Development of an 1D simulation model to optimize performance and emissions of large gas engines

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Abstract: *The main subject of this paper is the development of a multicylinder engine model for the prediction and optimization of engine performance based on one-dimensional (1D) simulation. 1D simulation is widely used to preoptimize engine geometry and operating parameters to achieve performance targets and comply with operational and emission constraints. Due to the short calculation times, 1D simulation allows the evaluation of a larger number of variants. As new engine concepts are developed, many operating parameters are first defined and optimized with a 1D multicylinder engine model. This model illustrates the full complexity of the engine with its geometry, turbocharging and combustion parameters. In this paper the design of experiments (DoE) method is used in connection with 1D simulation to determine the optimal engine configuration as well as parameters related to the combustion process, i.e., valve timing, compression ratio, ignition timing, excess air ratio. This approach enables the determination of the maximum engine efficiency while taking the boundary conditions and the constraints of nitrogen oxide emissions (NOx) and knock into account. The method also enables the reduction of the cylinder-to-cylinder deviations by improving the gas dynamics and the fuel metering in the main combustion chamber and in the pre-chamber, which is especially important for the multicylinder engine. The simulation results are validated with experimental investigations on a single cylinder research engine.*

Keywords*: GAS FUELED ENGINES, 1D SIMULATION*

1. Introduction

In recent years the demand for high-performance engines has increased, which drives their continued development. When a new gas engine is being developed, a global optimum for the operating parameters should be found so that the engine can be operated at the best possible efficiency and the required power output without the occurrence of knock and while complying with valid emission legislation. Whereas the current German legislation [1] for gas engines defines the nitrogen oxide emissions limit as 500 mg/m³ (norm) @ 5% O2, the trend is towards a further reduction to 250 mg/m³ (norm) @ 5% O2 (Gothenburg Protocol [2]) or 75 mg/m³ (norm) @ 15% O2 (EU Directive 2010/75/EU [3]). This paper describes the evolution and the important role of 1D simulation modeling in the development of a new high-performance gas engine. The required sub-models and boundary conditions are discussed and an application is provided as an example of successful use of the methodology.

2. LEC Development Methodology

The 1D simulation that is part of **LDM** (**L**EC **D**evelopment **M**ethodology) [4] is an efficient tool that meets the demands for flexibility, predictability and computational time for this type of investigations. LDM is based on the intensive interaction between simulation and experimental investigations on single cylinder research engines (SCE) and multicylinder engines (MCE), see Figure 1. This methodology makes use of 3D CFD simulation and 0D/1D engine cycle simulation. While 3D CFD simulation is mainly employed to optimize the details of relevant processes (e.g., mixture formation and combustion in the prechamber and main combustion chamber, determination of the location of knock), 0D/1D engine cycle simulation is applied to pre-optimize significant engine parameters (e.g., compression ratio, valve timing). When applying the LDM methodology, it must be guaranteed that the results from single cylinder tests can be transferred to the multicylinder engine. For this it is necessary to acquire boundary conditions at the SCE to get conditions comparable to the ones of the multicylinder engine. Not only the thermal boundary conditions but also the conditions at the beginning of the intake stroke (temperature, pressure, and in-cylinder gas composition) are required. These conditions are determined in an iterative process based on 1D engine cycle simulation of the multicylinder engine and the single cylinder setup. The design of the single cylinder test bed has some specific features. While the piping system of the single cylinder engine test bed is being designed, it is important to adapt the gas dynamics in the intake and exhaust piping system. The objective is to achieve similar conditions in the cylinder of the SCE and the corresponding multicylinder engine.

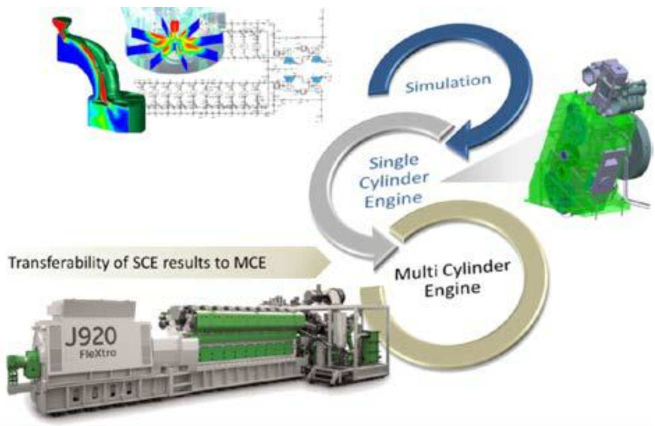

Fig. 1 *LDM: LEC Development Methodology*

3. Database and data analysis for the calibration and verification of the 1D model

For following the LDM, in a first step a reference case has to be created using measurement data from a physical engine with the purpose of further development and calibration of the simulation model. The SCE configuration, described in this paper, is equipped with gas scavenged pre-chambers and about 6 dm³ cylinder displacement volume. The available database includes measurements for variations of compression ratio, NOx emission level, ignition timing, intake charge temperature, pre-chamber energy and exhaust gas pressure. Configurations with two different valve lift profiles were used. Furthermore, measurement some performed at the knock limit.

Measurement data are required for the development and calibration of models as well as for the calculation of the rates of heat release for direct specification in the 1D simulation. Developed at the LEC, the engine cycle calculation program LEC CORA is used to analyze the operating points measured on the test bed. The software package CORA (Combustion Optimization, Research and Analysis) was designed to analyze and simulate the high-pressure cycle of the working process of combustion engines. It enables the analysis of measured pressure traces as well as simulation of cylinder conditions during the high-pressure cycle upon specification of the rate of heat release histories or the rate of heat release models. The software is used in combustion analysis mainly for pressure offset, compression ratio and top dead center adjustment as well as pressure history analysis (high-pressure cycle) and loss analysis.

The high demand on the quality of the measurements used as a basis for analysis, leads to the necessity to check this quality, whenever possible directly and automatically at the test bed, to allow early detection of errors [5]. In this context, a methodology for automated error diagnosis on engine test beds was developed at the LEC. The algorithms this system is relying on, are provided in the "LEC MCheck" (LEC Measurement Check System) software solution and are used directly on the test bed. A consistent use of these tools guarantees a high quality of measurement data and the resulting rate of heat release histories, which in turn is advantageous, when calibrating simulation models and interpreting the results.

4. Development of the MCE model

As baseline simulation model, the MCE model with pre-chambers for each cylinder, gas mixers and two stage turbocharging, is used. The compressors and turbines are depicted with corresponding maps. The model is created using the commercial software package GT Power. One challenge in the development of a pre-chamber gas engine simulation model is to determine the conditions, not only in the cylinder, but also in the pre-chamber (PC) as accurately as possible, because the combustion in the PC influences the behavior of the main chamber. For this reason, also the pre-chamber, pre-chamber gas valve and the piping system of the PC gas rail are depicted in the 1D model for each cylinder. The pre-chamber gas valve is a check valve, and it is modelled with high complexity: pin mass, valve spring stiffness, valve maximum displacement and flow coefficients. The pre-chamber gas rail is also modelled in detail, in order to reproduce the gas dynamics in the rail and the fuel flow into the pre-chamber thoroughly.

4.1. Modelling of the combustion process

1D simulation requires the rate of heat release in the cylinder and in the PC. Measurement data from relevant operating points, measured on SCE, are used to determine the actual rate of heat release history using engine cycle calculation. The combustion duration in the cylinder and the fraction of fuel burned are additionally adjusted as functions of excess air ratio (EAR), because those parameters are strongly dependent on EAR. Those functions are determined from measured EAR variations on the SCE test bed, Figure 2.

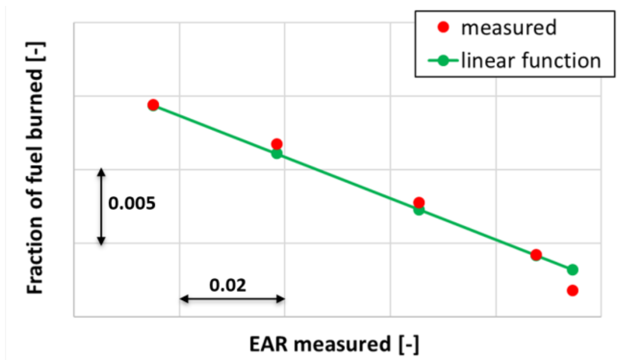

Fig. 2 *SCE measurement: Fraction of fuel burned as a function of EAR.*

Figure 3 represents the implementation of the functions for combustion duration and fraction of fuel burned in the cylinder module of the 1D MCE model.

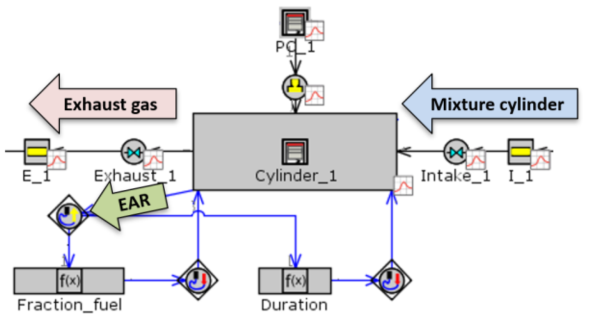

Fig. 3 *Implementation of the functions in the MCE model*

4.2. NOx model and knock prediction

The NOx concentration that arises during combustion is calculated from the well-known Pattas and Häfner model [6] in the used software, which accounts for the formation of thermal NO using an extended Zeldovich mechanism. The temperature of the burned zone for simulating the post-flame reactions is calculated from the heat release rate (ROHR) model with a two-zone sub-model. In addition, the two-zone modeling approach enables to determine the maximum temperature in the unburned combustion zone, which is assumed as a reasonable indicator of conditions for knock events and as a criterion for the knock limit. The assumption is, that the knock behavior of the engine stays unchanged in case that this temperature is constant. Another possibility for knock prediction is the application of the LEC knock model [7]. The basic idea behind this model is to ascribe the statistical phenomenon of the occurrence of knock-cycles to the similar statistical phenomenon of the ignition delay scatter. The method uses models for the ROHR, knock timing and knock intensity. Because the LEC knock model requires a wide measurement database with operating points at the knock limit for its calibration, typically it is not used at this stage of the engine development.

4.3. Other features of the MCE model

In most of the common applications, large-bore gas engines operate at constant NOx emission levels. For this reason, a NOx-controller is implemented in the MCE model, so that it continuously varies the EAR until the target NOx level is reached.

One issue, when using such a highly complex model, is the relatively long computing time. In order to reduce it, for some investigations the turbochargers are replaced with a block, which uses a function for calculation of the exhaust back pressure. The function is based on the turbocharger main equation [8], and in this case it is possible to use a constant turbocharger efficiency and constant compressor bypass ratio. For the adjustment of the exhaust back pressure in the model an orifice connection in the exhaust piping of the model is used.

With respect to NOx-emission, the 1D MCE model typically is calibrated by using NOx variations measured on a single cylinder research engine. With this approach very good agreement of the simulation results with the measured EAR at the same NOx level can be achieved. Due to the high complexity of the system and the large number of free parameters, the statistical method Design of Experiment (DoE) is a useful tool to support this calibration. The free parameters optimized on the basis of this approach are typically compression ratio, control of the combustion process, valve timing and turbocharger design. The typical goal of the investigations is to achieve the highest engine efficiency possible while fulfilling the boundary conditions of permissible NOx emission limits, maximum cylinder peak firing pressure and knock-free operation [9]. Figure 4 provides an overview of the optimization process using the DoE method.

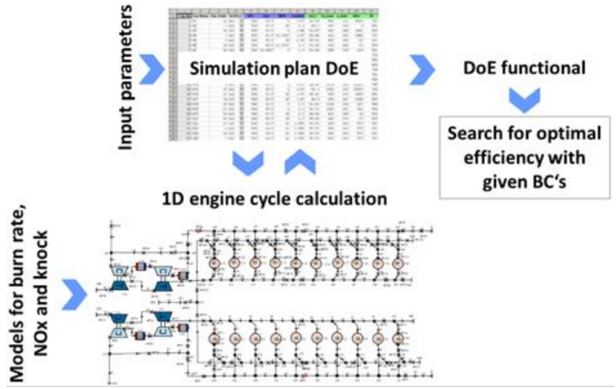

Fig. 4 *Procedure for applying DoE methods for 1D simulation.*

5. Applications of the 1D simulation model and results

Different engine configurations were compared with the 1D MCE model. First, the model was calibrated on the base of SCE measurements. Thereby different measurement series were used: Brake mean effective pressure (BMEP) variations, NOx variations, as well as measurements at the knock limit. The following configurations were investigated:

- base concept with Miller valve timing, compressor bypass and mixture preparation with a gas mixer,
- mixture preparation with port fuel injection (PFI) for each cylinder instead of a centrally located gas mixer for all cylinders and control of the peak firing pressure,
- mixture preparation with gas mixer and variable valve control.

The simulations with the 1D model have shown that all configurations have similar EAR deviations from the average value in the PC at ignition timing. In order to balance those EAR deviations in the pre-chambers, PC solenoid valves can be used instead of check valves.

The implementation of the PFI for each cylinder instead of a gas mixer is a potential improvement. In the case of PFI, a gas valve admits the fuel into the intake port in front of the intake valve, then the mixture of air and fuel flows into the cylinder, when the intake valve is open. The objective is a reduction of the cylinder-to-cylinder deviations of the multicylinder engine, because the PFI concept allows a cylinder-specific fuel control. As a consequence, the balancing of the peak firing pressure is possible.

The application of variable valve control, allows a zero compressor bypass and as a consequence an efficiency increase and a reduction of unburned hydrocarbon emissions (HC), but it also requires more procurement costs and leads to higher friction losses.

There is high potential in the layout of the valve lift curves for the first two configurations above. The valve lift curves influence the cylinder temperature, residual gas content and as a consequence the nitric oxide emissions formation and the knock tendency. In addition, the valve overlap is responsible for a part of the HC emissions.

With the defined BMEP and NOx-level as target values a high-end gas engine is optimized using the 1D MCE model. Thereby the design of experiments method is used. The target is to increase the engine efficiency, on the condition that NOx and peak firing pressure must not exceed the previously given values. Following factors for the DoE investigation are chosen: position of the ROHR (crank angle at 50% mass fuel burned in the cylinder, MFB_50%), intake valve opening, intake valve closing, exhaust valve opening and exhaust valve closing. The constraints are knocking combustion (described by the maximum temperature in the unburned zone) and EAR. Measurements on the SCE test bed have shown that the combustion stability deteriorates once the EAR exceeds a critical threshold. With the help of the commercial software MODDE a simulation plan with 26 cases is generated, the cases are simulated, and mathematical models for prediction of engine efficiency, temperature of the unburned zone and peak firing pressure are created. Figure 5 shows the very good agreement between the observed values and the predicted ones. With the help of the optimizer tool in the MODDE software the optimal variant is determined, and the valve timings for a new camshaft can be fixed. With the newly designed and machined camshaft measurements on the SCE test bed with variation of ignition timing and compression ratio have been performed.

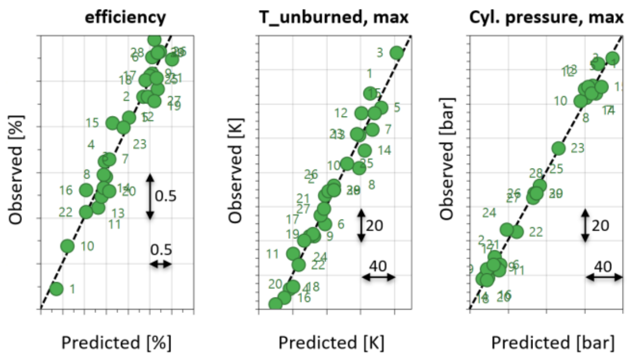

Fig. 5 *DoE investigation: observed vs. predicted values.*

The measurements have confirmed the optimal MFB_50% for maximal engine efficiency from DoE investigation. The efficiency gained by the compression ratio increase from simulation and from measurement are also in the same range. The measurements confirmed also the efficiency increase with the new valve lift profile.

6. Summary and outlook

This paper presents the relevance of 1D simulation during the development process of high-performance large bore gas engines by taking different development constraints into account. 1D simulation models of different designs and at different levels of detail were discussed in relation to each specific issue. The model was calibrated on the base of SCE measurements. As a result, it was possible to increase the BMEP and engine efficiency. The simulation results were confirmed by measurements at the SCE test bed.

Further investigations are planned with increased compression ratio and adaption of the MFB_50%.

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