Assessment of Water Injection in a SI Engine using a Fast Running Detailed Chemistry Based Combustion Model

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Summary

Water injection is investigated for turbocharged spark ignition engines to limit knock probability and therefore enable higher engine efficiency. This work presents an integrated simulation-based optimization process to assess water injection. The fast running quasi-dimensional stochastic reactor model is coupled with tabulated chemistry to account for water effects on laminar flame speed and combustion chemistry. The increase of the compression ratio and the shift of the spark timing to earlier crank angles are most beneficial for fuel consumption. Wherefore, the limitation of the compression ratio and the shift of the retarded spark timing are better for low knock probability. Overall, the water presence shows a decrease of fuel consumption and knock probability at the same time. The application of the quasi-dimensional stochastic reactor model with tabulated chemistry reduces the computational costs and is suitable for multi-objective optimizations.

1 Introduction

Today we experience the revival of water injection as a key technology for turbocharged, spark ignition (SI) engines [1]. It enables higher boost pressures and compression ratios, which results in increased engine efficiency [2]. The rising number of optimization parameters pushes the traditional test bench approach to its limits and demands sophisticated simulation tools to support the engine development and pre-calibration.

Detailed three-dimensional (3D) computational fluid dynamic (CFD) studies of water injection in gasoline engines are published by Berni et al. [3] and Netzer et al. [4]. The group of Berni et al. focused on the application of 3D CFD to investigate a specific

water injection concept. They show the feasibility of the simulation approach to evaluate water effects on thermodynamic conditions and auto-ignition. Netzer et al. emphasize the necessity to use detailed chemistry in 3D CFD simulations, to separate physical from chemical water effects. The authors found that water effects on laminar flame speed and combustion chemistry are not negligible. Furthermore, the 3D CFD results state the strong influence of water injection and vaporization on the local distribution of temperature and auto-ignition hot spots within the cylinder.

The physics-based quasi-dimensional (QD) SI stochastic reactor model (SRM) accounts for the mixture and temperature in-homogeneities within the cylinder [5, 6, 7, 8]. This approach allows to predict local effects of fuel composition on flame propagation, auto-ignition and emission formation. The QD SRM was already applied to investigate the effect of different octane number fuels on auto-ignition in the unburned zone as shown by Netzer et al. [9]. The detailed chemistry for multi-component fuels used in that work as well as in the presented work is based on the methodology of reaction mechanism development and reduction introduced by Seidel et al. [10, 11]. To reduce the computational cost of the QD SRM simulations, Matrisciano et al. published a reaction-progress-variable-based tabulation strategy [12]. Thereby, the detailed chemistry is pre-compiled in a look-up table based on thermodynamic conditions and reaction progress variable.

This work presents a simulation-based optimization method including the QD SRM with dual fuel (gasoline and water) tabulated chemistry and the optimization tool modeFRONTIER [13]. A multi-objective optimization process is defined to reduce fuel consumption and knock probability of a SI engine operating point by water presence and compression ratio increment. The first section introduces the simulation methodology to optimize the SI engine operating point. Following, the numerical test case is defined, and the optimization results are discussed.

2 Simulation Method

In the engine development process, the prototype engine and its base calibration must be tested for many operating conditions. Therefore, an integrated process based on detailed 3D CFD models, fast running two-zone QD SRM and multi-objective optimization tools can be incorporated (see Figure 1).

The detailed chemistry and its sensitivity to water presence is the fundament for the process since it will be applied to 3D CFD and QD SRM simulations. The 3D CFD data for turbulent kinetic energy k_{CFD} is used as input data for the QD SRM mixing time τ_{SRM} in equation (1):

$$\tau_{SRM} = C_{\phi} \cdot \frac{\left(\frac{6 \cdot V}{\pi}\right)^{\frac{1}{3}}}{\sqrt{k_{CFD}}} \qquad (1)$$

Therein, C_ϕ is a calibration parameter and integral length scale is modeled as a function of the instantaneous cylinder volume V. Due to the mixing time the QD SRM accounts for the turbulence-chemistry interaction in SI engines.

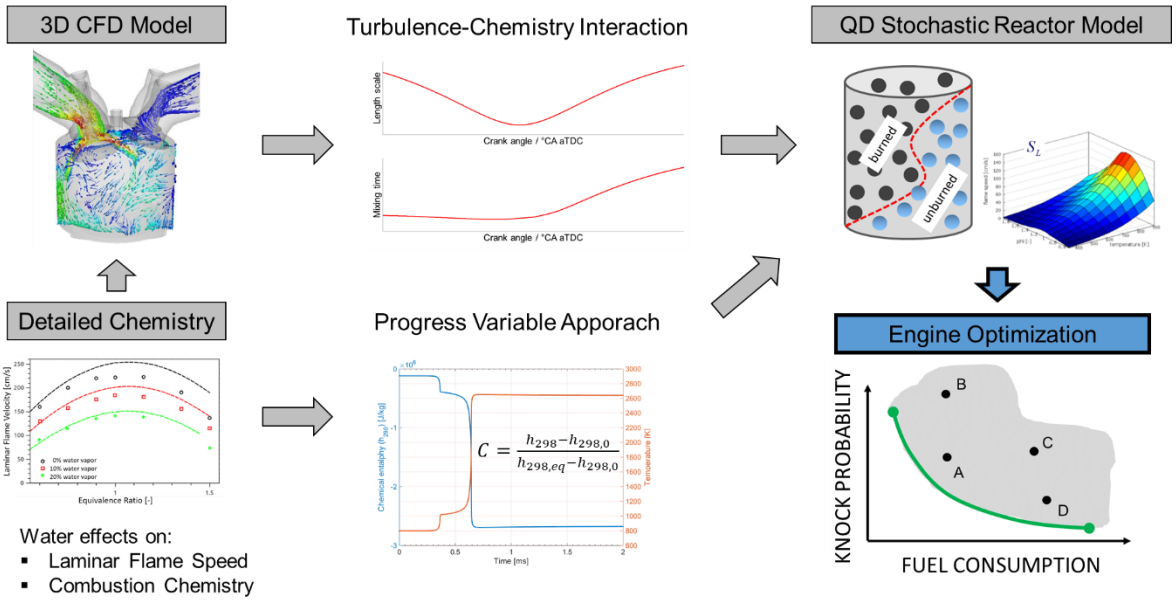

Figure 1: QD SRM and 3D CFD integrated simulation-based optimization process with detailed chemistry.

The laminar flame speeds and the combustion chemistry are stored in a pre-compiled look-up table (see table ranges in Table 1 and Table 2). A dual fuel approach for an Ethanol Toluene Reference Fuel (ETRF; ethanol, toluene, iso-octane, n-heptane) fuel surrogate and water is used. The first fuel stream is composed of 5.3% Ethanol, 49.2% iso-Octane, 9.1% n-Heptane and 36.4% Toluene in mass percent. The second fuel stream is composed of 100% water. During the simulation laminar flame speeds and chemistry sources are retrieved from the look-up tables based on the current thermodynamic conditions. Further, the progress variable (C) is used for the chemistry table look-up. The fuel-water-air mixture is initialized homogeneously-mixed at the start of the QD SRM simulation, assuming an idealized port-injection.

Table 1: Laminar flame speed dual fuel table specifications.

	Range	Steps
Temperature	350 - 1200K	50K
Pressure	1 - 100bar	1bar
Equivalence Ratio	0.5 - 1.5	0.05
Water/fuel ratio	0 - 60%	10%
EGR	0 - 20%	10%

Table 2: Combustion chemistry dual fuel table specifications.

	Range	Steps
Temperature	250 - 1400K	25K
Pressure	1 - 200bar	2.5bar
Equivalence Ratio	0.2 - 4.0	0.2
Water/fuel ratio	0 - 40%	10%
EGR	0 - 30%	10%

To account for the changes of thermodynamic conditions due to water injection and vaporization, a simplified approach is used. The water mass and vaporization enthalpy of water at 100°C ($q_{vap,water} = 2264 \frac{kJ}{kg}$) are used to calculate the energy Q_{water} needed to vaporize the liquid water. Following, based on the isobaric heat capacity of air ($c_{p,air} = 1.008 \frac{kJ}{kg\ K}$) and trapped mass $m_{trapped}$, the temperature drop ΔT of the cylinder gas temperature is calculated with $\Delta T = \frac{Q_{water}}{c_{p,air} \cdot m_{trapped}}$.

For the multi-objective optimization, a best practice setup is used. The Non-dominated Sorting Genetic Algorithm (NSGA-II) together with the Uniform Latin Hypercube (ULHC) space filler algorithm is applied [13]. The number of individuals is set to 10 and the number of generations is 150. In total 1500 designs are calculated. The optimization target is to reduce the fuel mass and knock probability of the numerical test case. To evaluate the knock probability, the best practice knock limit is defined as $6 \frac{J}{^\circ CA}$ maximum heat release rate in the unburned zone in the QD SRM. The optimization design parameters and the applied ranges are shown in Table 3. To compare the cases at the same engine load, the indicated mean effective pressure (IMEP) could vary within a range of $\pm$ 3%.

Table 3: Multi-objective optimization design parameter ranges.

	Minimum	Maximum
Compression Ratio	9.0:1	13.0:1
Water/fuel ratio	0%	40%
Pressure at IVC	1.7bar	2.7bar
Spark Timing	-25°CA aTDC	5°CA aTDC

3 Numerical Test Case

The 3D CFD test case for a boosted SI engine operating point at 2500 rpm and 16.2bar IMEP from Netzer et al. [4] is used to perform the multi-objective optimization with the QD SRM. The engine geometry and operating conditions are listed in Table 4. The base case without water presence is used for calibration of the QD SRM mixing time.

Additionally, three operating points with different spark timings, water/fuel (w/f) ratios (20%, 50% and 80% w/f ratio) and IMEPs are used to validate the QD SRM.

Table 4: Engine geometry and operating conditions for the base case without water presence.

Bore x Stroke	86 mm x 90 mm
Compression Ratio	10.0:1
Spark Timing	-4°CA aTDC
Fuel Mass	55 mg/stroke

4 Simulation Results

The QD SRM calibration and validation results for cylinder pressure, heat release rate and exhaust emissions (CO_2, H_2O, CO and NO_x) compared to 3D CFD are shown in Figure 2. The calibration case (a) shows a good agreement with the 3D CFD results. For the first validation case (b) with 20% w/f ratio, the spark timing was shifted to earlier crank angles in 3D CFD, wherefore the maximum cylinder pressure is as high as for the base case. For the validation cases (c) with 50% w/f ratio and (d) with 80% w/f ratio, the maximum cylinder pressure is decreasing due to a longer combustion duration in QD SRM and 3D CFD. Overall, the QD SRM matches the 3D CFD results accurately and the applicability of the mixing time modeling approach is proven. Subsequently, the validated QD SRM is used for the multi-objective optimization of the SI engine operating point.

The overall simulation time for the 1500 designs was 6h and 45m on three cores of a Intel i7-7820HQ CPU at 2.90GHz. The optimization was able to find an optimum solution and the resulting Pareto Front is shown in Figure 3. On the x-axis the fuel mass and on the y-axis the maximum heat release rate (HRR) of the unburned zone is plotted. The base case (A) is highlighted with the red color (see Figure 2 case (a)). The designs (black) are grouped into two clusters (Cluster-1 and Cluster-2) and are highlighted by the dark and light grey colored ellipses. The designs within these clusters share similar engine operating parameters. The green colored case (B) is the optimum case found in the optimization. The blue case (C) has the lowest fuel consumption, the yellow case (D) is closest to the target IMEP and the magenta colored case (E) has the lowest maximum HRR in the unburned zone.

In Figure 4 the average engine parameters of Cluster-1 and Cluster-2 are compared to the base engine parameters. On the one hand, to reduce fuel mass, one must increase compression ratio, decrease pressure at IVC and shift spark timing to earlier crank angles (light grey line). On the other hand, to reduce knock probability, one must limit compression ratio and retard spark timing (dark grey line). Both clusters share a similar water fuel ratio of 25% to 30%. This finding shows that a high w/f ratio is beneficial for low fuel mass and low knock probability at the same time.

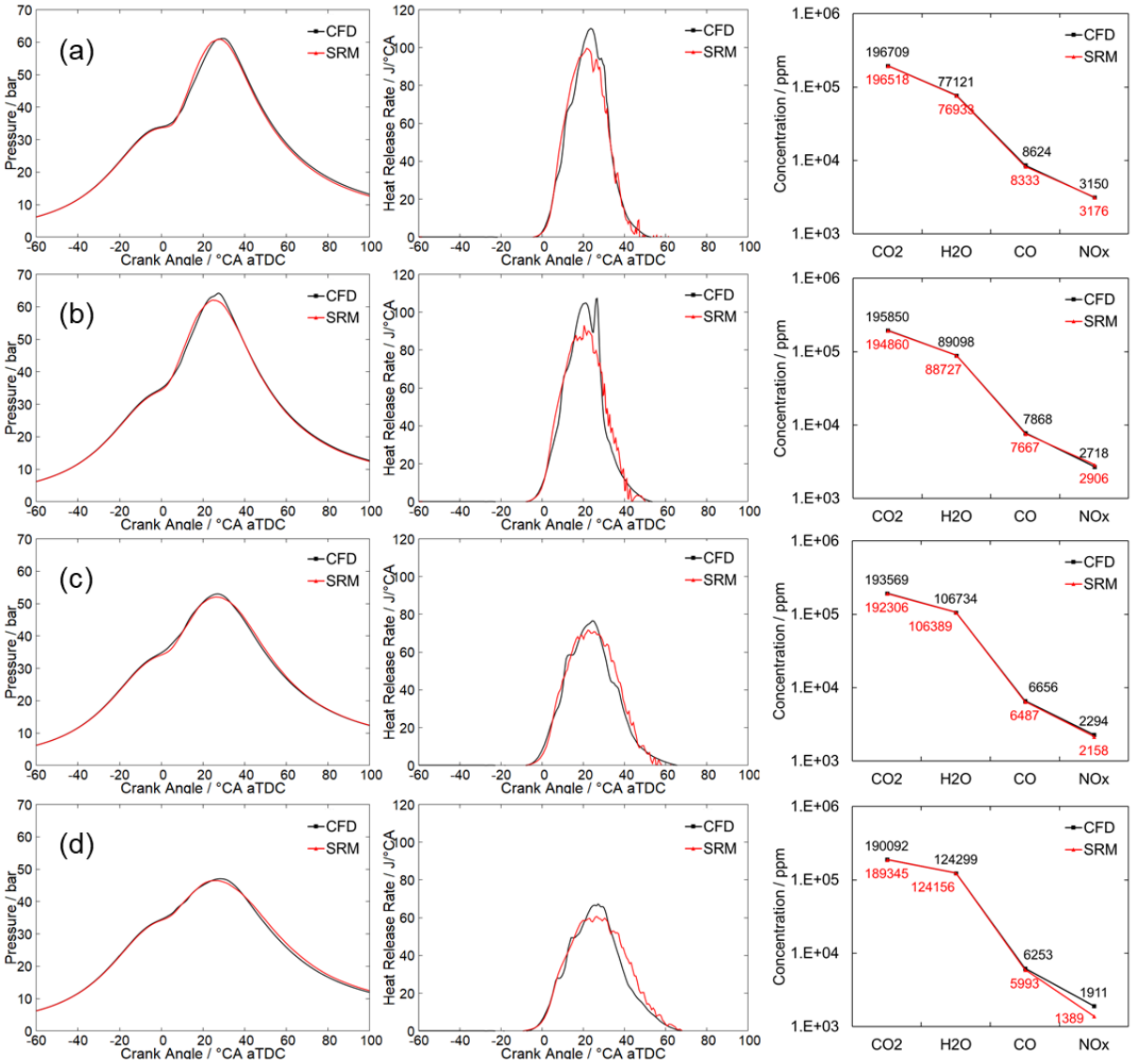

Figure 2: 3D CFD and QD SRM with detailed chemistry - Calibration results for case (a) with 0% w/f ratio and 16.2bar IMEP and the validation results for the cases (b) with 20% w/f ratio and 16.2bar IMEP, (c) with 50% w/f ratio and 15bar IMEP and (d) with 80% w/f ratio and 14.1bar IMEP.

The calculated cylinder pressures and heat release rates of the unburned zone of the QD SRM with tabulated chemistry, for the base case and the optimized cases, are compared in Figure 5. For cases (B), (C) and (D) a higher peak cylinder pressure is predicted due to the higher compression ratio and earlier spark timing. For case (E) a lower peak cylinder pressure is found because the spark timing is retarded. All optimized cases show a reduced HRR in the unburned zone due to water presence.

The computational time of the 3D CFD simulation for one closed-engine-cycle is 16h on 24 cores. The QD SRM with detailed chemistry (without tabulation) takes 3min for one closed-engine-cycle on 16 cores. Finally, the QD SRM with tabulated chemistry takes 3s for one closed-engine-cycle on 1 core.

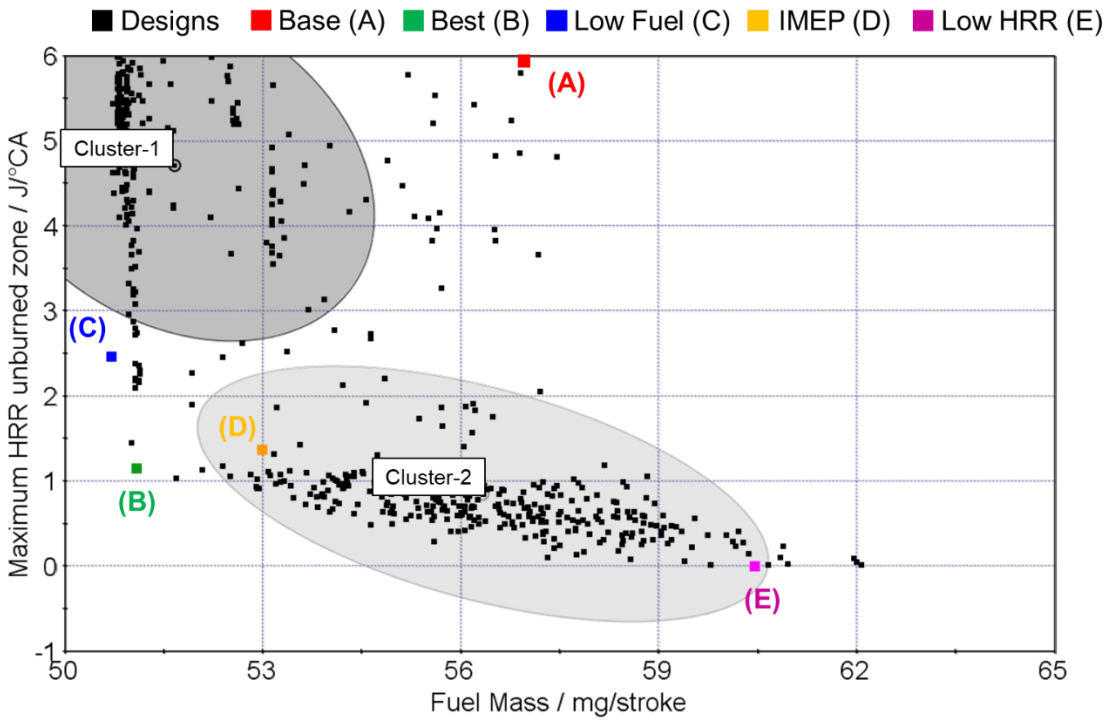

Figure 3: QD SRM optimization results with tabulated chemistry. The dark and light grey colored ellipses highlight clusters of designs sharing similar sets of engine parameters.

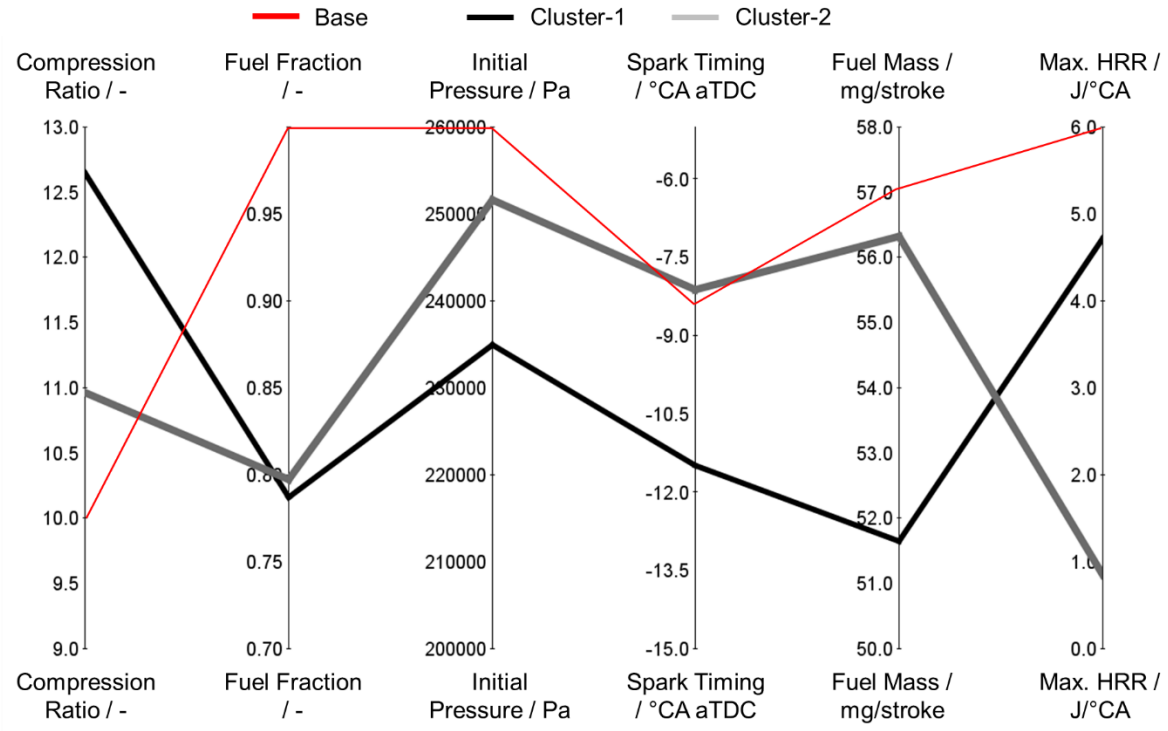

Figure 4: QD SRM optimization results with tabulated chemistry. The red line shows the base engine parameter values. The black and grey colored lines highlight the average engine parameter values for Cluster-1 and Cluster-2.

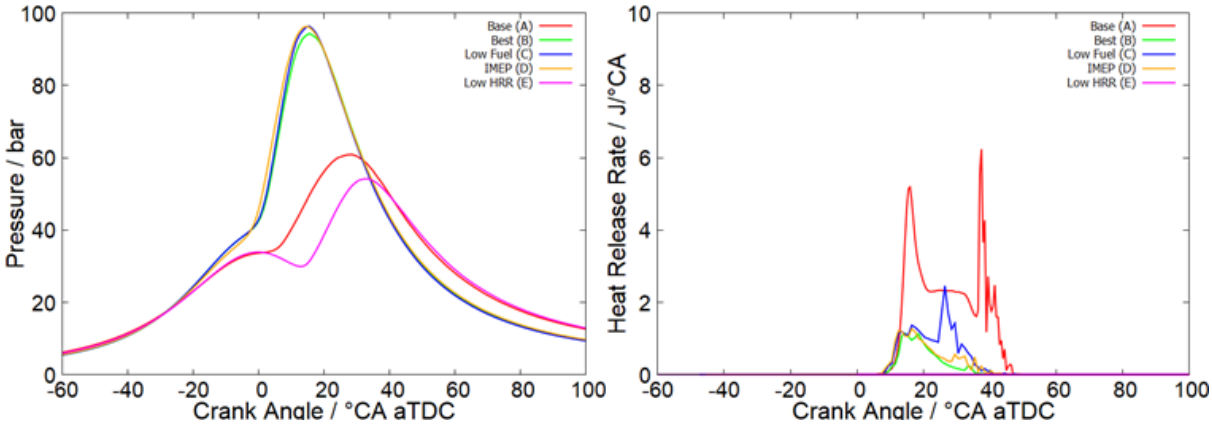

Figure 5: QD SRM optimization results with tabulated chemistry. The calculated pressure of the base case and the optimized cases is shown on the left side. The calculated heat release rate of the unburned zone on the right side.

5 Conclusions

An integrated simulation-based optimization process is successfully tested for the assessment of water injection in turbocharged SI engines. The process includes the 3D CFD simulation results of a 2500rpm and 16.2bar IMEP operating point as reference. The QD SRM with tabulated chemistry is coupled with the optimization tool modeFRONTIER to perform a multi-objective optimization of fuel consumption and knock probability.

The general knowledge from SI engine development could be confirmed by the QD SRM optimization. The reduction of fuel consumption is favored by increased compression ratio and earlier spark timing. In contrast, the lower knock probability is influenced by low compression ratios and later spark timings.

The presence of water is beneficial for reducing fuel consumption and knock probability at the same time. An optimum w/f ratio in the range of 25% to 30% is determined from the QD SRM simulation.

Overall, the QD SRM with tabulated chemistry is a fast running tool, which can be applied for complex integrated optimization processes.

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7 References

[1] B. Durst, G. Unterweger, S. Rubbert, A. Witt and M. Böhm, "Thermodynamic effects of water injection on Otto Cycle engines with different water injection systems," in *The Working Process of the Internal Combustion Engine*, Graz, 2015.

[2] F. Bozza, V. De Bellis and L. Teodosio, "Potentials of cooled EGR and water injection for knock resistance and fuel consumption improvements of gasoline engines," *Applied Energy,* vol. 169, pp. 112-125, 2016.

[3] F. Berni, S. Breda, M. Lugli and G. Cantore, "A Numerical Investigation on the Potentials of Water Injection to Increase Knock Resistance and Reduce Fuel Consumption in Highly Downsized GDI Engines," *Energy Procedia,* vol. 81, pp. 826-835, 2015.

[4] C. Netzer, T. Franken, L. Seidel, H. Lehtiniemi and F. Mauss, "Numerical Analysis of the Impact of Water Injection on Combustion and Thermodynamics in a Gasoline Engine using Detailed Chemistry," in *SAE Technical Paper*, 2018.

[5] M. Pasternak, F. Mauss, M. Sens, M. Riess, A. Benz and K. G. Stapf, "of a Turbocharged Gasoline Engine under High Load Condition of a Turbocharged Gasoline Engine under High Load Condition stochastic reactor model and three-dimensional computational fluid dynamics engine model," *International J of Engine Research,* vol. 17, no. 1, p. 76–85, 2016.

[6] M. Sens, A. Benz, M. Riess, F. G. Lage, X. S. Bjerkborn, F. Mauss and M. Pasternak, "Multiple Spark Plug Approach: Potential for Future Highly Diluted Spark Ignited Combustion," in *SIA Powertrain*, Versailles, 2015.

[7] M. Pasternak, C. Netzer, F. Mauss, M. Fischer, M. Sens and M. Riess, "Simulation of the Effects of Spark Timing and External EGR on Gasoline Combustion Under Knock-Limited Operation at High Speed and Load," in *Knocking in Gasoline Engines*, Berlin, 2017.

[8] LOGE AB, "LOGEsoft Manual v1.08," 2016. [Online]. Available: www.logesoft.com.

[9] C. Netzer, L. Seidel, M. Pasternak, C. Klauer, C. Perlman, F. Ravet and F. Mauss, "Engine Knock Prediction and Evaluation Based on Detonation Theory Using a Quasi-Dimensional Stochastic Reactor Model," *SAE Technical Paper,* 2017.

[10] L. Seidel, Development and Reduction of a Multicomponent Reference Fuel for Gasoline, Cottbus: Brandenburg University of Technology Cottbus-Senfenberg, 2017.

[11] L. Seidel, C. Netzer, M. Hilbig, F. Mauss, C. Klauer, M. Pasternak and A. Matrisciano, "Systematic Reduction of Detailed Chemical Reaction Mechanisms for Engine Applications," *Journal of Engineering for Gas Turbines and Power,* vol. 139, no. 9, 2017.

[12] A. Matrisciano, T. Franken, C. Perlman, A. Borg, H. Lehtiniemi and F. Mauss, "Development of a Computationally Effcient Progress Variable Approach for a Direct Injection Stochastic Reactor Model," *SAE Technical Paper,* 2017.

[13] ESTECO, "modeFRONTIER User Guide 2017R4," 2017. [Online]. Available: https://www.esteco.com/modefrontier.