1D SIMULATION AS AN ELEMENT OF AN EFFICIENT METHODOLOGY FOR ENGINE CONCEPT DEVELOPMENT

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Abstract: *The development of highly efficient combustion concepts for internal combustion engines requires a suitable development methodology. In recent years, the LEC has created LDM (LEC Development Methodology), which is based on the intensive interaction between simulation and experimental investigations on single cylinder research engines. 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. The design of experiments (DoE) method is used in connection with 1D simulation to find the optimal engine configuration as well as parameters related to the combustion process, i.e. valve timing, compression ratio, ignition timing, excess air ratio. The maximum engine efficiency is found by taking into account the boundary conditions (brake mean effective pressure, turbocharger efficiency), where NOx level and knock limit are constraints.*

Keywords: INTERNAL COMBUSTION ENGINES, DEVELOPMENT METHODOLOGY, 1D SIMULATION

1. Introduction

The trend toward higher efficiencies and increasingly stringent emission legislation are greatly pushing forward engine development. A variety of degrees of freedom emerge in the optimization of engines because of the various possible ways to reach the targets as well as the interaction between individual operating parameters. A global optimum for these operating parameters should be found so the engine can be operated with the best possible efficiency and the required power output without the occurrence of knock and while complying with emission legislation [12].

Simulation is a central component of a development and optimization methodology for new engines. While commercially available software (AVL Boost, GT-Power) is relied upon to simulate the engine cycle, most of the required 0D submodels are developed or expanded at the Large Engines Competence Center (LEC).

This paper explains the basic characteristics of the development methodology and the important role that 1D simulation plays in the development of new engines. The required models and boundary conditions are discussed and several applications are provided as examples of successful use of the methodology.

2. LEC Development Methodology

LDM (**L**EC **D**evelopment **M**ethodology) is used to develop and optimize combustion concepts for engines at the LEC. 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 employed above all 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). In order that this methodology can be applied, it must be guaranteed that the results from single cylinder tests can be transferred to the multicylinder engine. To this end, it is necessary to achieve boundary conditions comparable to those of the multicylinder engine. Not only the thermal boundary conditions but also the conditions at the beginning of the intake stroke (temperature, pressure, and working 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. [2]

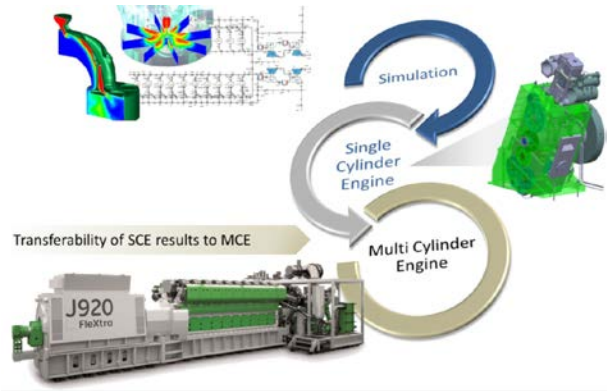

Fig. 1 *LDM: LEC Development Methodology.*

3. Submodels required for 1D simulation

1D simulation requires not only the standard boundary conditions but also the rate of heat release in the cylinder. Measurement data from comparable operating points on similar engines can also be used to determine the actual rate of heat release history using engine cycle calculation. However, this has the disadvantage that the rate of heat release history does not fit exactly to the actual boundary conditions. Ideally, the rate of heat release history is calculated with a 0D rate of heat release model implemented in the cylinder of the engine cycle calculation software based on the conditions at intake valve closing calculated in 1D simulation. 0D models for calculating NOx formation and knock models can also be implemented in this manner.

The rate of heat release models discussed below are particularly suitable for use in this development methodology as they contain few empirical assumptions due to their physical basis and thus only a few model parameters must be calibrated. In addition, they have very short calculation times.

3.1. Rate of heat release models for open chamber gas engines, prechamber engines, DI diesel engines and dual fuel engines

The basic principle of the 0D rate of heat release model for open chamber gas engines and prechamber gas engines rests on the propagation of a hemispherical flame of finite thickness that rushes through the pre-mixed charge in the combustion chamber [4]. The calculation of laminar flame speed, which is dependent on fuel type, temperature, pressure and mixture quality, and its increase due to effects of turbulent density and density differences between the unburned and the burned gas zones help to describe the reaction rate. The gas mass available in the flame front can either be converted into a rate of heat release according to the Magnussen model or by applying the well-known entrainment model [14].

To describe the ROHR in the prechamber engine, the effects of the gas jets issuing from the prechamber are modeled [7].

The main combustion chamber and the prechamber are treated as two combustion chambers connected by a restriction. After ignition occurs in the prechamber, the initially hemispherical surface of the flame front is restricted soon after combustion starts due to contact with the prechamber walls. The flame front moves away from the spark plug in the direction of the transfer ducts at the turbulent flame speed; the volume of the flame front is determined by the combustion chamber geometry. The burning gas jets issuing from the transfer ducts mingle with a part of the surrounding unburned charge and act as the starting point for the progression of a flame front in the main combustion chamber.

The LEC has also developed models for DI diesel engines that describe combustion as well as ignition delay and pre-mixed combustion, all of which are either based on the MCC approach (mixing controlled combustion) [5], [6], or on a package model [17]. The quality of the results improves when an injection rate curve is specified and a quasidimensional spray model is applied.

Taking these requirements into account, a 0D simulation approach that predicts the rate of heat release in dual fuel engines was developed [15],[16]. The characteristics of dual fuel combustion require a two-stage simulation approach that combines the first phase of combustion, which is dominated by diesel fuel combustion, with the second phase of combustion, which involves homogeneous combustion of a background mixture consisting of natural gas and air. A package model similar to models used to simulate diesel engines is applied to describe the first phase; the second phase is modeled using an entrainment model [14].

3.2. NOx model

The NOx concentration that arises during combustion is calculated from the well-known Pattas and Häfner model [8], which only accounts for the formation of thermal NO using an extended Zeldovich mechanism with a total of six chemical equations. The differential equation derived in this model was adopted unchanged. The required equilibrium concentrations of the individual species are calculated with a gas properties program based on the JANAF thermochemical tables. The temperature of the burned zone for simulating the post-flame reactions was calculated from the ROHR model with a two-zone model.

In the case of a prechamber engine, the prechamber and the main combustion chamber must be treated separately; nevertheless, their interaction has to be considered. The detailed approach for calculating NOx emissions from prechamber engines is described in [13].

3.3. Knock model

Simple 0D models were developed to describe and predict the phenomena associated with knocking combustion in gas engines [9], [10]. An Arrhenius equation that calculates the rise in the concentration of radicals in the unburned charge is used to determine the onset of knock. The reaction rate is determined between intake valve closing and knock onset from the cylinder pressure, the temperature of the unburned zone and the methane number and then the integral is taken. A simulated combustion cycle is described as knocking if the integral value between the start and end of combustion reaches a certain threshold. At the same time, a specific amount of unburned fuel mass must still be present in the cylinder at the calculated start of knock and the knock intensity of the simulated cycle (pressure amplitude of the high-frequency oscillations at the start of knock) must also exceed a given threshold value. All these thresholds must be calibrated from existing measurements or from empirical values before simulation.

3.4. Measurement data analysis as the basis for calibrating 0D models

Measurement data is required for development and calibration of 0D models as well as calculation of the rates of heat release for direct specification in 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 analysis of measured pressure histories as well as simulation of cylinder conditions during the high pressure cycle upon specification of rate of heat release histories or rate of heat release models. The software is used in combustion analysis mainly for pressure level adjustment, pressure history analysis (high pressure cycle) and loss analysis of direct injection diesel engines and spark ignition gas engines with external mixture formation.

The great demands on the measurements that form the basis of analysis also make it necessary to check the quality of measurements automatically whenever possible directly at the test bed to allow early detection of errors [1]. In this context, a methodology for automated error diagnosis on engine test beds was developed at the LEC. The algorithms it relies upon are provided in the “LEC-MCheck” (LEC Measurement Check System) software solution and are used directly on the test bed.

Intensive use of these tools guarantees the high quality of measurements and the resulting rate of heat release histories, which in turn is advantageous when calibrating simulation models and interpreting the results.

4. Application of 1D simulation as part of the development methodology

The following section provides examples of applications that show how 1D simulation is used in a variety of areas in the process of developing a new engine.

4.1. Design of a single cylinder test bed and determination of boundary conditions for testing

Single cylinder research engines were set up at the LEC in order to optimize the thermodynamics of large engines; one example of an engine setup can be seen in Figure 2.

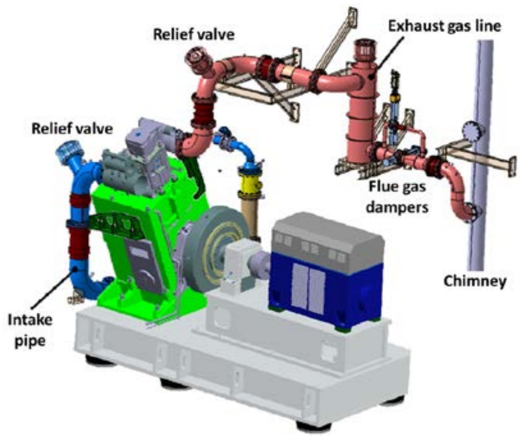

Fig. 2 *Single cylinder research engine (SCE).*

The main dimensions of the single cylinder research engine correspond to those of the multicylinder engine. When the single cylinder research engines are supplied with conditioned charge air (temperature, pressure and humidity), it is possible to adjust the conditions to those of the multicylinder engine and maintain them, thereby guaranteeing the transferability of the results of single cylinder tests to the multicylinder engine.

To ensure comparable operating conditions between the single cylinder research engine and the multicylinder engine in the broadest area possible, the intake and exhaust system is specially calibrated using comparative analysis with the multicylinder engine model based on 1D engine cycle analysis and adapted to the specific situation on the test bed. To evaluate the quality of the calibrated result, Figure 3 shows the simulated gas exchange pressure histories on the intake and exhaust sides of the MCE and the histories measured on the single cylinder research engine at the same operating point. The following procedure is used to ensure the same conditions at the start of the high pressure cycle (temperature, pressure and composition of the working gas).

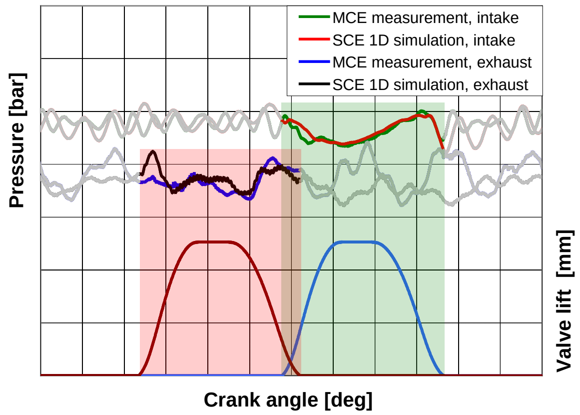

Fig. 3 *Calibration of gas dynamics in the intake and exhaust system of the single cylinder research engine.*

Based on 1D engine cycle simulation with the multicylinder engine model, the conditions in one representative cylinder at intake valve closing are determined using a simulated rate of heat release history as well as the parameters of the turbocharger and the specifications for load and excess air ratio. These results provide the basis for 1D engine cycle simulation with the model of the setup of the single cylinder research engine. Charge air and exhaust back pressure are varied until identical starting conditions appear at intake valve closing when the same conditions are set as with multicylinder engine simulation (rate of heat release history, load and excess air ratio). Measurements are conducted on the single cylinder research engine with the values thus determined for charge air pressure and exhaust back pressure. The rate of heat release history is then inserted into the calculation with the multicylinder engine model and run through a second time. Normally satisfactory agreement between the rate of heat release histories already appears after the second iteration loop and the procedure can be completed by determining the relevant values from multicylinder engine simulation. [3]

4.2. Detailed analysis of various processes within the engine

A great variety of processes within the engine can be analyzed using a 1D model. This section analyzes how NOx formation is determined in detail using the example of an engine with a prechamber and discusses the reasons for differences between the cylinders in multicylinder engines.

The prechamber concept is applied to large gas engines in particular. Figure 4 shows the modeling of both combustion chambers in the commercial GT-Power software.

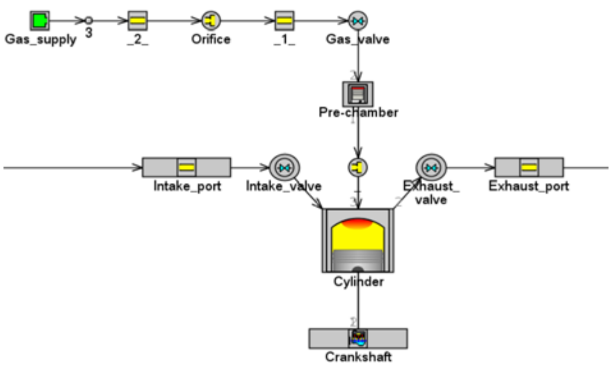

Fig.4 *Screenshot of the 1D model of a single cylinder research engine with a prechamber.*

The model is especially helpful for investigating knock behavior and NOx formation in both combustion chambers. Combustion is modeled using a thermodynamic two zone model because the determination of the temperature in the burned zone is required in order to simulate NOx accurately. The amount of NOx in the prechamber is determined separately from the amount in the cylinder using the NOx submodel described above. Results from measurements and from 3D CFD simulation are used to calibrate the NOx models. NOx concentrations in the prechamber and in the main combustion chamber are calculated with 1D simulation, results are shown in Figure 5. For low NOx concepts without exhaust gas aftertreatment, the engines are run with a leaner mixture (Lambda > 1.6) [11]. The enleanment of the cylinder produces several negative effects, for example a rise in HC emissions and subsequent loss in efficiency.

The goal of the investigation is to discover an optimal configuration that does not exceed the NOx limit and at the same time has the fewest losses. The following factors can be optimized:

- Charge composition in the prechamber at ignition timing. The excess air ratio in the prechamber can be controlled by the amount of gas that flows through the gas valve before the prechamber, see Figure 4.
- Prechamber size. Larger prechambers produce more NOx, but a certain amount is required for the momentum of the flame torches with which the mixture is ignited in the cylinder.
- Charge composition and combustion phasing in the cylinder.
- Prechamber geometry. It is depicted in the 1D model by the rate of heat release history. The rate of heat release histories used are obtained from the combustion analysis of measured operating points or from 3D CFD simulation.

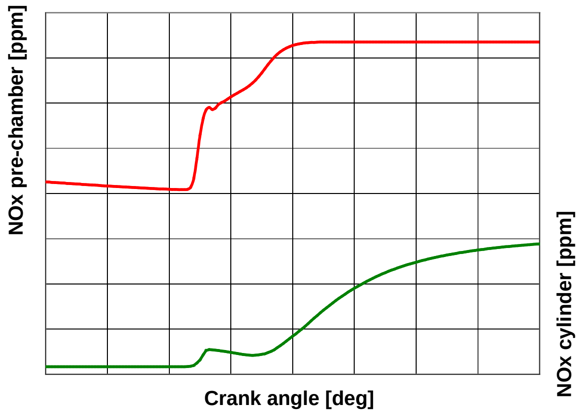

Fig. 5 *Simulated NOx concentrations with the NOx submodel in the prechamber and in the cylinder of a large gas engine.*

Another issue with the multicylinder engines that were investigated are the cylinder specific differences that are mainly detected as differences in peak firing pressure. They increase pollutant formation and knock tendency in spark ignition gas engines. Possible reasons for these differences are:

- Different cylinder masses due to gas dynamics in the intake system
- Different amounts of residual gas in each cylinder due to gas dynamics in the exhaust system and during valve overlap
- Different gas mixtures in the cylinders due to the characteristics of mixture formation (e.g., differences in air mass with gas engines with port fuel injection)
- Different combustion phasing in the cylinders due to the different charges and gas mixtures

With a calibrated 1D model, these effects can be modeled and measures can be taken that reduce these differences. Control strategies that can be applied to the multicylinder engine can also be elaborated.

3D CFD simulation is used to analyze the processes in the combustion chamber in detail. It can model spatial events such as the location of knock or the mixture distribution. The required boundary conditions are prepared with a 1D model.

4.3. Preoptimization of the overall system using simulation

Based exclusively on simulation, virtual combustion process development places very great demands on the quality of the used simulation methodology. Preoptimization is crucial in the area of large engines in particular. First, stroke/bore ratio, compression ratio, excess air ratio, turbocharger configuration and valve timing are predesigned using engine cycle simulation based on ROHR, NOx formation and knock behavior models that have been calibrated on other research engines. 3D CFD methods are applied to preoptimize the fuel-mixture concept, the design of the prechamber, and combustion in detail. Preoptimization of the combustion results in a rate of heat release history that is used to calibrate 0D simulation models.

To apply the methodology, it is necessary to link together the 0D, 1D and 3D calculation models intensively so that the boundary conditions required for the calculations can be exchanged. This is largely carried out using standardized and automated processes.

The entire system is then optimized using 1D engine cycle simulation; Figure 6 provides an overview of the optimization process.

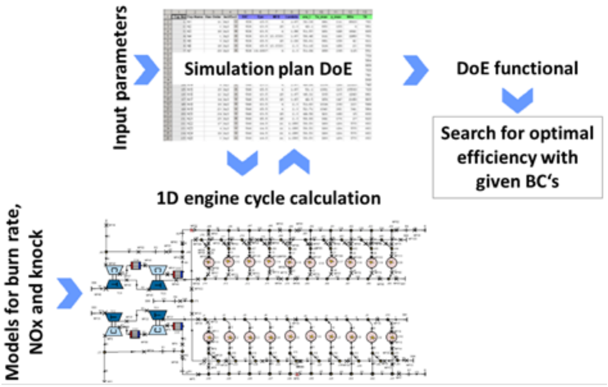

Fig. 6 *Procedure for applying DoE methods for 1D simulation.*

Due to the high complexity of the system and the large number of free parameters, the statistical method Design of Experiments (DoE) is heavily relied upon. 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 goal of design is to achieve the greatest engine efficiency possible while staying within the boundary conditions of permissible NOx limits, maximum cylinder peak firing pressure and knock-free operation [2].

5. Summary and Conclusions

This paper presented the LEC development methodology, focusing in particular on the role 1D simulation plays in the methodology. The submodels as well as the required boundary conditions were presented and discussed. Selected examples of applications were used to show how the methodology can be put into practice.

In summary, the following conclusions can be drawn: LEC Development Methodology combines simulation with experimental investigations on single cylinder research engines in order to optimize fuel consumption and emissions. 1D simulation has become an important part of the process of developing highly efficient combustion concepts. The predictive quality of the simulation models also allows reliable thermodynamic predesign of a new engine on the basis of simulation alone. Using this approach, development time can be kept to a minimum and development costs can be significantly reduced.

6. References

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