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APPLICATION OF CFD SIMULATION TO OPTIMIZE COMBUSTION IN PRECHAMBER GAS ENGINES WITH PORT INJECTION

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Abstract. The combustion engine technologies of the future must reduce fuel consumption and CO_2 emissions while maintaining high power density. In addition, large stationary gas engines have to meet high demands with respect to emission legislation, fuel flexibility and robustness. Cylinder-specific fuel gas admission (port injection) allows lean burn gas engines to meet these requirements. To further increase efficiency, it is key to avoid knocking combustion. With port injection, high efficiencies can be accomplished, but at the same time a high level of mixture homogeneity must be ensured.

This paper describes the use of CFD simulation to investigate and optimize combustion in a large prechamber gas engine. The focus is on a methodology that enables the evaluation of different mixing concepts and the interaction between the prechamber and main combustion chamber. Due to the three-dimensional nature of the mixing phenomena, CFD simulation is critical to understanding and optimizing these processes. Calculation methods and models are discussed and a methodology for the detailed assessment of the quality of mixture homogeneity is presented.

The CFD methodology is verified by assessing the combustion and knock behavior of a single cylinder research engine that includes optical combustion diagnostics. The flame front propagation is recorded by a large number of fiber optic sensors in the prechamber and the main combustion chamber. A tomographic post-processing routine calculates local flame intensities, flame distribution in relation to crank angle degree and probable knock locations in the main combustion chamber.

Finally, the paper compares analyzed and simulated flame propagation in the prechamber and the main combustion chamber and presents the knock locations identified in several example cases. The results confirm the statements derived from CFD simulation. It is shown that CFD simulation is a valuable tool in the predesign of prechamber gas engines that contributes to a thorough understanding of the combustion process at the operating limits.

1 INTRODUCTION

The key to the energy technologies of the future will be reduced fuel consumption and CO_2 emissions whilst maintaining a high power density. In addition, large stationary gas engines have to meet high demands with respect to emissions legislation, fuel flexibility and robustness. With regard to efficiency, large gas engines now reach values that are far beyond those of diesel engines, see [5]. A variety of measures were responsible for the remarkable increase in efficiency. Two key points were the increased efficiency in the turbocharging system and the decrease in cylinder-specific differences by using selective gas admission in the intake duct upstream of each cylinder (port injection) [6]. It was also critical to raise the compression ratio and at the same time make the engines more resistant to knocking. With port injection, high efficiencies can be accomplished; however, a high level of mixture homogeneity must be ensured. A less homogeneous mixture is obtained with cylinder-specific mixture formation via port injection (PI) than with the variant with a central gas mixer. One issue in this investigation was to evaluate to what extent the reduced homogeneity of the charge in port injection influences the tendency for knocking to occur in the engine. Since there is only a brief time window during which the mixture can be homogenized when port injection is used, special emphasis was placed on simulation-based pre-optimization. 3D-CFD simulation was conducted of a number of PI variants with the goal of obtaining the most homogeneous mixture possible with a predefined pressure difference between the intake and exhaust sides. Since poor homogenization has an unfavorable impact on knock tendency especially at the periphery of the combustion chamber, an assessment can be made only in combination with the entire combustion sequence. As a result, it was also necessary to provide a good description of the combustion sequence of the prechamber combustion concept using simulation and to verify the models with measurements on a single-cylinder research engine. In addition to standard measurement technology, optical combustion diagnostics was used on the single-cylinder research engine to obtain local information about the prechamber (PC) and main combustion chamber (MC) and their interaction.

2 GENERAL APPROACH TO SIMULATION-BASED COMBUSTION SYSTEM DEVELOPMENT

The LEC Development Methodology (LDM) [1] is used to develop and optimize combustion concepts for large engines. LDM is based on the intensive interaction between simulation (SIM) and experimental investigations on single-cylinder research engines (SCE) and multi-cylinder engines (MCE). The simulation-based development of combustion processes with LDM presupposes the availability of a single-cylinder research engine derived from the multi-cylinder engine under investigation. New concepts are developed and validated following this methodology as illustrated in **Figure 1**. Typical application examples are the development of new prechamber concepts, lowest emission concepts, combustion system design for specific gas mixtures and alternative ignition concepts.

In many cases, 3D-CFD simulation is relied upon to pre-optimize a new concept. The engine cycle of the multi-cylinder engine is simulated in order to generate the boundary conditions.

Initial assumptions have to be made about the expected rate of heat release and the operating parameters. As a rule, rate of heat release, NOx formation and knock behavior are simulated with zero-dimensional models extensively validated by measurements taken on the engine under investigation (SCE and MCE). The engine cycle model must be calibrated to measurements from the multi-cylinder engine and best illustrate the geometry of the intake and exhaust system, valve timing and turbocharging.

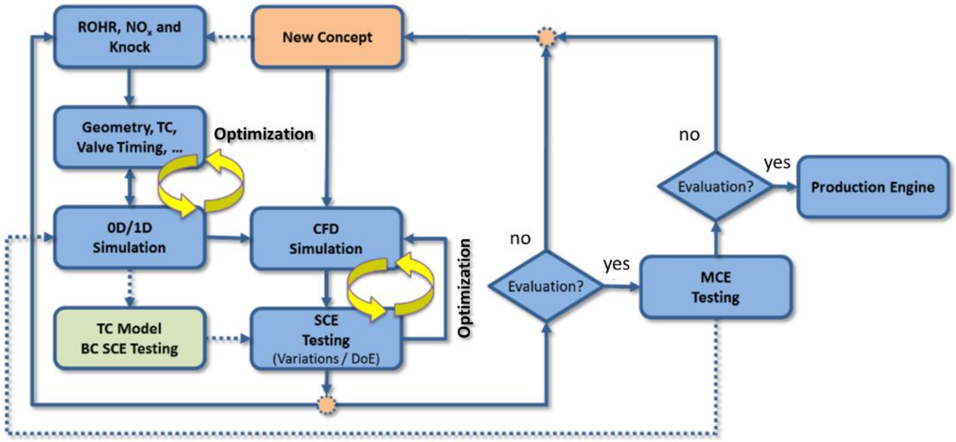


Figure 1: Simulation-based combustion process development (LDM)

Using these boundary conditions, the concept is preoptimized with 3D-CFD simulation. The most promising variants are then tested on the single-cylinder engine. The boundary conditions required for single-cylinder engine tests are derived once again from engine cycle simulation. The simplified turbocharger model implemented into the test bed software that is normally used generates the pressure difference between the intake and exhaust sides as a function of engine operating parameters. The concept is assessed based on the test results and optimized if necessary (e.g., further simulation calculations, DoE tests). In most cases, the implementation of the concepts on the MCE also requires the entire system to be optimized with one-dimensional engine cycle simulation. This process is carried out with zero-dimensional models calibrated using the measurement results of the new concept and statistical methods (cf. the section “Virtual Combustion Process Development”). After a positive assessment of the measurement results from single-cylinder testing and the statements regarding the impact on the entire system, the concept can be transferred to the multi-cylinder engine. The multi-cylinder test bed results then provide the basis for deciding whether the concept should be introduced into series production.

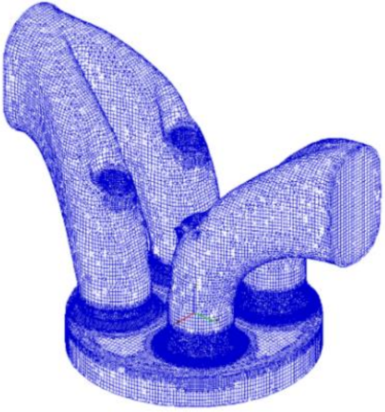
3 3D CFD SIMULATION

The present investigations were conducted with the CFD software FIRE (version 2013) from AVL List GmbH Graz [7]. The base module of the program permits simulation of reactive gases in complex geometries. In addition, numerous models are available for handling special tasks such as mixture formation, combustion simulation and pollutant formation. The core of the flow simulation is the SIMPLE algorithm for coupling pressure and velocities according to Patankar [8]. The preprocessor permits the creation of moving grids.

The following section describes the basic procedure, mentioning the grid topology appropriate for this task and the applied models. The generation of the required boundary conditions will be explained and the limitations of the method will be discussed.

3.1 Grid and topology

The geometry of the combustion chamber of the single-cylinder research engine and the intake and exhaust ports were modeled and interconnected. An overview is provided in **Figure 2**; gas admission is not represented in the figure. The mesh was prepared with FAME Engine Plus. FAME Engine Plus [7] is based on the FAME Hexa meshing and smoothing technology. Over 80% of the mesh consists of hexahedron cells. The remaining cells are tetrahedrons, pyramids and prisms. The total number of cells in the mesh is around 3.5 million. The table on the right-hand side of **Figure 2** presents the solver settings that were used.



Discretisation			
	Calculation of boundary values		Mirror
	Calculation of derivates		Least Sq. Fit
Equation control			
	Differencing scheme		
		Momentum	MINMOD Relaxed
		Continuity	Central Differencing
		Turbulence	Upwind
		Energy	Upwind
Linear solver			GSTB for all Eq.
Convergence criteria			0.0001 for all Eq.

Figure 2: CFD grid and solver settings

3.2 Models used

All the models used in these investigations that were applied during simulation are available in AVL FIRE. The k-zeta-f model was employed as the turbulence model. To simulate combustion, the multi-species PDF model [9] was used. NO concentration was simulated with the Extended Zeldovich Model. The two equations initially proposed by Zeldovich along with an additional equation were used.

3.3 Boundary conditions generated by 1D simulation

As explained above, boundary conditions on the intake and exhaust sides must be set for CFD simulation. These conditions are determined with 1D simulation. Boundary conditions for pressure are used on the air intake side and on the exhaust side. A mass flow boundary condition was set at the location of the gas intake. The principle behind the port injection system is illustrated in **Figure 3**. The gas is added at the location of the gas valve. A large number of variations were made in the geometry of the gas intake port as well as in mass flow in terms of the timing and duration of injection (see **Figure 3**, right); in 1D simulation, care is taken that the desired pressure to obtain the required load is reached with each configuration. Based on the boundary conditions from 1D simulation, 3D-CFD simulations were conducted and the homogeneity of the mixture at ignition timing was evaluated. The detailed discussion of the evaluation is found in section 4.

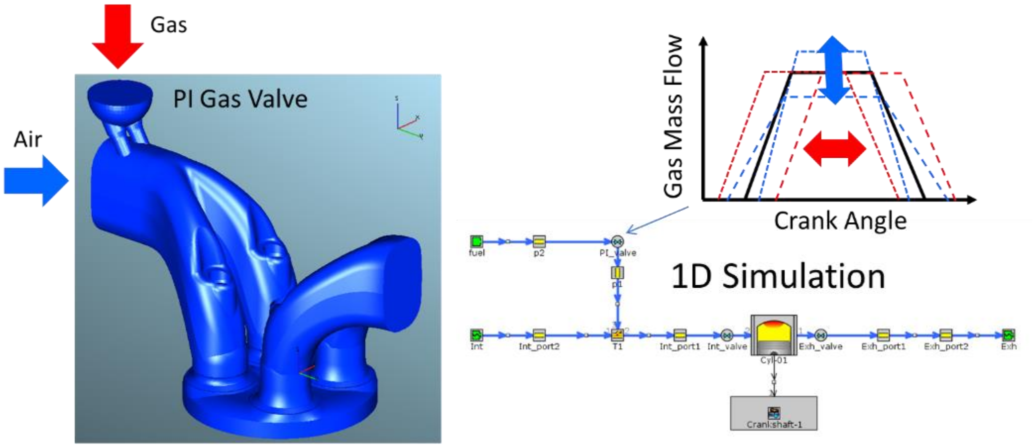


Figure 3: CFD boundary conditions from 1D simulation

3.4 Limitations

In principle, 3D CFD simulation provides good predictions of charge motion and mixture formation. The processes within the engine are reproduced with sufficient accuracy by the models provided by the software. In terms of inflammation and combustion sequence, the model parameters must be calibrated based on engine measurements. A well calibrated combustion model is able to predict NO and HC emissions. The availability of suitable boundary conditions is equally important for successful prediction. As a consequence, the limitations regarding the robustness of the results are ultimately dictated by combustion modeling. In particular, RANS simulation of the complex processes of the interaction between the prechamber and main combustion chamber has nearly reached a limit. For example, it has not been possible to use a uniform set of parameters for combustion in the prechamber and in the main combustion chamber. In this case, a combustion model in connection with large eddy simulation (LES) may bring about an improvement. With the resources available at present, however, calculation of the entire combustion chamber with LES still appears to involve too much effort. Nevertheless, the investigation of certain parts of the model may also be helpful in simulation with RANS. In general, RANS methods in combination with the methodology described above can be used to optimize the qualitative details of specific processes (mixture formation and combustion in the prechamber and main combustion chamber, determination of possible knock locations, etc.).

4 EVALUATION AND VERIFICATION

To guarantee the robustness and reliability of the simulation methodology, above all when a variety of coupled submodels are applied, a special emphasis should be placed on verifying the individual elements. Only with models that can be easily compared to engine measurements can the combustion concepts be predesigned and optimized effectively. In predesign with simulation, it is also effective to define suitable criteria for assessing the quality of the results. The following section presents and discusses evaluation criteria that have proven to be effective in the predesign of a combustion concept for gas engines with port injection. To evaluate the quality of the calibration of the combustion model, a comparison of the measured and simulated pressure curves and burn rate curves are presented and discussed below. The methodology used for mixture formation, NO formation and knock tendency is described. It was verified by measurements on a single-cylinder research engine, a brief description of which is thus provided. Also described is the special optical combustion diagnostics for flame propagation and determination of the location of knock. Finally, CFD calculations and SCE measurements are compared.

4.1 Evaluation criteria for combustion concept predesign using simulation

- **Mixture homogeneity**

Along with the design of the prechamber and the main combustion chamber, the mixture formation unit of the port injection concept has a significant impact on combustion and knocking. The main target was to achieve the most homogeneous mixture distribution possible in the cylinder at ignition timing and a specific maximum excess boost pressure in the gas supply in order to minimize losses from pressurization. A flammable mixture must appear near the spark plug and richer zones must be avoided at the periphery of the main combustion chamber since they might increase the tendency for knocking to occur. The main influencing parameters were the geometry of the air and gas intake system and the injection cycle (in essence the injection timing and the duration of injection). **Figure 4** presents the results obtained with both a baseline variant and an optimized variant (see also [2]). The homogeneity was evaluated by comparing the mass fractions in the respective lambda range. 90% of the mixture mass of the optimized variant fell within the defined target range. Moreover, knock behavior clearly improved as well. Virtually the same knock limit was achieved as with the homogeneous variant that was implemented on the test bed with an external gas mixer.

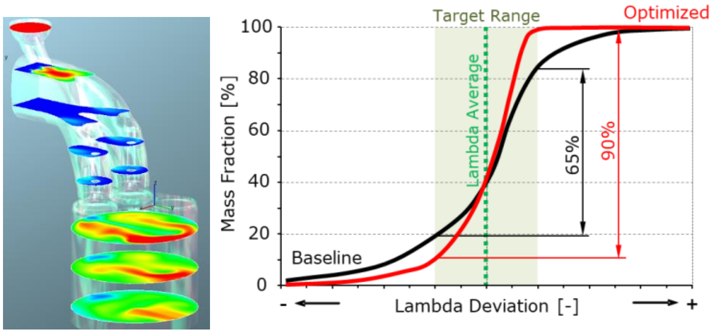


Figure 4: Assessment of mixture homogeneity

- **Combustion**

The prerequisite for successful preoptimization of a combustion concept is good simulation of combustion. Since engine performance, pollutant formation and knock tendency are significantly influenced by combustion, special care should be taken. The combustion model is first calibrated based on a measured operating point (whenever possible). **Figure 5** provides an example of the calibration of a combustion model. In this prechamber combustion concept, the lean mixture with an excess air ratio of around 2 is ignited by flame torches from the prechamber with an excess air ratio of around 1. The parameters of the combustion model were chosen so that the best possible agreement was obtained between the burn rate, the pressure in the prechamber (PC) and the pressure in the main combustion chamber (MC). Calibration with the deviation shown in the figure proved to be sufficiently accurate for preoptimization.

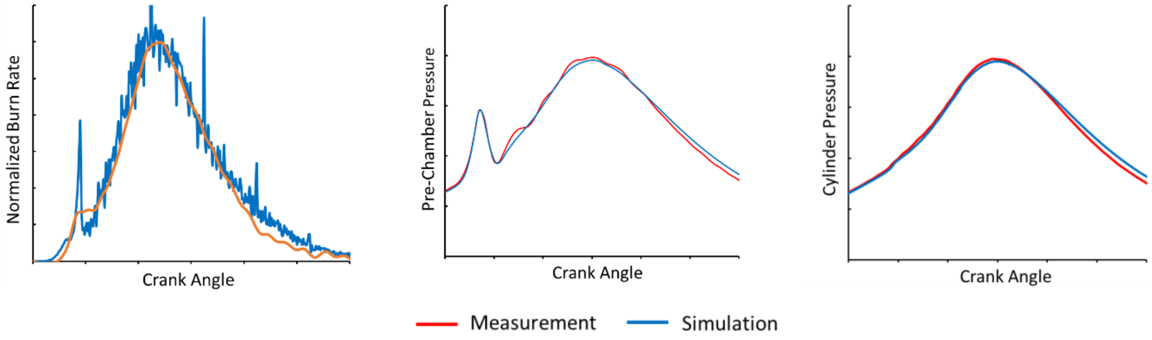


Figure 5: Prechamber combustion: normalized burn rate, pressure in prechamber and in main chamber

- **NO formation**

If combustion is calibrated properly, the NO model also reproduces NO production well. The NO level is determined by the progression of combustion. Since the engine is normally operated so that it complies with a specific NO limit, lambda must be set to ensure that compliance is achieved with the required NO limit. In the predesign phase, lambda is varied in three steps, thereby yielding three corresponding NO limits. **Figure 6** presents the workflow for this. An interpolation curve is determined from the three NO levels that appear at the end of calculation. Based on this information, an appropriate target lambda can be set for the NO target value. With this lambda, the desired NO concentration is obtained. Four CFD loops in general are required.

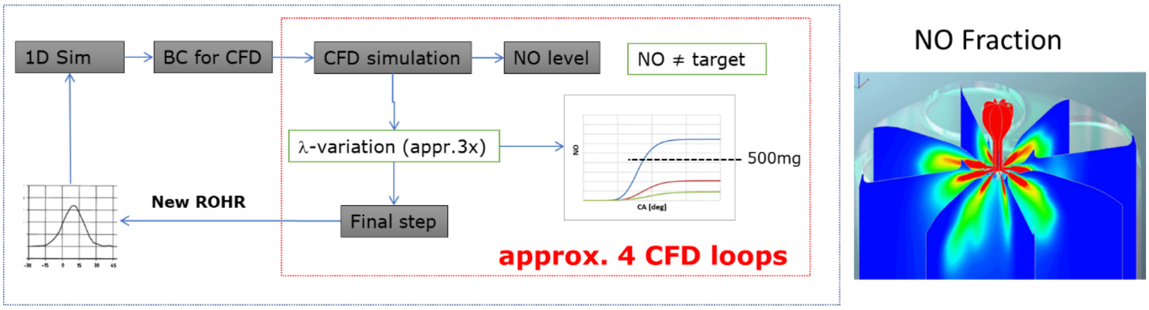


Figure 6: NO formation, achievement of required NO level

- **Knocking**

To assess knock tendency, the maximum temperature in the unburned end gas zone was investigated during the predesign phase. Output scripts were used to examine every location in the combustion chamber where this temperature exceeded a specific threshold value. The potential knock locations obtained in this manner were compared with regards to number and location of the simulated variants. **Figure 7** compares the knock tendency of the PI variants (left) with the homogeneously premixed variants (right). It compares the results of a preoptimized PI version with those of a homogeneous variant. There appears to be only a slight difference in the distribution of potential knock locations. The knock locations of the homogeneous variant are more evenly distributed on the periphery. The results showed very good agreement with measurements that were carried out later.

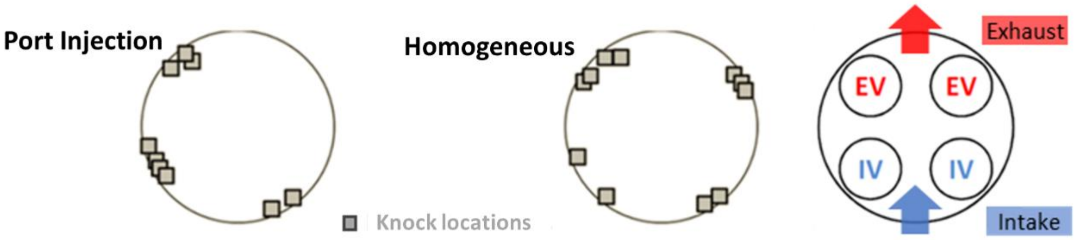


Figure 7: Comparison of potential knock locations, homogeneous operation and port injection

4.2 Single-cylinder research engine

The single-cylinder research engine shown in **Figure 8** was set up for thermodynamic optimization. A large part of the test bed infrastructure had to be adapted so that it was possible to operate the research engine with the power reserves required. The single-cylinder research engine corresponds to the multi-cylinder engine in its dimensions and is designed with the same V-angle as the multi-cylinder engine. To guarantee comparable operating conditions between the single-cylinder research engine and multi-cylinder engine in the widest possible range, the intake and exhaust piping system was calibrated with the multi-cylinder engine model using comparative analysis based on 1D engine cycle simulation and adapted to the local conditions at the test bed.

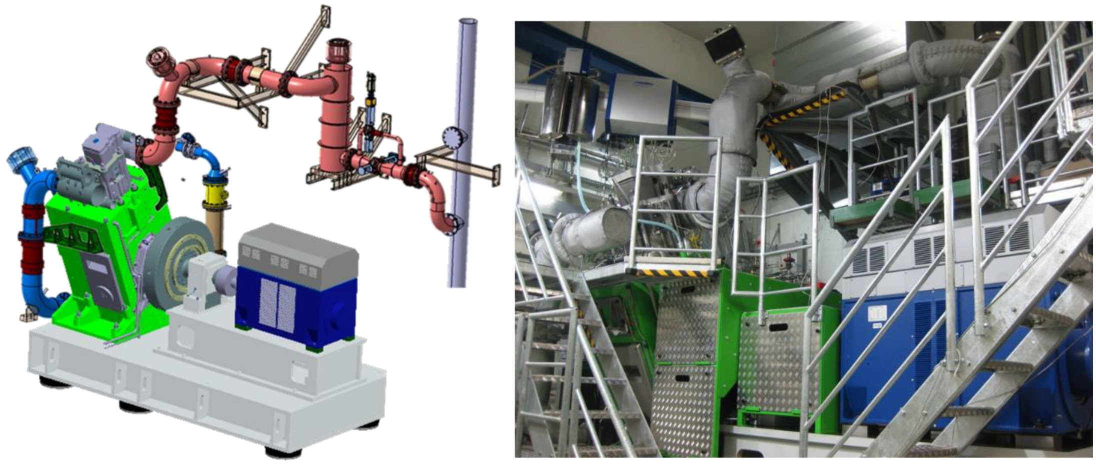


Figure 8: Single-cylinder research engine with adapted intake and exhaust system

4.3 Special measurement system

Along with the standard measurement technology, special measurement technologies were used to verify flame propagation and knock behavior. The optical investigations shown below were conducted with the Visiolution measurement system from AVL [3] [4]. This system is based on fiber optics and facilitates an evaluation of combustion. The combustion chamber sensors can be arranged with a great degree of flexibility; possibilities range from a single sensor to an optical cylinder head gasket. The measuring system records the total light emission of radiation due to combustion via very small optical openings in the individual measuring ducts. The time the flame arrives in the individual measuring ducts is determined by defining an intensity threshold value. Thus, flame propagation can be described in general terms in areas that are not easily optically accessible – e.g., a prechamber with a small number of measuring ducts. Tomography is used to make more detailed statements about the combustion process. In this case, a fine mesh extends out from a large number of single optical sensors (max. 160) into the measuring plane. The number of measuring ducts from which the optical observation mesh extends determines the spatial resolution of the system. The distribution of the location of flame propagation is reconstructed from the intensities recorded synchronously over time in the individual ducts at selected times or crank angle positions with knowledge of the geometry of the lines of sight. Seven sensors with four lines of sight (A, B, C, D) each were applied around the circumference of the prechamber in order to conduct flame propagation investigations (**Figure 9**).

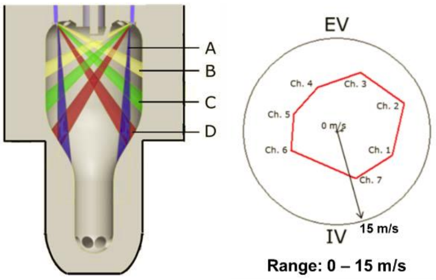


Figure 9: Spatial arrangement of the optical sensors in the prechamber with an evaluation example

From the assessment described above, polar diagrams are obtained in which flame arrival time and flame speed can be represented at the seven sensor positions. In the main combustion chamber, eight combustion chamber sensors with sixteen lines of sight each were built into the circumference of the liner. A narrow mesh network of lines of sight extended out from the sensors into the measuring plane. The measuring plane was normally aligned with the cylinder axis around 20 mm below the fire deck. This distance was chosen to fulfill mechanical strength requirements and to position the measurement plane as close as possible to the outlet bores of the prechamber so that as much information as possible was acquired about the initial flame growth in the main combustion chamber (**Figure 10**). With a tomography post-processing routine, it is possible to obtain flame propagation images in relation to crank angle as well as flame intensities at discrete times in this combustion chamber plane. Since knocking combustion manifests itself in highly frequent fluctuations in flame intensity, knock locations can also be detected by a special analysis with a high pass filter (lower right).

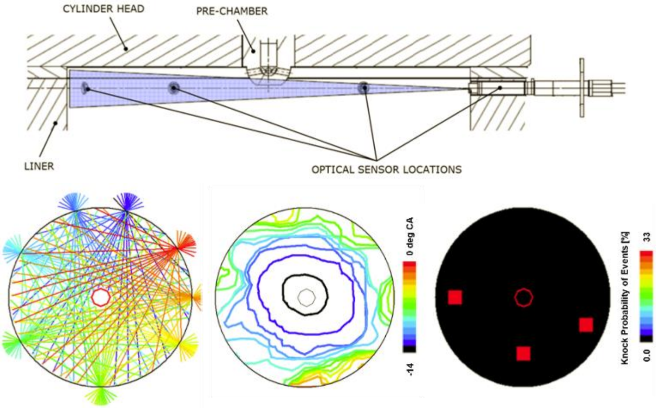


Figure 10: Spatial arrangement of the optical sensors in the main combustion chamber (AVL system) with an evaluation example

4.4 Comparison of CFD simulation and measurement

In addition to the calibration of combustion using global pressure and burn rate curves shown above, local and temporal distributions of specific parameters can also be investigated with optical combustion diagnostics. This is of particular interest for the interaction of combustion between the prechamber and the main combustion chamber. **Figure 11** depicts flame propagation in the prechamber.

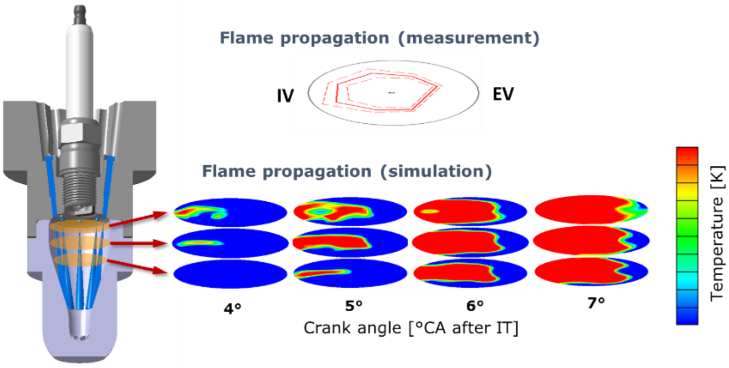


Figure 11: Flame propagation in the prechamber

The measurement results (top) reveal an increased propagation velocity in the direction of the intake valve (IV). 3D-CFD simulation also reveals the same phenomenon. Temperatures in three different cross-sectional planes are presented at four different times (4° to 7°). Triggered by a tumble flow in the prechamber, the flame is initiated asymmetrically. This asymmetry continues to propagate and goes on to initiate asymmetric combustion in the main combustion chamber (**Figure 12**). The left flame torch forms earlier and more strongly (left). As a result, flame propagation in the main combustion chamber increases slightly to the left in the direction of the intake valve as indicated by the measurement (right).

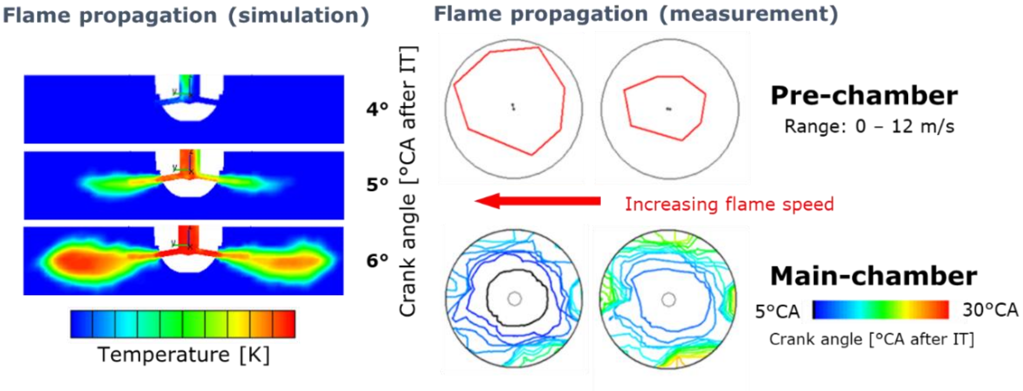


Figure 12: Interaction between the prechamber and the main combustion chamber

The quality of homogenization is ultimately assessed by knock behavior on the single-cylinder research engine. The left-hand side of **Figure 13** presents the measurements of the optimized PI variant (bottom) and those of the homogeneous variant (top). On the right is the simulated mixture distribution in the same cross-sectional plane.

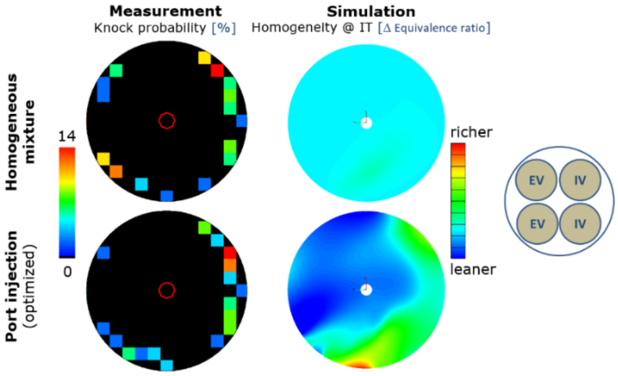


Figure 13: Comparison of knock behavior and homogeneity (PI – homogeneous mixture)

5 CONCLUSIONS AND OUTLOOK

Systematic research that follows the development methodology presented in this paper has revealed that 3D-CFD simulation is already a very efficient tool for developing combustion concepts for large gas engines. The choice of appropriate submodels must be made with care so that the underlying physical processes can also be depicted reliably. Both the choice of a mesh topology and calculation using RANS methods in combination with a multi-species PDF model that depicts combustion have proven to be appropriate. The optical investigations to verify flame propagation and knock behavior generated additional data whose detailed analysis confirmed the important characteristics of the combustion processes that were underway. This analysis was able to be used for qualitative validation of CFD simulation of combustion and knock. In any case, the great effort involved in using this measurement technology to validate the CFD models is worthwhile in order to guarantee the very highly developed simulation technology and apply it in predictive simulation in the future.

NOMENCLATURE

MCE	Multi-cylinder engine	CA	Crank angle
SCE	Single-cylinder engine	IT	Ignition timing
LDM	LEC Development Methodology	PC	Prechamber
MC	Main combustion chamber	PI	Port injection
TDC	Top dead center of the piston	EAR	Excess air ratio
BMEP	Break mean effective pressure	SIM	Simulation
IV	Intake valve	EV	Exhaust valve
RANS	Reynolds-averaged Navier-Stockes equations		
ROHR	Rate of heat release		

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