ISSN: 1231-4005
e-ISSN: 2354-0133
DOI: 10.5604/01.3001.0012.2860

MULTIDIMENSIONAL SIMULATION OF COMBUSTION AND KNOCK ONSET IN GAS ENGINES

Reinhard Tatschl, Peter Priesching, Jürgen Schneider

AVL List GmbH, Advanced Simulation Technologies
Hans-List-Platz 1, A-8020 Graz, Austria
tel.: +43 316 787 618, +43 316 787 1294, +43 316 787 1198, fax: +43 316 787 777
e-mail: reinhard.tatschl@avl.com, peter.priesching@avl.com, juergen.schneider@avl.com

Abstract

Natural gas fuelled internal combustion engines enable efficient energy conversion with relatively low environmental impact. Depending on the specific application, the available fuel quality, and the emission regulations to be fulfilled, different types of gas-engine combustion systems are in use. The major performance and hence efficiency limiting factors in gas fuelled engines are related to the lower ignitability of natural gas at part load and the appearance of abnormal combustion (knock) at high load conditions. This article provides an overview of the multidimensional CFD simulation workflow for the investigation and assessment of flame propagation and knock onset characteristics in different types of natural gas fuelled internal combustion engines. The most common approaches for simulating flame propagation/combustion under engine conditions are presented together with selected models for describing the pre-flame reactions finally leading to knock onset in the unburned in-cylinder charge ahead of the flame. Based on selected application examples, the models' performance and capabilities with respect to reflecting the essential characteristics of flame propagation and knock onset are presented.

Keywords: *gas engines, simulation, combustion, efficiency, knock onset*

1. Introduction

In the last decades, constantly increasing effort has been spent on reducing the impact of internal combustion engines on the environment, particularly concerning the emission of CO_2 and the various regulated pollutants, such as NOx, particulates, unburned hydrocarbons, etc. Natural gas is an effective alternative to gasoline and diesel fuels in many internal combustion engine applications. Due to its combustion properties, natural gas is well suited for lean burn operation with low NOx emission levels, and its high research octane number allows combustion at higher compression ratios. Both features are particularly attractive regarding engine efficiency and emission characteristics for a broad range of applications for transportation as well as power generation. Due to their high efficiency and low environmental impact, natural gas fuelled engines are already well established for stationary power generation and are gaining further increased attention for marine, locomotive and automotive applications.

However, the lower flame speed of natural gas can cause issues regarding spark-induced flame initiation at part load operation, while port-fuel admission can lead to power density losses due to displacement of intake air by the low-density natural gas. In addition, despite its higher research octane number, which allows combustion at higher compression ratios, the undesired onset of knock is still one of the major efficiency limiting factors at high load operating conditions. Diesel pilot injection, active and passive pre-chamber concepts and gas direct injection into the main combustion chamber can help to master these challenges, however, at the expense of considerably increased combustion system development and optimization effort. The need for shortened development times and hence fewer hardware prototypes during the development and field testing phase leads to the necessity of reliable simulation tools for accurate prediction of the governing in-cylinder processes.

In recent years, 3D-CFD has been successfully established for the calculation of fluid flow, mixture formation, and combustion in internal combustion engines as a complementary tool to in-

cylinder pressure analysis and optical mixture formation and combustion diagnostics. The accuracy of the calculation results and hence the potential contribution of the CFD simulation to major design decisions in the engine development process strongly depends on the achievable simulation project turnaround times and the reliability of the models adopted for the treatment of the individual in-cylinder physical and chemical processes.

Based on models and methods available today, 3D-CFD simulations are able to provide quantitative space and time resolved information about the various in-cylinder flow and mixture formation quantities and already today considerably contributes to a better understanding of the combustion process in natural gas fuelled engines. Such detailed information on the governing in-cylinder processes is an invaluable contribution to gaining an in-depth insight into the cause and effect chain and forms the basis for combustion system optimization with respect to efficiency and pollutant emission characteristics.

The present article provides an overview of the methodology on how to utilize multidimensional CFD for the investigation and assessment of flame propagation and knock onset characteristics in different types of natural gas fuelled internal combustion engines. After a short overview on the numerical solution approach, dedicated models for simulating flame propagation/combustion under engine conditions are presented together with selected methods for describing the pre-flame reactions finally leading to knock onset in the unburned in-cylinder charge ahead of the flame. Based on selected application examples, the models' performance with respect to reflecting the essential characteristics of flame propagation and knock onset are presented and discussed.

2. CFD Simulation Methodology

The present chapter provides an overview of the overall CFD methodology for simulation of internal combustion engine flow, mixture formation, and combustion. The workflow description including the CFD solver and modelling details as well as the calculation results shown are based on the commercial CFD code AVL FIRE™.

2.1. Simulation Kernel

AVL FIRE™ enables the simulation of turbulent reactive flows in moving contracting/expanding engine geometries adopting all kinds of different liquid and gaseous fuel types. The simulation kernel solves the general conservation equations of mass, momentum and enthalpy as well as additional transport equations for turbulence related quantities and chemical species. Depending on the physical and chemical sub-models adopted, additional scalar quantities, such as fluid volume fraction, mixture fraction, reaction progress variable, flame surface density, etc. are accounted for.

The solution method is based on a fully conservative Finite-Volume approach supporting general unstructured computational grids with elements containing an arbitrary number of cell faces (polyhedral elements). All dependent variables for momentum, pressure, density, turbulent kinetic energy, dissipation rate, and further scalar quantities, such as chemical species, flame surface density, etc., are evaluated at the centres of the computational cells. Special connectivity and interpolation practices for gradients and cell-face values are introduced to accommodate the polyhedral calculation volumes. The overall solution procedure is iterative and is applicable to turbulent flows at all speeds, including super-sonic flows.

For solving, the large sets of linear equation systems evolving from the discretization of the governing equations, efficient preconditioned Conjugate Gradient Methods and Algebraic Multigrid Methods are adopted. Various initial and boundary conditions are supported to match the setup of any simulation to the real flow problem, such as gas mixing, coolant flow and heat transfer [1, 2, 20], as shown in Fig. 1. Meeting the requirements of different fields of applications, simulations may be set up in steady or transient (time stepping and crank angle) mode. For execution on multi-

processor hardware, a domain decomposition parallelization approach, enabling efficient solution of flow problems comprising of a large number of computational cells, is employed.

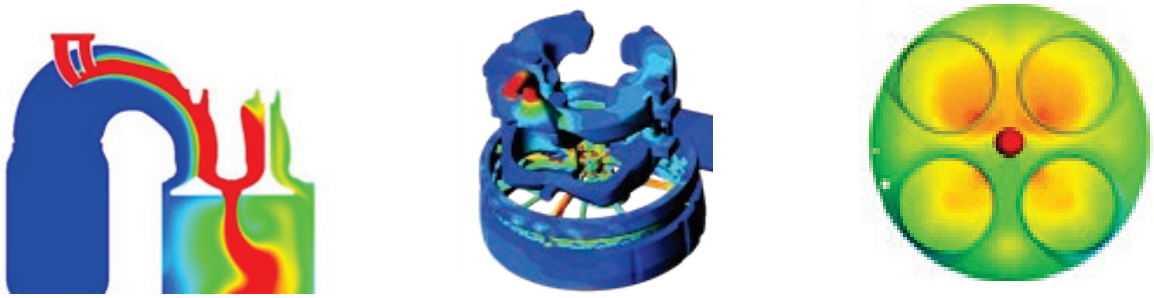

Fig. 1. Selected CFD simulation results of turbulent flow and heat transfer in engines; intake port gas admission (left) coolant flow (middle), combustion chamber gas-side heat transfer (right)

2.2. IC-Engine Geometrical Modelling

The computational representation of the moving engine geometries is enabled by appropriate grid generation methods applicable to all types of spark-ignition and compression-ignition engines. The meshing module of AVL FIRE™ comprises advanced grid generation techniques, enabling fast and seamless meshing of all types of engine geometries, including complex pre-chamber, spark plug and injector details, as shown in Fig. 2.

Depending on the adopted meshing technology, the resulting computational grids consist of polyhedron elements, of hexahedron elements with prisms and pyramids in the vicinity of local refinement and transition areas, or of hexahedron elements arranged in a block-structured manner. Automated mesh movement techniques and algorithms for resolution of geometrical details provide maximum flexibility for all relevant grid generation tasks. Mesh movement is based upon an interpolation between grids of identical topology set up at different positions of the moving domains, typically at different piston/valve positions. In order to ensure optimum mesh quality during piston/valve movement over the entire crank-angle interval under consideration, a so-called rezoning procedure is applied.

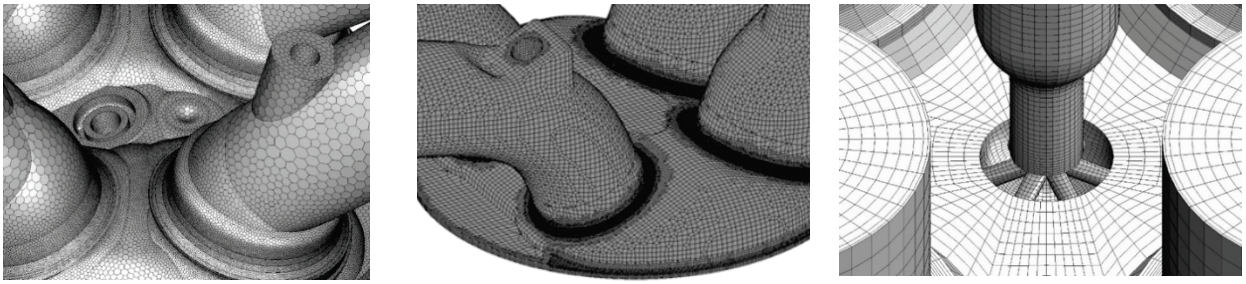

Fig. 2. Computational grids generated by adopting different meshing technologies; polyhedron mesh (left) unstructured hexahedron mesh (middle), block structured hexahedron mesh (right)

3. Combustion and Knock Onset Modelling

The combustion behaviour in IC-engines is mainly determined by the in-cylinder turbulent flow, the mixture stoichiometry, and the in-cylinder pressure and temperature conditions in the unburned charge. The local turbulent reaction rate is thereby governed by the fuel chemistry and the related laminar burning velocity, as well as by the impact of the turbulent flow field on the reaction zone. For calculating premixed, partially premixed, as well as non-premixed combustion in IC-engines, models of different level of complexity are available in AVL FIRE™. These can be distinguished by the turbulence/chemistry interaction modelling, the adopted hydrocarbon reaction mechanisms, and the numerical treatment of the turbulent reaction zone itself.

3.1. Premixed Flame Propagation

The Flame Tracking Model for simulating premixed flame propagation is based on the assumption that under typical engine operating conditions the chemical reactions in the turbulent flame front are much faster than the turbulent mixing processes. Thus, the flame front can be considered as thin compared to the length scales of the turbulent flow field and can hence be approximated by a connected surface propagating across the combustion chamber [8]. The propagation characteristic of the flame surface is determined by the combined effects of the turbulent reactions, the expansion of the hot combustion products behind the flame and convective transport due to in-cylinder charge motion. The mathematical representation of the flame propagation process itself is achieved on the basis of a surface-tracking algorithm, such as the level-set approach [11], which is efficiently coupled with the relevant conservation equations governing the in-cylinder flow, temperature and mixture composition fields.

The local turbulent flame speed, determined by the chemical kinetics in the reaction zone and the wrinkling of the flame front due to its interaction with the turbulent in-cylinder charge, is described via suitable turbulent flame speed correlations, e.g. [9, 16, 8]. On this basis, the impact of the local fuel/air equivalence ratio, the local residual gas concentration, the in-cylinder pressure, and temperature conditions as well as of the local turbulence intensity on the propagation velocity of the flame surface can be well reflected by the simulation. For a representative set of liquid and gaseous fuels these correlation functions are readily available, for future fuels these can be derived from experimental studies.

The application of the Flame Tracking Model enables seamless analysis of the flame propagation characteristics in open chamber gas-engines, such as the assessment of the impact of different in-cylinder charge motion, piston bowl geometry and spark-ignition system features.

Fig. 3. Open chamber gas engine combustion; flame front position at 5 deg. CA after TDC (left) and 25 deg. CA after TDC (right)

Figure 3 shows in a top view of the combustion chamber the flame propagation characteristics in an open-chamber research engine. The considered engine is based on a small turbo-charged 4-cylinder in-line diesel engine. The diesel injector of the original engine is replaced by a centrally located 7-hole gas injector. Methane is injected during the early compression stroke with a pressure of about 40 bar directly into the combustion chamber, leading to good homogenisation of the fuel with the in-cylinder charge prior to combustion. The engine features a spark plug ignition system with an off-centred spark plug position. The flame front is represented by the iso-surface separating the unburned and burned mixture ahead and behind the reaction zone, respectively. In the left picture, displaying the flame front location at 5 deg. CA after firing TDC, the remnant of the asymmetric spark plug location is still clearly visible. At 25 deg., CA after TDC the flame shows a more symmetric pattern in the late burning phase. The results clearly demonstrate the insight the adopted Flame Tracking Model is able to provide into the detailed flame propagation characteristics and into the cause-and-effect relations between in cylinder flow field, piston shape, and spark plug location.

3.2. Cycle-to-Cycle Combustion Variations

The Coherent Flame Model for simulating premixed and partially premixed combustion in engines is based upon solving a transport equation for the flame surface density, and accounting for flame surface production due to wrinkling of the flame by turbulence effects and for flame surface annihilation due to chemical reaction. The laminar flame speed information required in the coherent flame modelling approach for premixed combustion is obtained either from empirical correlations, such as [15], or from detailed chemical kinetic calculations and tabulation of the laminar flame speed data as a function of temperature, pressure, equivalence ratio and residual gas content [4, 5]. The detailed kinetic calculations and the tabulation of the laminar flame speed data are performed independently of the CFD calculation. A fast interpolation algorithm adopted for processing of the tabulated flame speed information ensures CPU efficient use of the detailed chemical kinetic information within the CFD simulation. In order to describe the fuel oxidation chemistry in the reaction zone, a reduced hydrocarbon chemical kinetic scheme combined with an equilibrium chemistry approach is used in order to model the high temperature oxidation process within the flame and in the post-flame region, respectively.

Based on a Large-Eddy-Simulation (LES) variant of the Coherent Flame Model, cycle resolved simulations of the premixed flame propagation enable the analysis and assessment of cycle-to-cycle variations of engine combustion processes [24, 25]. Suitable extensions of the Coherent Flame Model with respect to treatment of flame stretch and curvature ensure its successful application in the context of the LES simulations. In order to quantitatively reflect the variation of the cycle resolved in-cylinder pressure traces, the adopted spark flame initiation model accounts for the impact of subgrid-scale processes on the size, location, and initial flame surface density of the initial flame kernel [24].

Large gas engines have the flexibility to be operated with different types of gaseous fuels like biogas, weak gases and pit gases. However, the gas composition has a strong impact on the heating value and the methane number and therefore on the ignitability, power output and knocks resistance. It is therefore an important goal for gas engine development to optimise the combustion process for a given gas quality in order to achieve reliable ignition behaviour and similar efficiencies as for gas engines that are operated with methane.

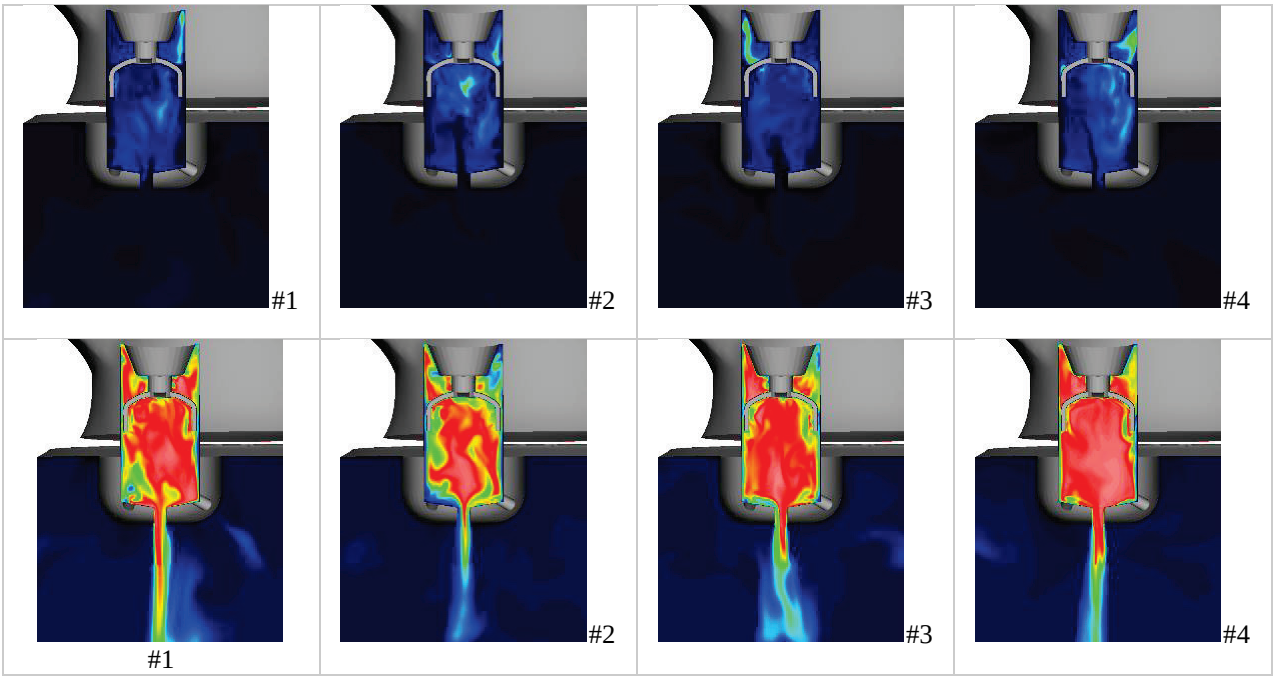

Fig. 4. Cycle-to-cycle variations of combustion in a passive pre-chamber spark-plug; temperature field for individual cycles at 20° CA bTDC (top row) and 14° CA bTDC (bottom row)

A major prerequisite for the development of strategies for reliable ignition and minimized cycle-to-cycle combustion variations is a detailed understanding of the causes leading to the cyclic dispersion of the combustion process from one cycle to the other. Conventional cylinder pressure indication provides information on the appearance of cycle-to-cycle combustion variations and also enables a quantification of the in-cylinder pressure evolution variations from one cycle to the other. However, in order to identify the origins of the cycle-to-cycle combustion variations, a detailed cycle-resolved insight into the locally governing in-cylinder flow, mixture formation, and early stages of flame propagation including their complex mutual interactions is required.

Figure 4 shows the simulated cycle resolved temperature distribution in a passive pre-chamber spark plug for four engine cycles at two different crank-angle positions adopting LES. Specifically in the results obtained for the crank-angle position of 14° CA before TDC, the cycle-to-cycle differences in the temperature fields become clearly evident for both the conditions in the pre-chamber itself and the jet of hot combustion products exiting from the pre-chamber and entering the main combustion chamber. Results of this kind provide clear indications to the combustion system development engineer how to specifically adapt the pre-chamber size and shape in order to achieve optimum combustion stability for all relevant operating conditions.

3.3. Diesel-Gas Dual Fuel Combustion

Adopting tailored extensions, the Coherent Flame Model is also applicable to dual fuel combustion, capable of simultaneously accounting for all relevant combustion regimes [7, 14]. Extension of the original model formulation enables proper simulation of the dual fuel combustion sub-processes, namely the treatment of the dual fuel mixture ignition delay, the initial flame surface density following auto-ignition, and the flame front propagation across the lean gas/air mixture. Detailed chemistry calculations using a dual fuel compatible reaction mechanism form the basis for the ignition delay tabulation, which covers the two different fuels natural-gas and diesel, usually adopted in the dual fuel combustion mode [6]. The extensions related to the initial flame surface density deposition in the burned areas following diesel pilot spray auto-ignition account for thermal expansion of the combustion products and local turbulence effects. The subsequent flame front propagation process is then governed by the flame surface density transport, adopting laminar flame speed data accounting for varying mixture composition of natural gas and diesel.

The validity of the dual fuel version of the Coherent Flame Model is proven for a large high-speed four-stroke single cylinder diesel-gas dual fuel engine with a displacement of approximately 6 litres [7]. The measurements are carried out on an engine testbed with all media supplied to the engine (e.g. charge air, burning gas, cooling water and lubricating oil) properly conditioned. A lean natural gas-air mixture is used to investigate the combustion process. A common rail system with up to 1600 bar rail pressure provides the high-pressure diesel fuel supply for the pilot injection that ignites the gas-air mixture. The injector is positioned in the centre of the cylinder head and has four symmetrically arranged nozzle holes.

An injection timing variation at nominal engine power is chosen as the basis for validating the dual fuel simulation model. From a baseline operating point, the injection timing is varied between -10 °CA and +10 °CA. The results in Fig. 5 clearly show that a variation of the injection timing within a range of 20 °CA at very small diesel fractions has a significant influence on the combustion process. Diesel, gas, and air mass flow vary according to the efficiency of the operating point. Thus, the three operating points chosen provide a good basis for investigating the ability of the simulation model to depict the differences in combustion behaviour. As can be seen from the space and time resolved results in Fig. 5 the injection timing strongly influences the mixing of the diesel with the background mixture, the ignition locations for the mixture as well as the flame front propagation characteristics, which are linked to the individual mixing and ignition phenomena.

Figure 5 on the left shows a comparison of the measurement and simulation results for the three

operating points, comparing the heat release rates post-processed using a 0D engine-cycle tool. With early injection, the heat release rate exhibits a very symmetrical shape with the simulation results being in good agreement with the measured values. With the baseline injection timing, the heat release rate exhibits a slightly different behaviour, reaching a kind of premixed peak most likely linked to the diesel auto-ignition. In the case of late injection timing, the measured premixed peak of the diesel auto-ignition is even more significant.

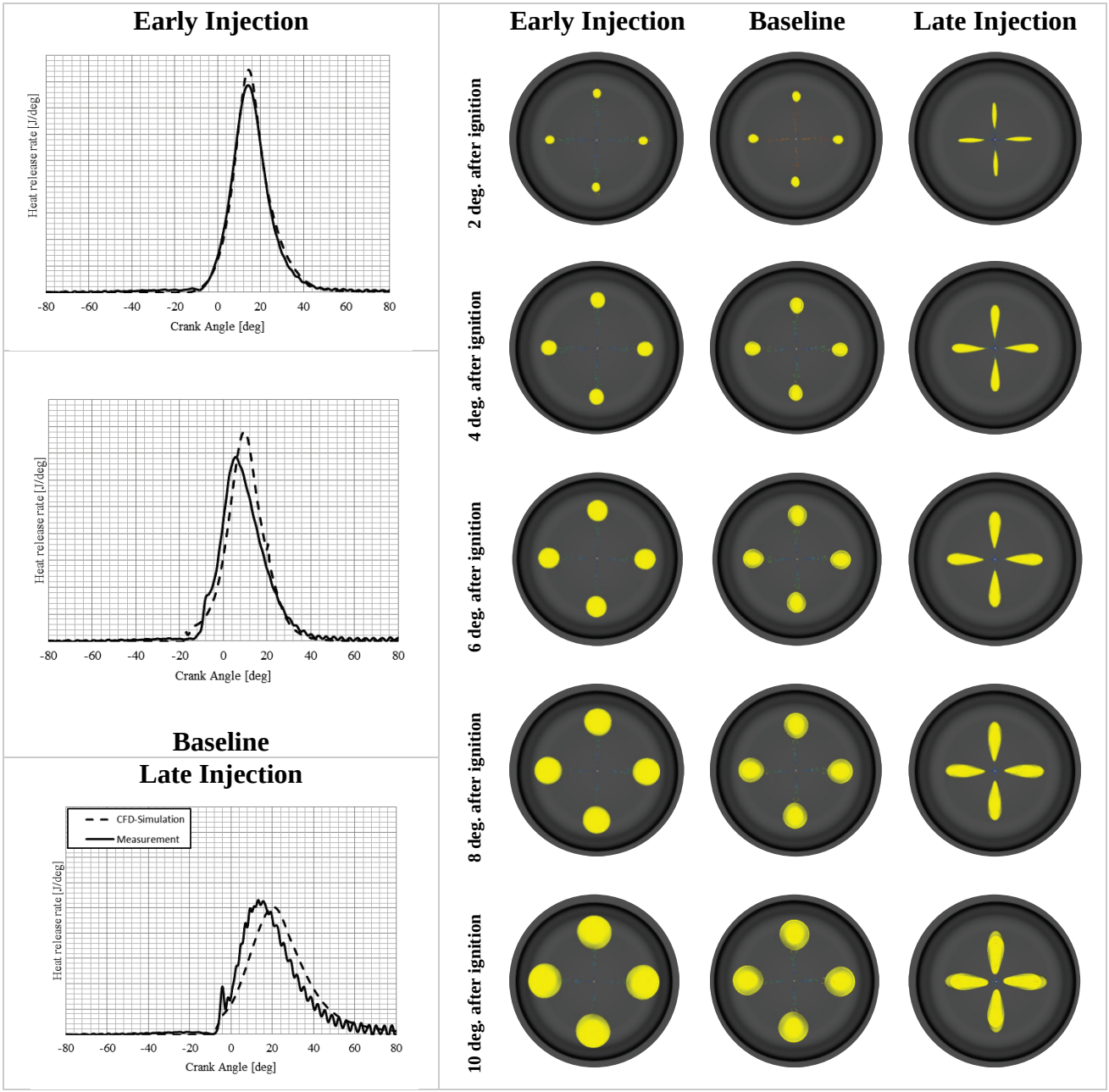

Fig. 5: Dual-fuel engine combustion; simulated vs. measured heat release rate (left) and iso-surface of the reaction progress variable (right) for three different injection timings [7]

The above results clearly demonstrate the possible insight into the auto-ignition timing and location, the detailed flame propagation characteristics and the impact of combustion system parameter variations onto the global combustion behaviour the newly developed dual fuel Coherent Flame Modelling is able to provide. Besides the injection timing variation, the impact of varying diesel injection quantities, number of injector holes, nozzle tip protrusion and angle variation, as well as background mixture stoichiometry variations can be easily analysed and assessed.

3.4. Detailed Chemistry Combustion Modelling

Modelling the combustion chemistry and the turbulence/chemistry interaction during hydrocarbon oxidation is the major challenge in simulating turbulent reacting flows in engines. The chemical kinetic reactions of typical hydrocarbon fuels involve hundreds of intermediate species and their reaction paths usually comprise of several hundred up to several thousand of reaction steps. Are the reaction details and the related rate coefficients of the common hydrocarbon neither fuels known in detail nor would it be feasible to account for the entire set of reactions within an engineering environment due to excessively high computational demands.

The coupling between the chemistry and the turbulent flow field results from the high non-linearity of the chemical reaction rates under the presence of local stochastic fluctuations of the flow and composition fields. The common practice adopts an averaging procedure replacing the instantaneous flow field quantities by its mean and fluctuating components. Mathematically these results in the appearance of terms in the conservation equations, which contain correlations of fluctuating components, that needs to be expressed by known mean flow quantities. A variety of models of various levels of complexity and sophistication has been proposed in the last decades in order to model the complex hydrocarbon combustion chemistry and to account for the turbulence/chemistry interaction, e.g. [3, 13, 19].

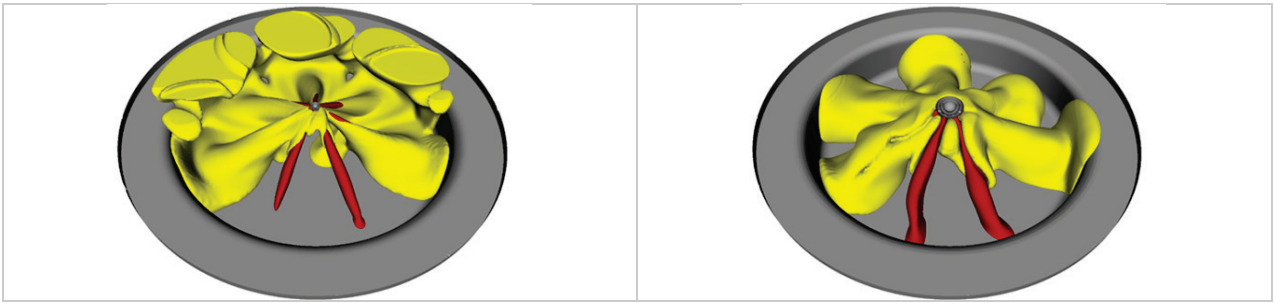

Fig. 6. Detailed chemical kinetic simulation of gas direct-injection with diesel pilot fuel spray ignition, adopting pilot spray configuration A (left) and pilot spray configuration B (right)

The Flamelet Generated Manifold modelling approach perfectly masters the above challenges related to the efficient treatment of complex chemical kinetics and proper handling of the turbulence/chemistry interaction in the context of a complex multidimensional CFD simulation, [22]. This is achieved via pre-calculation of the detailed chemical kinetic reactions prior to the CFD simulation and storage of the relevant information about the reaction paths and the related conversion rates in tabulated form. For premixed natural gas combustion these tables are set up on the basis of the free parameters pressure, temperature, mean and variance of the mixture fraction and reaction progress variable. In the context of dual fuel combustion systems, the parameter range is further extended by the fuel composition dimension, e.g. natural gas, diesel (usually represented by n-heptane) in order to account for the transition from diesel/gas mixture auto-ignition to a self-sustaining freely propagating flame front in the pure gas/air mixture.

The detailed/tabulated chemical kinetics based simulation approach is specifically well suited for the simulation of highly complex combustion processes, characterized by the simultaneous appearance of premixed, partially premixed and non-premixed combustion regimes. By adopting the Flamelet Generated Manifold approach, combustion systems utilizing gas direct-injection and diesel pilot fuel sprays can be handled in the simulation in a highly efficient manner. Fig. 6 shows representative simulation results of the application of detailed chemical kinetic simulation for analysis and assessment of the impact of different diesel pilot fuel sprays on the spatial and temporal evolution characteristics of the combustion details. Such kinds of simulations offer a seamless way of virtual analysis and assessment of different gas-injection, diesel pilot spray injection and operation strategies prior to hardware testing of the different configurations.

3.5. End Gas Reactions and Knock Onset

Engine knock is caused by the rapid auto-ignition of a portion of the in-cylinder charge that generates a local pressure pulse leading to pressure oscillations in the combustion chamber. This auto-ignition is usually initiated from one or more locations in the end gas, the unburned mixture ahead of the flame front. The thermodynamic state of the end gas in the cylinder is determined by the in-cylinder pressure, temperature, and mixture composition conditions including their history during the intake and compression strokes. Critical parameters that affect the in-cylinder and hence end gas conditions are inlet pressure and temperature, air-fuel ratio, spark timing, compression ratio, engine speed, charge preparation, and combustion chamber geometry. Hence, coupling of suitable semi-physical or detailed/reduced chemical kinetics based auto-ignition models with the flame propagation and combustion models introduced above enables identification of the location of the pre-reactions that finally lead to the onset of knock.

Fig. 7. Open chamber gas-engine combustion and knock onset; local temperature distribution (left) and pre-flame progress variable (right) [18]

Semi-physical knock models are typically based on describing the growth of a knock precursor representing the progress of the auto-ignition pre-reactions [10, 23]. The knock precursor production rate is usually based on an Arrhenius-like expression with the rate parameters as functions of the specific fuel type under consideration. Alternatively, tabulated auto-ignition data based on detailed chemical kinetic calculations are used for representative hydrocarbon fuels to calculate the knock-precursor formation rates. In the kinetic knock, modelling approaches the pre-reactions in the end gas are directly calculated according to detailed or reduced chemical kinetic schemes [18]. The currently available chemical kinetic mechanisms for the description of natural gas/methane oxidation, e.g. [12, 17, 21], are capable of properly reflecting the auto-ignition behaviour for a broad range of initial conditions. Local effects of fluctuating temperature and mixture composition are accounted for in the CFD simulation by adopting a presumed probability density function (PDF) approach or by directly solving for the transport equation of the joint scalar PDF by adopting suitable particle methods, as shown in Fig. 7.

8. Summary

An overview of the multidimensional CFD simulation workflow for the analysis and assessment of flame propagation and knock onset in different types of gas fuelled internal combustion engines is provided together with selected results of the application of the individual models to specific gas engine combustion systems.

The simulation results demonstrate the applicability of the Flame Tracking Model to the analysis of the combustion characteristics in an open chamber gas engine. The applicability of the LES version of the Coherent Flame Model is successfully demonstrated for the analysis of the cycle-to-cycle combustion variations in a passive pre-chamber spark ignition gas engine. A comparison of simulation results with measurement data regarding the impact of pilot diesel fuel injection on the combustion characteristics in a large diesel-gas dual fuel engine demonstrates the capabilities of the dual fuel version of the Coherent Flame Model. Results of the application of a detailed chemical kinetic combustion modelling approach prove to reflect the impact of different diesel pilot injection configurations on the overall combustion characteristics of a gas direct injection engine. Different modelling approaches to simulate the pre-reactions in the end gas are presented together with results showing the knock onset locations in an open chamber gas engine.

Acknowledgements

The research was partially done in the frame of the KNOCKY project, which received funding from the European Union's HORIZON 2020 Research and Innovation Programme under grant agreement No. 691232.

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Manuscript received 24 March 2018; approved for printing 29 June 2018