimental data and simulations was achieved when using a combination of the uniform droplet size and KHRT models. This model was therefore used in all subsequent engine simulations. As far as modelling is concerned, the code’s modelling capabilities were enhanced by implementing and developing models relevant to the turbulent burning of stratified gasoline-air mixtures at the elevated temperatures and pressures associated with combustion in a GDI engine. More specifically, two relevant issues were addressed. First, a semi-detailed chemical mechanism for the combustion of a gasoline surrogate in air was developed and validated. The gasoline surrogate consisted of iso-octane, toluene, and n-heptane in volumetric proportions of 55%:35%:10%, respectively. The mechanism includes 120 species participating in 677 reactions. It was validated against experimental data on the ignition delay times and laminar flame speeds of different mixtures at a range of pressures and temperatures. The mechanism was then used to compute laminar flame speeds for gasoline-air mixtures at equivalence ratios of $0.2 \leq \phi \leq 2.0$, unburned gas temperatures of $298 \leq T_u \leq 800$K, and pressures of $1 \leq P \leq 30$ atm. The results of these calculations were approximated and the approximations were implemented into OpenFOAM® for subsequent CFD modelling of stratified turbulent combustion in a GDI engine. In order to study stratified burning in a GDI engine, the Flame Speed Closure (FSC) model of premixed turbulent combustion was combined with a so-called presumed Probability Density Function (PDF) method that made it possible to account for the influence of turbulent fluctuations in local mixture composition on the local burning rate. The combined model based on the FSC and presumed PDF approach was implemented into OpenFOAM® and the roles played by its various submodels were investigated in a step-wise fashion. Finally, the so-extended code was used to simulate a GDI engine burning a globally lean mixture. Good agreement between results computed by me and experimental data provided by my colleagues was obtained. In addition, the model’s sensitivity was investigated.

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Anne Kösters

Diesel Fuel Spray Formation and Combustion - A Modeling Approach

PhD Thesis, 2014

The formation, ignition and combustion of fuel sprays are highly complex processes, and the models that are traditionally used to describe them have a range of shortcomings. The introduction of commercial and non-commercial computational fluid dynamics (CFD) software has facilitated the development and application of new and improved multidimensional CFD models describing these phenomena. Spray modeling is generally done using the Eulerian-Lagrangian method, in which the gas phase is modeled as a continuum and the droplets are tracked in a Lagrangian way. Existing spray models vary widely in their accuracy and robustness, and the performance of spray simulations is strongly dependent on their discretization, as is the predicted level of spray-generated turbulence. The work presented here concerns the prediction of spray formation and combustion behaviors using improved models implemented in the free open source software package OpenFOAM. To enable improved RANS simulation of spray formation, the VSB2 spray model was implemented, refined, and tested under diverse ambient conditions. This model mainly differs from standard spray models in the way it describes the breakup and evaporation of the liquid fuel. It was designed to be unconditionally robust, have a minimal number of tuning parameters, and be implementable in any CFD software package that supports particle tracking. The results of VSB2 spray simulations were compared to data from the Engine Combustion Network (ECN) and experiments conducted at Chalmers University of Technology. In addition the Volume Reactor Fraction Model (VRFM), a novel partially stirred reactor model, was implemented in OpenFOAM. This model defines a reactor fraction based on the mixture fraction, a chemical progress variable, and their variances rather than defining mixing and chemical time scales. The effect of exhaust gas recirculation (EGR) on n-heptane sprays formed under Diesel engine-like conditions was studied using the VRFM and the results of these simulations were compared to experimental data from the ECN. Finally, results obtained using the VRFM were compared to data generated using the well stirred approach and the multiple RIF model.

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Andreas Matsson

THE EFFECTS OF VARIOUS NOZZLE HOLE CONFIGURATIONS ON DIESEL ENGINE PERFORMANCE

PhD Thesis, 2013

Any improvement that can be done with the diesel engine to reduce emissions and fuel consumption is of importance. The aim of the studies presented in this thesis was to determine whether changes in the nozzle geometry of the fuel injection systems used in diesel engines might improve their emissions and fuel consumption. This project started with the question if elliptical or non-circular nozzle holes instead of the conventional circular designs would have any effect on emissions and fuel consumption in a heavy duty diesel engine. It was speculated that non-circular holes might increase air entrainment in the lift-off zone and thereby reduce smoke emissions. Increased air entrainment in the lift off zone would allow more of the fuel to burn under relatively lean conditions in the rich premixed zone and thus reduce soot formation. Experiments were conducted using a single cylinder engine whose emissions and fuel consumption were measured. An optical cylinder head was also designed and manufactured, and used to investigate flame propagation during combustion using fuel injectors with non-circular nozzles. The effects of varying the nozzle hole inlet geometry were also investigated by conducting experiments with single-hole axisymmetric nozzles that had been subjected to different grades of hydrogrinding. These studies were performed using a high temperature high pressure combustion chamber, and a variety of techniques were used to characterise the resulting sprays and flames. Impingement measurements were also performed to ensure that the studied nozzles produced fuel jets with the same momentum. From the impingement measurements velocity, discharge coefficient and loss of kinetic energy was calculated. Finally, the effects of changing the nozzle hole inlet geometry were investigated using a single cylinder heavy duty diesel engine. The engine's emissions and fuel consumption were measured and an endoscope technique was used to capture images from inside the combustion chamber during the combustion sequence. Two-colour pyrometry was used to determine the soot and temperature distributions inside the cylinder from the images, and the results of this analysis were compared to the emissions data.

ISBN 978-91-7385-953-0

Markus Grahn

Model-Based Diesel Engine Management System Optimization - A Strategy for Transient Engine Operation

PhD Thesis, 2013

To meet increasingly strict emission legislation and stronger demands on fuel consumption, typical passenger car diesel engines become increasingly complex with more and more controllable systems added. These added systems open up for the possibility to operate the engine at more efficient conditions, but it also becomes more challenging to optimize the settings in the engine management system. Methods to optimize settings in an engine management system based on steady-state engine operation are well developed and described in the literature, and also used in practice. Methods to handle transient engine operation are not as well developed, and typically various compensations are added in an engine management system to account for effects during transient engine operation. Calibration of these compensations is currently a manual process and is largely performed to meet regulations rather than to optimize the system. This thesis consists of papers that describe the introduction of a novel method to optimize settings in a diesel engine management system with an aim to minimize fuel consumption for a given dynamic vehicle driving cycle while keeping accumulated engine-out emissions below given limits. The strategy is based on existing methods for steady-state engine operation, but extended to account for transient effects in the engine caused by dynamics in the gas exchange system in a systematic manner. The strategy has been evaluated using a simulation model of a complete diesel engine vehicle system. The optimization strategy has been shown to decrease fuel consumption for a diesel engine vehicle compared to existing methods based only on steady-state engine operation. Using the simulation model, the strategy has been shown to decrease fuel consumption for a vehicle driving according to the New European Driving Cycle with 0.56%, compared to a strategy based only on steady-state engine operation. This thesis also consists of papers that describe the complete diesel engine vehicle system simulation model. The model can perform a simulation of a vehicle driving according to a predefined dynamic driving cycle, and it estimates fuel consumption together with NOx and soot emissions throughout the simulation depending on settings in the engine management system. The model accounts for transient effects on fuel consumption and emissions caused by dynamics in the engine gas exchange system. The simulation model is implemented in the Simulink environment, and the simulation time is in the range of 10 to 20 times faster than real-time.

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Mikael Thor

Torque based combustion property estimation and control for diesel engines

PhD Thesis, 2012

Modern diesel engines are becoming increasingly complex as a result of demands on the reduction of both fuel consumption and emissions. This escalating complexity not only applies to the engine itself, but also to its control system. In this context, the interest in closed-loop engine control is growing as this control strategy offers increased accuracy and robustness, as well as a reduced need of control system calibration, compared to traditional open-loop engine control systems. However, the concept of closed-loop control requires information about the controlled process, in this case the combustion events in the cylinders, and additional sensors are thus needed. The most suitable sensor configuration for the acquisition of combustion information is still subject to research. This thesis deals with estimation and control of diesel engine combustion properties based on crankshaft torque measurements. Methods are presented that describe a combustion event in the torque domain and estimate combustion properties either directly or by first reconstructing the corresponding cylinder pressure. The proposed combustion property estimation methods are evaluated using both simulations and experimental data. Combustion net torque, a novel torque domain combustion description, is a central concept in this thesis. Techniques for combustion net torque based estimation of both entire burned mass fraction traces and the 50% burned mass fraction combustion phasing measure are presented. These techniques are also implemented in a real-time engine control system and used in order to successfully demonstrate torque based closed-loop combustion phasing control online. This experimental demonstration illustrates how disturbances that effect the combustion phasing can be detected and counteracted using crankshaft torque measurements.

ISBN 978-91-7385-705-5

Monica Johansson

Fischer-Tropsch and FAME Fuels as Alternatives for Diesel Engines; an Experimental Study

PhD Thesis, 2012

Research into alternative fuels is necessitated by our heavy reliance on limited oil reserves and increasingly strict emissions legislation. The studies reported in this thesis involved conducting engine tests using alternatives to fossil Diesel fuel in both heavy-duty and light-duty single cylinder engines. The combustion modes considered were conventional Diesel combustion and two more advanced modes: low temperature combustion (LTC) and homogeneous charge compression ignition (HCCI). Both Fischer-Tropsch (FT) and Fatty Acid Methyl Esther (FAME) fuels were considered; in both cases, the formation of emissions, fuel consumption and combustion behavior were compared to those of conventional Diesel fuels. The overall objectives of these studies were to determine whether it is possible to operate conventional Diesel engines with the alternative fuels and to operate the engines in a fashion that will minimize the emissions of species covered by legislation such as soot and NOx. It was also expected that the results obtained would provide new insights into soot and NOx formation when burning alternative fuels in a Diesel engine. The first experiments were performed in a light-duty engine with Fischer-Tropsch fuels, Swedish environmental class 1 (MK1) and European Diesel (EN590), using both conventional and HCCI combustion. In the conventional Diesel combustion mode, it was found that the soot emissions were up to 30 percent lower than those obtained using MK1. It was further seen that the high cetane number of the tested F-T fuels reduced the ignition delay and over-leaning, which resulted in lower HC emissions. Despite the high cetane number of the F-T fuels, HCCI combustion could be achieved with increased levels of EGR. The FT fuels are less dense than conventional Diesel fuel, which may reduce the extent of spray-wall interactions and would thus reduce CO emissions. The FT fuels had heating values that were similar to those for conventional Diesel fuels and therefore exhibited comparable specific fuel consumption. In the heavy-duty engine tests, the FT fuels yielded soot emissions that were up to 60 percent lower than those for MK1 Diesel. However, there was no clear difference between the two in terms of NOx emissions, which appeared to be more sensitive to the engine's operating parameters than to the nature of the fuel. For example, they could be reduced by up to 90 percent by increasing the level of EGR from 0 to 40%. The FAME fuels also yielded very substantially lower soot emissions than European Diesel in the heavy-duty engine, being up to 90% lower for the FAME fuels. This was attributed to the absence of aromatics (which are precursors in soot formation) in the alternative fuels and to the high oxygen content of the FAME fuels. In addition, the flame lift-off was longer for FAME fuels, which improves the mixing of fuel and air and thus generates lower soot emissions. Unfortunately, the FAME fuel also yielded NOx emissions that were up to 20% higher than those for conventional Diesel, which was partially due to the FAME flame temperature being 40°C higher than that for Diesel fuel. The oxygen content of the FAME fuels also gave leaner fuel-air mixtures and thus higher NOx emissions. When assessing alternative fuels, it is important to consider ethical and environmental factors throughout their

entire lifecycle and also to be aware that there is unlikely to be a single alternative that can fully replace all fossil fuels currently in use.

ISBN 978-91-7385-677-5

Junfeng Yang

Biodiesel Spray Combustion Modeling Based on a Detailed Chemistry Approach

PhD Thesis, 2012

Replacing conventional diesel fuels with biodiesel has the potential to drastically reduce engine-out emissions of soot, carbon monoxide, and total unburnt hydrocarbons, at the cost of slightly increased nitrogen oxide emissions. However, to realize the full benefits of using biofuels in this way, there is a need for theoretical models describing their combustion in internal combustion engines. While master models of this kind have been developed recently, they involve very large numbers of reactions and intermediates, making them difficult to study using current computing resources even when using one-dimensional flame modeling. In order to derive a more computationally tractable semi-detailed mechanism (~500 species/2000 reactions) for engine studies, the detailed mechanism has been subjected to a sophisticated reduction strategy based on methods such as Directed Relation Graph and its variants. The aim was to generate a reduced mechanism that would accurately reproduce the key features of the combustion process, including the fuel's auto-ignition behavior and the concentrations of the various intermediate species involved. The reduced mechanism was therefore validated against experimental data and results obtained using the master model for combustion under various simplified conditions, e.g. shock-tube, jet stirred reactor, laminar flame propagation, opposed-diffusion flame. To provide input data for flame modeling, the transport species properties of the fuels studied using the reduced biodiesel mechanism were estimated using semi-empirical methods. The estimated thermo-physical properties and the outputs of the spray combustion models were compared to real spray characteristics measured in a spray chamber. The liquid penetration, flame lift-off and average Sauter Mean Radius (SMR) for sprays of different fuels were calculated and compared. Ignition Quality Tester modeling was conducted to assess the Cetane Number of the fuels studied using the biodiesel oxidation mechanism and spray sub-models, e.g. spray atomization, droplet breakup and evaporation models. The results obtained indicated a potential direction for mechanism optimization since there was found a considerable uncertainty regarding the thermodynamics of the master mechanism. In addition, IQT modeling also provides a way to understand a relative influence of physical spray dynamics and combustion chemistry on the overall ignition delay for biodiesel. To study the impact of bio-diesel fuels on engine performance, 3D CFD simulations for both heavy duty (Volvo D12C) and light duty (Volvo NED5) engines were carried out under different operating conditions. Predictions were validated against measured in-cylinder parameters and exhaust emission concentrations. The semi-detailed mechanism was shown to provide an efficient and accurate representation of actual biodiesel combustion and emissions formation. Moreover, the engine modeling also suggested that using biodiesel in place of conventional diesel fuel increases nitrogen oxide emissions by 10%. Quantitative analyses of the in-cylinder temperature, equivalence ratio and nitrogen oxide distributions provided deep insights into the origin of these elevated NOx emissions. It was found that oxygen-containing fuels such as biodiesel increase the concentration of molecular and atomic oxygen present in the cylinder during combustion, and this is likely to be the cause of the elevated NOx emissions.

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Malin Ehleskog

Low Temperature Combustion in a Heavy Duty Diesel Engine

PhD Thesis, 2012

In recent years, there have been major efforts to reduce engine emissions and fuel consumption. The studies described in this thesis were conducted with the aim of identifying methods for reducing harmful engine-out emissions of soot and nitrogen oxides (NOx) under high load without increasing fuel consumption. The first part of the project focused on low temperature combustion using very high levels of EGR. It was found that very low soot and NOx emissions could be achieved at low loads. Unfortunately, these conditions resulted in high fuel consumption as well as high emissions of HC and CO. The increased emissions could be mitigated by optimising the timing of the SOI and increasing the injection pressure, but the high fuel consumption remained problematic. Intermediate levels of EGR can be used to increase the ignition delay and thereby achieve partially premixed combustion. When soot and NOx emissions are plotted against the amount of EGR, there is an intersection point at which the soot emissions are just beginning to increase but the recirculated exhaust gas has greatly reduced the NOx emissions. At this point, the HC and CO emissions and the fuel consumption remain acceptably low. If the onset of the increased soot emissions could be shifted to a higher EGR level or if the peak soot emissions could be reduced in magnitude, the tradeoff between soot and NOx emissions at intermediate EGR levels could be improved. By increasing the charge air pressure, the size of the soot bump is reduced and the point of intersection between the soot and NOx curves is shifted to a higher EGR percentage. The soot-NOx tradeoff can also be improved by increasing the injection pressure to reduce the soot peak while using EGR levels that are high enough to suppress NOx formation. To further investigate the potential of partially premixed combustion, the effects of varying the timing of late inlet valve closure were investigated. The results show that reducing the effective compression ratio increased the ignition delay and thus increased premixing for both late and early intake valve closing (IVC). In the absence of EGR, this reduced NOx emissions without increasing soot emissions as long as the combustion phasing and equivalence ratio remained unchanged. When EGR was used, this approach reduced soot emissions while maintaining low NOx emissions. These emissions reductions were achieved without associated increases in unburned hydrocarbon emissions or fuel consumption.

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Stina Hemdal

Optical Diagnostics Applied to Internal Combustion Engines: Catalysis, Sprays and Combustion

PhD Thesis, 2011

Gasoline direct injection with spray-guided charge formation is one of the most promising concepts to reduce fuel consumption and CO_2 emissions of spark ignited engines. The advantages with the system are owing to un-throttled operation and stratification of the injected fuel resulting in a globally lean combustion. In these engines, the mixture formation, which is controlled by the fuel injection system, play a crucial role for the success of the combustion event. The stratification of the fuel creates locally fuel rich areas promoting efficient soot formation, and one of the drawbacks of stratified combustion is increased engine-out soot levels. In this work optical diagnostics were applied to fuel sprays in order to investigate the overall spray formation, the internal structure and to some extent the rate of evaporation. The formation of hollow cone sprays from an outward opening injector, at conditions corresponding to start-up in stratified mode, was studied in more detail. Sprays of gasoline-ethanol blends and ethanol were compared to sprays of gasoline. The obtained sprays were highly reproducible and had large recirculation zones that were somewhat reduced for low fuel temperatures. Optical diagnostics were also applied to investigate stratified combustion inside a firing engine. The aim was to investigate the sources of soot formation at stratified combustion. The charge formation, and the OH chemiluminescence and soot luminescence of the flame were visualized from below, through a quartz window in the piston. The in-cylinder observations showed that the fuel formed a compact cloud in the centre of the cylinder with fuel rich islands. Soot was efficiently formed and also efficiently oxidized except late in the cycle. The in-cylinder observations were compared to engine out emissions. Engine-out emissions of HC, CO and NO_X may be removed by oxidation or reduction promoted by a catalyst. The amount of desorbed species outside a catalyst gives information about the reaction kinetics. In this work the concentration of desorbed OH molecules, formed during the water formation reaction, was measured outside a platinum catalyst using cavity ringdown spectroscopy.

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Fabian Peng Kärrholm

Numerical Modelling of Diesel Spray Injection, Turbulence Interaction and Combustion

PhD Thesis, 2008

This thesis covers two main topics. The first is numerical modelling of cavitating diesel injector flows, focusing on describing such flows using a single-phase cavitation model based on a barotropic equation of state together with a homogenous equilibrium assumption. The second topic is Euler-Lagrangian simulations of diesel sprays, focusing on attempts to reduce the high grid/timestep dependencies in numerical simulations of diesel sprays. In addition, the ability of two CFD codes to predict flame lift-off length and ignition delay time, and the advection scheme's influence on fuel distributions, are considered. A long-term goal was to develop a new atomization model based on calculated flows in injector nozzles, which did not have the drawback of requiring either non-physical parameters or information derived from specific experiments. To validate the cavitation simulations, comparisons were made with experimental data obtained at AVL. The experimental data (which are practically 2D) provide information on velocity profiles and pressure contours. These data were used to validate the code. However, since the code is not stable for diesel-type pressures, no atomization model was developed. The main part of the thesis describes how diesel sprays were simulated using the discrete droplet model (DDM), in which the liquid is described by Lagrangian coordinates and the vapour by an Eulerian approach. The simulations have been used to investigate how the k-ε family of turbulence models influence spray behaviour, and a simple but efficient way to reduce the dependency of the mesh resolution, by limiting the turbulence length scale in the liquid core region, is proposed. This constraint is shown to have a positive effect on the spray behaviour, and to reduce both grid and timestep dependencies. In addition, the ignition delay time and flame lift-off lengths have been investigated, since these two properties are believed to be important for emissions formation. The simulations used a complex chemical mechanism involving 83 species and 338 reactions. The effects of the numerical scheme, the turbulence model and physical parameters (like ambient temperature and oxygen content) on these variables have also been investigated.

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Mikael Skogsberg

A Study on Spray-Guided Stratified Charge Systems for Gasoline DI Engines

PhD Thesis, 2007

Innovative technologies are required to meet ongoing challenges to reduce the CO_2 emissions from passenger cars and their fuel consumption. Such technologies are usually complex and require detailed analyses to deliver efficient, reliable systems. One proposed approach to meet these challenges is to use Direct Injection Stratified Charge (DISC) combustion systems, which consequently have received great interest, especially in Europe and Japan. A key component for realizing stable, lean operation in a DISC engine is the fuel injector. In this type of engine, the time available for fuel atomization and mixture preparation is significantly shorter than in conventional port fuel injected engines. Furthermore, the position of the spray and structure of the fuel cloud generated by the injector must remain stable, regardless of the speed and load, and must not be sensitive to in-cylinder cycle-to-cycle variations. The objectives of the work presented in this thesis were to investigate the spray formation, fuel distribution and combustion of sprays generated by the most common types of fuel injectors used for spray-guided DISC engines and thus gain a better understanding of the physical properties and parameters governing the mixture formation and combustion processes. The presented results were obtained from both spray chamber and single cylinder engine tests, using advanced laser-based measuring methods and high speed video photography in conjunction with measurements of emissions and standard engine operating parameters, such as pressure, temperature and heat release. In the investigations the main focus was on the stratified charge operating mode, due to its great potential to improve fuel consumption and CO_2 emissions in parts of the speed-load operating range in which the efficiency is normally very low for conventional gasoline engines. The results show that two types of injectors (multi-hole and outward-opening A-nozzle injectors) can be used for spray-guided systems. The flexibility in terms of spray shape offered by multi-hole nozzles can be very advantageous, but the sprays they deliver have tendencies to over-penetrate and to create steep fuel concentration gradients near the spark plug. Furthermore, careful optimization of the multi-hole injector geometry is necessary to ensure misfire-free combustion in stratified charge operation. A-nozzles provide additional means to control the mixture formation since their needles are directly actuated by a piezo crystal, enabling multiple injections and variation of the fuel flow. The results show that this can help reduce the spray penetration and provide means to extend the operational window of misfire-free, stable stratified charge combustion in terms of both ignition and injection timing parameters. Furthermore, tests performed in an optical single-cylinder engine have shown that a DISC combustion system fitted with a piezo-actuated A-nozzle has the potential to lower the fuel consumption and CO_2 emissions by over 40% at low load and speed when operated in stratified charge mode compared to homogenous charge operation. A further investigation showed that a dual-fluid air-assisted injector which uses compressed air to internally atomize the fuel displays favorable atomization properties, but limitations in possible injection timings due to high cylinder back-pressures and low fuel injection pressure severely limit the scope for using it when the engine is operated in stratified charge mode.

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Rickard Ehleskog

The Influence of Multiple Injections on Combustion: an Experimental Investigation

PhD Thesis, 2007

The high fuel efficiency and torque of the diesel engine has made it the obvious choice for heavy duty applications for a long time. In addition, these characteristics of the modern super-charged HSDI diesel engine also make it very suitable and popular for car applications. However, since all engines emit combustion products that can be harmful to the environment, and the transport sector makes a major contribution to total anthropogenic emissions of potentially harmful substances, increasing legislative demands are being placed on manufacturers of diesel (and other) engines to minimise emissions. One of several possible strategies to reduce pollutant formation is to use multiple injections, i.e. to divide injections into two or more parts. In the studies underlying this thesis the effects of multiple injections on diesel combustion were investigated experimentally, in both spray chamber experiments and engine tests. The main objectives of the work were to investigate ways in which multiple injections could be used to reduce engine-out emissions from diesel engines and to increase the efficiency of diesel engines. Split injections consisting of two injection pulses were shown to have significant effects on the combustion processes in both a heavy duty and a light duty engine, although the effects differed somewhat between the two types of engine. In the light duty engine splitting injections into two pulses lowered the engine-out particulate and CO emissions and increased the fuel efficiency. However, they also resulted in increased NOX emissions. Increased air-fuel mixing is believed to be the main reason for this. In the heavy duty engine a split with a very short dwell time, resulting in a rate-shaped injection rather than a true split injection, resulted in shortened combustion durations, which simultaneously reduced fuel consumption and NOX emissions. Use of multiple injection regimes alone will not meet the tough emissions legislation of the future. However, they seem likely to play a significant role in the continuing efforts to develop cleaner diesel engines.

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Arjan Helmantel

Low Emission Concepts for Diesel Engines

PhD Thesis, 2006

In the recent past, the Diesel engine has been improved considerably in the areas of performance, fuel efficiency and exhaust emissions. In Europe, these improvements have resulted in a strong increase in the sales of passenger cars equipped with a Diesel engine. Since the emission of the greenhouse gas CO2 is directly linked to engine efficiency, the Diesel engine is also attractive from an environmental point of view. However, despite the emission reductions achieved by improvements to the combustion process, the stringent emission legislations of the near future will be difficult to meet without exhaust gas after-treatment systems. Disadvantages of after-treatment systems are the considerable cost as well as durability and servicing issues, which is a motivation to continue studying possibilities to reduce the engine-out emissions. This thesis discusses an experimental study of some of these possibilities, including modifications to conventional Diesel combustion and Homogeneous Charge Compression Ignition (HCCI). An experimental high speed DI Common Rail engine was used in all of the experiments. The effects of post injection and swirl ratio on emission formation have been studied by optical diagnostics of the combustion process. Processing the obtained data with the two- colour pyrometry method provided temporally resolved soot concentration and flame temperature data, which proved to be beneficial in answering the raised questions. Adding a third, post-injection after the main injection showed significant reductions of soot emissions with only minor changes of NOx emissions and fuel consumption. The reason is believed to be the increased turbulence caused by the extra injection and to some extent the increased flame temperature during the second half of the combustion process, both of which contribute positively to the soot oxidation rate. Increasing the swirl ratio of the intake charge also showed significant reductions of soot emissions. Similar to post injection, the increased turbulence increased the soot oxidation rate late in the combustion process. HCCI combustion is known for its potential to significantly reduce NOx and soot emissions. The experiments involving HCCI combustion of conventional Diesel fuel were focused on investigating the modifications to the engine hardware and the injection strategy that are necessary for operation in HCCI mode. A major difficulty of HCCI operation with Diesel fuel was found to be preventing over-advanced ignition and excessive combustion rates. The compression ratio was therefore reduced to delay ignition and high loads of EGR were used to further delay ignition and to reduce the combustion rate. Fuel was injected during the compression stroke in five subsequent short duration injections, so that a homogeneous mixture was created before start of combustion. Initially, compression ratios of 11.5 and 13.4 were used, while later in the development, the compression ratio was raised to 15. The higher compression ratio was used in combination with retarded intake valve closing timing, which reduced the effective compression ratio. Both NOx and soot emissions were reduced to near-zero levels, while the HC and CO emissions increased significantly. The increase in HC and CO emissions reduced the combustion efficiency, which was the main cause of the significant increase of fuel consumption. With the use of more accurate piezo injector and with modifications to the injection strategy, HC and CO emissions as well as fuel

consumption could be reduced significantly, while maintaining low NOx and soot emission levels for most operating loads of up to 0.5 MPa IMEP.

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Stefan Larsson

Torque based combustion phasing control

PhD Thesis, 2005

Due to environmental aspects and emission legislations the automotive industry is striving towards more efficient combustion engines. Many engine control systems in production today are based on look-up tables which are calibrated for different operating conditions. Improvements can be done by constructing better control systems to make the engine run in optimal operating conditions more often than conventional control systems are able to do today. One such improvement could be to replace some look-up tables with feedback control of wisely chosen properties of the combustion process. However, even if a promising property is found and quantified it must be measurable either directly or indirectly. Also, the property must be controllable using a suitable actuator. This thesis concentrates on estimating individual cylinder combustion phasing using a torque sensor mounted on a crankshaft. The combustion phasing is quantified using a measure called 50% torque ratio and it is controllable by modifying the spark advance for each cylinder. A control system has been implemented in an engine test bench to be able to test the ideas. Several test cases have been designed to demonstrate the capability of the system to control the combustion phasing individually for each cylinder and to compensate for simulated external disturbances in steady-state conditions. The control system is also equipped with self-optimising functionality by using an extremum seeking controller to detect for which value of the torque ratio that maximises generated work from each cylinder. The resulting implemented control system is capable of maintaining a desired set-point for the torque ratio in steady-state conditions. Transient conditions have not been evaluated. The extremum seeking controller is demonstrated to be able to find a torque ratio for each cylinder which maximises the generated work.

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Johan Wallesten

Modeling of Flame Propagation in Spark Ignition Engines

PhD Thesis, 2003

Developers and manufacturers of gasoline engines are struggling to improve fuel economy and minimize negative environmental effects. Hence, lean burn and direct injection (DI), in particular stratified charge (SC), spark ignition (SI) engines are of special interest. These engines have the potential to reduce the fuel consumption by 20-25% compared with conventional SI engines. However, the combustion process, is governed by complex interactions between chemistry and fluid dynamics, some of which are incompletely understood. Improved knowledge of combustion is, therefore, of vital importance for both direct use in the design of engines, and for the development of reliable simulation tools for engine development. In this thesis, a brief review is presented of the theory of flame propagation under conditions found in engines, to provide a basis for the formulation of a combustion model. This model, called the turbulent Flame Speed Closure (FSC) model, predicts the instantaneous flame speed, in both laminar and turbulent cases. It is also able to predict the flame development characteristics such as burning velocity and flame brush thickness during propagation. The model is based on time-dependent turbulent diffusivity found in the early phase of flame kernel growth and it includes a single universal model constant that needs to be tuned. To consider local mixture properties, a complex chemistry mechanism consisting of 100 species and 475 reactions is used to determine chemical time scales, required by the model. Validation against multiple databases for spherical flames shows that the model is capable of predicting the flame propagation in a variety of conditions for different fuels and mixture ratios. The combustion processes in two different SI engines are simulated using the commercial CFD-code FIRE? connected with 1-D gas exchange simulations. The FSC model was implemented in the code for the simulations of combustion processes Four speed/load combinations were simulated of which one featured SC combustion. The computations show good agreement with experimental data over a range of speeds and loads using the same value of the single model constant as in all the validation computations. The computations also show that the developed engine combustion simulation system is time effective, robust and able to reproduce the main features of homogeneous and stratified combustion, in a particular triple flame formation. Current DI SC engines suffer from too high unburned hydrocarbon (HC) emissions. Approximately 60-70% of the total HC emissions from the SC engine case is found to be due to overmixing, i.e. the fuel has mixed beyond flamability limits. To improve this, further development of the SC engine should be focused on reducing mixing time available between start of injection and ignition.

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Tao Feng

Numerical Modeling of Soot and NOx Formation in Non-Stationary Diesel Flames with Complex Chemistry

PhD Thesis, 2003

A complex chemistry model of reduced size (65 species and 268 reactions) derived on the basis of n-heptane auto-ignition kinetics, small hydrocarbon oxidation chemistry, polyaromatic hydrocarbon (PAH) and NOx formation kinetics together with a phenomenological soot model has been implemented in the KIVA code for multidimensional Diesel spray combustion simulations. An EDC (Eddy Dissipation Concept) based partially stirred reactor model is used to handle the turbulence-chemistry interaction. The results obtained from numerical simulations for direct-injection (DI) Diesel sprays, injected into a high-pressure combustion vessel at engine-like conditions or a real engine geometry, show that the approach is able to reproduce the transient Diesel auto-ignition and combustion processes as observed in optical imaging studies. The simulated results (for the cases tested) indicate that the auto-ignition of DI Diesel spray occurs at a site close to the mean stoichiometric surface. The ignition spot grows on the lean side, crosses over the mean stoichiometric surface, enters into the rich zone and develops further in a very short time. The prediction demonstrates that the post-ignition, fully developed combustion process occurs in a lifted diffusion flame stabilized at a large distance from nozzle exit. The spatial distributions of soot and NOx in the predicted lifted flame are similar to those described in Dec's conceptual Diesel combustion model. Further numerical investigations performed show that, the lower the ambient gas pressure and temperature, the longer the auto-ignition delay times of the sprays and vice versa. Increase in ambient gas pressure or temperature causes a reduction in the flame liftoff length. The results demonstrate also that the flame liftoff length is more sensitive to the change in the ambient temperature. The liftoff has a strong influence on the soot and NOx formation. The farther the flame is stabilized, the lower the emissions. Studies of air dilution effects were also performed to investigate the EGR effects on ignition delay, soot and NOx emissions of Diesel flames. The simulations suggest that Diesel auto-ignition delays are controlled by the oxygen concentrations not by the nature of diluents. The soot and NOx formation is suppressed by the dilution. Moreover, studies demonstrate that the initial temperature has a strong effect on soot formation whereas the pressure effect is much weaker. For the same amount of fuel injected, the longer the fuel injection duration time, the higher the maximum value of the averaged soot mass concentration produced. It is expected that the present numerical study combined with experimental studies may provide a better insight into Diesel spray combustion and pollutant formation in Diesel flames.

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Lionel Christopher Ganippa

Atomisation and Combustion Studies of Diesel Sprays

PhD Thesis, 2003

This thesis addresses two potential problems facing investigators involved in Diesel engine development: fuel atomisation and soot formation. A particular concern has been cavitation in nozzles and its influence on the spray and combustion, investigated through impingement studies, scaled-up transparent nozzle studies and evaluation of hydro grinding effects in a real-size nozzle. Besides cavitation, air dilution effects on soot formation were studied using Laser Induced Incandescence (LII) and two-colour pyrometry. A method was developed to study the instantaneous fuel jet momentum and nozzle discharge coefficient for a non-stationary injection process. The time-resolved fuel jet momentum and nozzle discharge coefficient provides information about the transient phenomena taking place during the injection period due to cavitation. Scaled-up transparent nozzles were used to observe the flow structure within the nozzle hole and to evaluate its effect on the jet emerging from the nozzle flow. The asymmetric distribution of cavitation discovered within the hole had a strong influence on the spray pattern. Under realistic engine conditions, two nozzles each with a hole along the nozzle axis and the same momentum distribution in time, but different inlet geometries, were chosen to study the cavitation effects on combustion. Even though there were differences in the internal turbulence and nozzle discharge coefficient due to cavitation, no major differences were observed in spray angle, penetration, ignition delay, flame structure, temperature or soot concentration between these two equivalent nozzles. LII measurements revealed that soot formation occurred on the inside boundary of the flame periphery where the temperatures are high and oxygen concentration is depleted. In addition, no soot formation was observed initially in the central core of the spray. During later stages, soot production in the interior of the flame caused the soot concentration to be higher in the central region close to the tip of the flame. In diluted environments, the effective ambient oxygen concentration available for reactions is lower, so the reaction rates and flame temperatures are reduced, which delays the first appearance of soot near the nozzle tip and decreases the overall soot formation. However, due to lack of oxygen, the soot that is formed is not effectively oxidised in the later stages, particularly close to the flame tip where very low temperatures were observed.

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Niklas Nordin

Complex Chemistry Modeling of Diesel Spray Combustion

PhD Thesis, 2001

The thesis illustrates the application of computational fluid dynamics (CFD) to turbulent reactive two-phase flows in piston engines. The focus of the thesis lies on numerical simulations of spray combustion phenomena with an emphasis on the modeling of turbulence/chemistry interaction effects using a detailed chemistry approach. The turbulence/chemistry interaction model accounts for the effects of turbulent micro-mixing on the chemical reaction rates. The models have been implemented in the {\bf KIVA3-V} code and successfully applied to spray combustion analysis in a constant volume and a DI Diesel engine. The limitations and difficulties of representing the spray in a Lagrangian fashion are also addressed. Three different liquid fuels have been used in the simulations: n-heptane, methanol and dimethyl ether (DME). Detailed and reduced chemical mechanisms have been developed and validated for all these fuels and reasonable agreement between experimental data and numerical simulations has been obtained.

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Michael Försth

Laser Diagnostics and Chemical Modeling of Combustion and Catalytic Processes

PhD Thesis, 2001

The $H_2 + 1/2 O_2 \leftrightarrow H_2O$ reaction on hot platinum surfaces has been studied. A stagnation flow geometry was used with a gas mixture of H_2 and O_2 at subatmospheric pressures. Experimental data of the OH concentration outside the surface were measured with Planar Laser Induced Fluorescence, PLIF, while Second Harmonic Generation, SHG, was used to determine the coverage on the surface. Detailed simulations of surface chemistry, mass-transport effects, and gas-phase chemistry, as well as the interaction between them, were performed with Chemkin. The formation energy of H_2O and OH was found to be 67 kJ/mol, while the desorption energy of OH was 250 kJ/mol. It was also found that, for pressures up to 130 Pa, the OH molecules that desorb from the surface are not influenced by the gas-phase chemistry. At higher pressures the desorbed OH molecules are partially consumed in reactions with gas-phase species. Increasing the pressure even more will result in a reactive gas phase where water is produced. Comparison with an inert glass surface showed that the catalytic surface strongly inhibits the gas-phase ignition. An explanation of this behaviour is that gas-phase radicals adsorb onto the surface and form less reactive species, such as water. In this way the gas phase outside a catalytic surface becomes depleted of reactive radicals. Sensitivity analysis was also used to study the complex surface/gas interaction. In another study elastic light scattering from a fuel spray was studied. Image processing was used in an attempt to reproduce the internal structure of the spray, despite the problems with strong attenuation due to substantial scattering from the spray. The numerical implementation was based on the Beer-Lambert's law for an inhomogeneous medium. The method was partially successful, although, calibration studies of the scattered light dependence on spray structure and droplet density will need to be included in future work.

ISBN 91-7291-034-8

Håkan Sandquist

Emission and Deposit Formation in Direct Injection Stratified Charge SI Engines

PhD Thesis, 2001

A promising approach to increase the efficiency of the spark ignition (SI) engine is to inject the fuel directly into the cylinder to form a stratified charge. There is a potential to reduce the fuel consumption at low speeds and loads by 20 - 25% compared with conventional SI engines with stoichiometric homogeneous charge. The main drawbacks to contemporary direct injection stratified charge (DISC) engines are high hydrocarbon (HC) and soot emissions. An experimental investigation of the sources of HC emissions, from a production Mitsubishi GDI® direct injection stratified charge SI engine which uses wall-guided mixture preparation, is presented in this thesis. The engine-out HC emissions were 50% higher for stratified operation than for homogeneous operation for the engine tested under the low load and speed conditions investigated. A comparison of cycle-resolved HC and NOx emissions was made for homogeneous and stratified operation. Distinct differences observed in HC concentration traces indicate clearly that the sources of hydrocarbon emissions are not the same as in conventional SI engines. The measurements indicate that over mixing (quenching), at the boundaries of the air/fuel mixture cloud, and under mixing, both in the spray center and on the surface of the piston bowl, are the dominating mechanisms for HC emission formation in this engine. The engine tested is more sensitive to fuel composition than conventional SI engines. While there is only a marginal potential to reduce the HC emissions from DISC engines by altering the distillation curve of the fuel, there is much greater potential to decrease the emissions by improving the fuel and combustion systems. Injector fouling was found to have a detrimental effect on HC emissions and engine stability when the engine was subjected to a 60 h deposit accumulation cycle. The frequency of misfires and/or partial burns became unacceptable after such short time intervals as 6 - 30 h for some of the gasolines tested. Although the deposit levels depend on fuel composition, it is concluded from this study that the formation of combustion chamber deposits did reduce HC emissions, due primarily to reduced heat transfer. It is clear from these tests that preventing injector deposit formation is essential for direct injection SI engines.

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Åsa Håkansson

Combustion Chemistry Investigation of Liquid and Solid Fuels

PhD Thesis, 2000

The aim of this work was to study the combustion of liquid and solid fuels with the emphasis on intermediates and products. Depending on the structure and the complexity of the fuel different reactors and methods were used. Small-scale laboratory reactors were built and chemical analysis and evaluation methods were developed. Heptane. N-heptane was combusted in an atmospheric premixed laminar flame burner (fuel/air ratio 1.0). Quantification and identification of the species profiles were performed using GC/MS, which was directly connected to the sampling probe. Complementary, the flame was modeled using a semi empirical heptane mechanism. Gasoline. Two gasoline qualities were combusted in an atmospheric premixed laminar flame burner (fuel/air ratio 1.0). The gasolines were European certificate gasoline (EUCG) and California phase 2 reformulated gasoline (P2 RFG). The EUCG contained higher amounts of aromatics and cyclohexane compared to P2 RFG. P2 RFG contained approximately 11% MTBE (EUCG none) and also higher amounts of isooctane. GC/MS was used for the identification and quantification of the species profiles. Bio Diesel. Rapeseed oil, rapeseed methyl ester (RME), and diesel (Swedish environmental class 1) were combusted at 550°C in a reactor. Similarities and differences between the combustion products were qualitatively investigated. Solid phase extraction (SPE) followed by GC/MS analysis was used for the sampling and identification of combustion species. Wood. Wood from eight conifer species, eight birch species, and two willow clones were examined. The samples were pyrolysed in nitrogen at 550°C using a small reactor and the results were analyzed qualitatively. Both direct sampling of the gaseous emissions and SPE technique were used. GC/MS and GC/FTIR/FID performed the chemical analysis. The results showed that different fuels demands detailed analyses of their combustion products, due to their environmental and health effects and also from a technological point of view. The combustion products could be derived from the original fuel components and the major part of the emissions consisted of unburned and partly burned fuel components. Seemingly, the results obtained from the small reactors can be valuable in the predictions of experiments performed in full-scale devices.

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