Ammonia as carbon free fuel for internal CombusTion engIne driVen AgriculTural vEhicle (ACTIVATE)

Work package 3
Deliverable report 3

Optimised engine performance map for the targeted engine

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Contents

1 Introduction

Scope of work

This report presents works carried out within the third deliverable (D3.3) of the third work package (WP3). It describes activities related to the application of the 0D stochastic reactor model (SRM) for the analysis of combustion and emissions formation from the engine operated with direct injection of ammonia and biodiesel.

The work focused was twofold. Firstly, we evaluated the possibility to map engine performance parameters and exhaust emissions over different engine speed and load conditions using the 0D SRM while having limited set of data for calibrating the model, and with having ammonia and biodiesel as fuel; extrapolating the application of the model to wider range of operating points is understood here as "engine performance mapping". Secondly, preliminary optimization of engine performance map was conducted to estimate the potential benefits of using ammonia for reducing engine out CO2 without affecting engine output performance.

Method

Simulations were carried out using framework presented previously that relies on the 0D SRM and detailed chemistry integrated with modeFRONTIER®©. The SRM along with a detailed reaction mechanism for ammonia and biodiesel is embedded in the multi-objective optimization (MOO) platform. The same setup of the were carried out using the SRM from LOGEengine package that we used previously for the works in WP3.

2 Engine data and simulation setup

Engine

Simulations in this report refer to the same engine that we used previously for the works in WP3. This the engine from Silesian University of Technology (SUT) that is described in details in the reports by project partner from SUT who investigated it experimentally. The basic specification of the engine is given in Table 1.

Table 1: Engine basic specification.

Engine type	Compression ignition
Bore (mm)	86
Stroke (mm)	70
Compression ratio (-)	16.5:1
Number of valves (-)	4
Rated power (kW @3500rpm)	6.4

Engine operating points

In total, 16 operating points were considered for the analysis. The points are characterized in Table 2, and Figure 1 shows in-cylinder pressure histories and IMEP corresponding to these points.

Table 2: Reference operating points for engine performance mapping.

No.	Speed [rev/min]	IMEP [rev/min]	NH3 [-]	MD [-]	Phi [-]	AES [-]	SOI NH3 [deg aTDC]	SOI MD [deg aTDC]
1	1000	1.96	0.5	0.5	0.21	0.34	-17	-21.1
2	1000	2.85	0.41	0.59	0.27	0.42	-15.1	-21.1
3	1000	3.64	0.41	0.59	0.3	0.42	-15	-15
4	1000	4.23	0.36	0.64	0.35	0.47	-5	-15
5	1000	6.68	0.43	0.57	0.66	0.40	-4.6	-10.1
6	2000	2.79	0.76	0.24	0.17	0.13	-7.3	-18
7	2000	3.95	0.69	0.31	0.25	0.18	-3.6	-17.1
8	2000	4.24	0.66	0.34	0.32	0.21	-4.3	-17.1
9	2000	4.97	0.6	0.4	0.38	0.25	-9.2	-18.5
10	2000	5.75	0.54	0.46	0.43	0.30	-15.9	-21
11	2000	7.34	0.49	0.51	0.57	0.34	-13.6	-20
12	2500	3.41	0.72	0.28	0.22	0.16	-7.4	-20
13	2500	4.02	0.8	0.2	0.3	0.11	-4.1	-19.7
14	2900	3.38	0.74	0.26	0.24	0.15	-7.5	-22
15	2900	4.03	0.74	0.26	0.3	0.15	-4.6	-22
16	2900	4.77	0.93	0.07	0.35	0.04	-4.6	-22

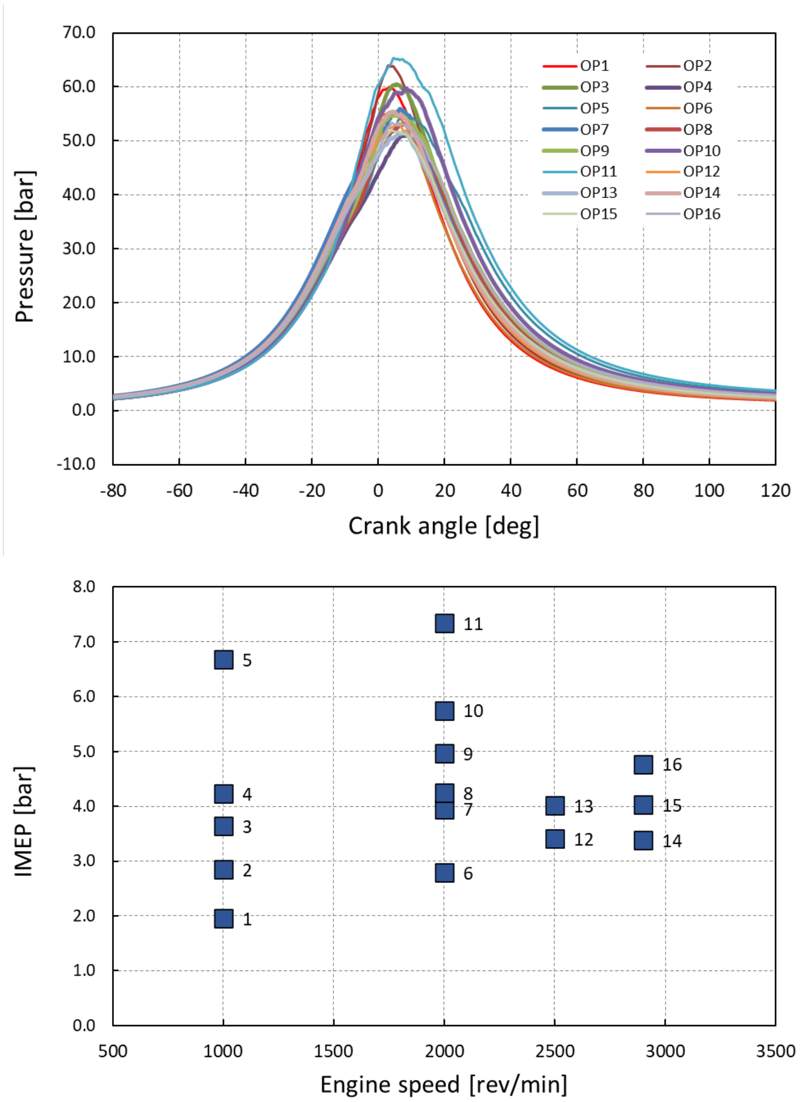

Figure 1: In-cylinder pressure histories and IMEP corresponding to operating points listed in Table 2.

Computational setup

Simulations were carried out using the SRM configured, in terms of number of particles, consecutive cycles and time step, as determined in previous investigation in the project. The parameters are summarized in Table 3.

Table 3: Setup of the SRM parameters.

Parameter	Value
Number of particles (-)	500
Number of cycles (-)	30
Time step (-)	0.5
Stochastic heat transfer coefficient (-)	15
Mixing model	Curl

3 Results

3.1 Baseline model results

Calibration of the baseline SRM follows the procedure presented in the millstone and deliverable reports. For the present work, out of 16 points from Table 2, we selected 4 points for model calibration. These are OP3, OP6, OP12 and OP15. They represent different load and speed conditions.

Figure 2 compares the experimental and and the simulated in-cylinder pressure histories for the selected four training operating points. The simulated histories follow reasonably well the experimental counterparts, though some mismatches are visible too. However, it needs to be point out that at the time of performing calculations we had information about injection timings, but there was no information about the injection rates for each fuel. These had to be presumed/calculated that introduced some in-accuracy into the modelling and obtained results. The lack of detailed rates data influences the modelling of vaporization process that is specifically important in predicting pollutants formation that are most sensitive parameters to simulate. Given these obstacles, here we limited the evaluation of the calibration quality to the in-cylinder pressure data (Figure 2), and we consider the obtained quality satisfactory.

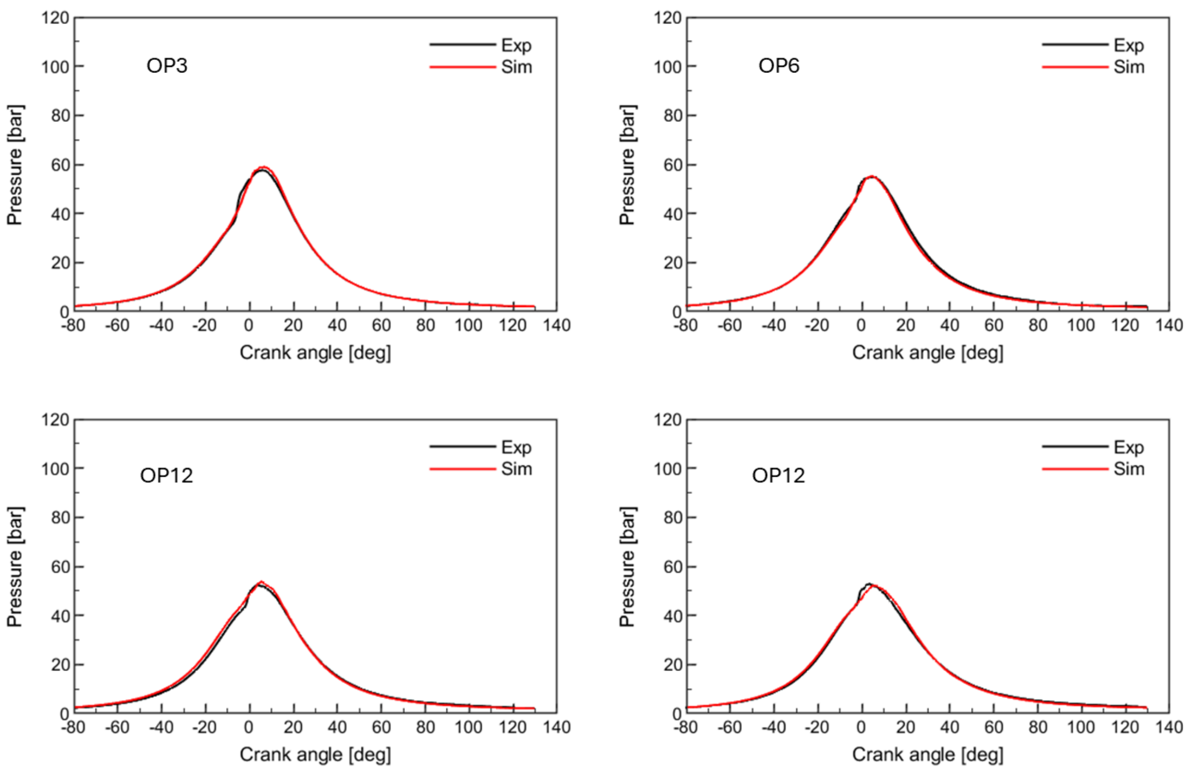

Figure 2: Comparison between the experimental and the simulated in-cylinder pressure histories for four operating points selected for training of the SRM.

SRM constants, that affect $k-\epsilon$ turbulence model, and hence the predicted combustion rates, and in consequence quality of the simulated in-cylinder pressure histories in Figure 2 were obtained through an automate calibration procedure using optimization algorithms. They are listed in Table 4, where $C_{\epsilon,1}$ and $C_{\epsilon,2}$ denote model parameters for in-cylinder flow and inflow/back squish flow, respectively. C_{inj} is the model parameter that influences the flow velocity due to fuel injection. C_{τ} is a general model parameter that enables scaling the history of mixing time.

Table 4: Constants of $k-\epsilon$ turbulence model in the calibrated SRM.

Parameter	$C_{\epsilon,1}$	$C_{\epsilon,2}$	C_{inj}	C_{τ}
Value	1.69	2.25	0.0089	9.22

3.2 Engine performance mapping

Having determined $k-\epsilon$ turbulence model (Table 4) the SRM was applied to simulate engine performance parameters for all 16 operating points listed in Table 2. The results obtained are presented in Figure 3 and Figure 4. Similarly as it was obtained for training operating points, here also reasonable agreement is observed between the simulated pressure histories and the experimental counter parts. The simulated pressure and RoHR histories and corresponding to them emissions are considered baseline results for the optimization task presented in the next paragraph.

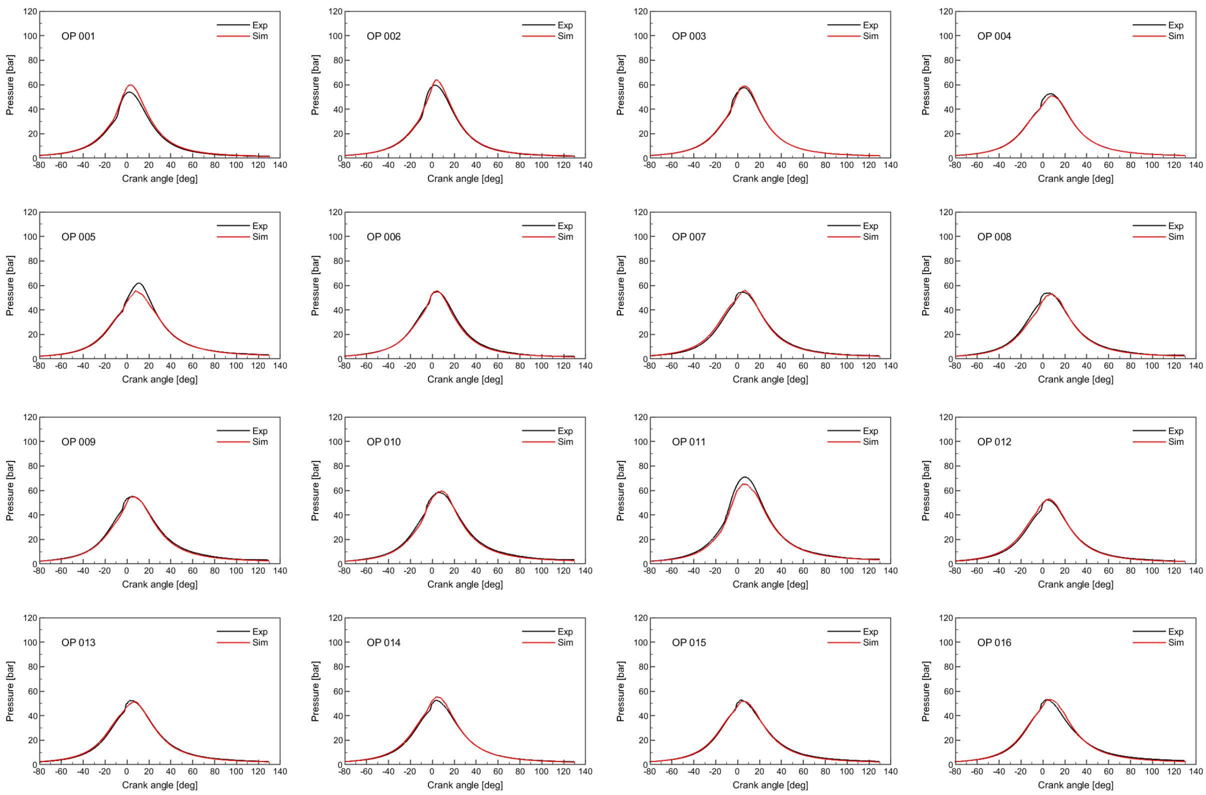

Figure 3: Comparison between the experimental and the simulated in-cylinder pressure histories for operating points listed in Table 2; results based on SRM setup determined from calibrating OP3, OP6, OP12 and OP15.

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Silesian University of Technology
NTNU Norwegian University of Science and Technology
LOGE
University of Agriculture in Krakow

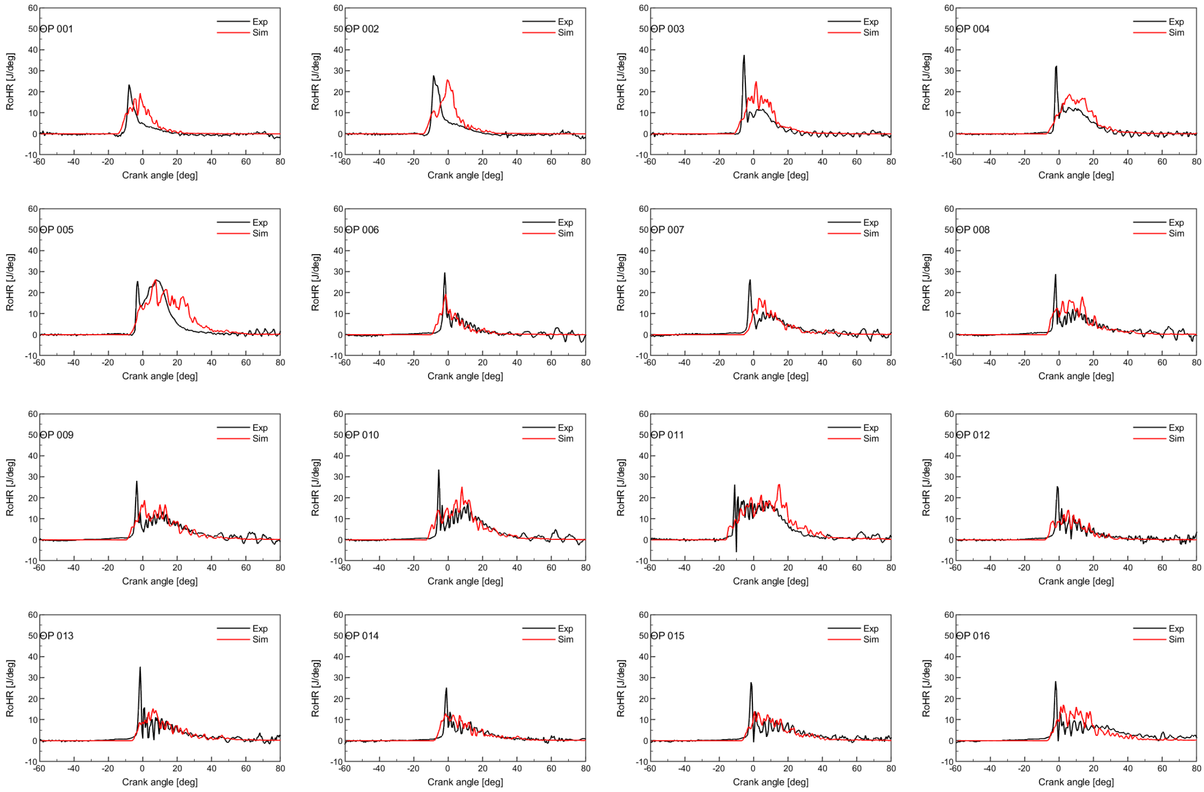

Figure 4: Comparison between the histories of RoHR from experimental pressure and the simulated RoHR for operating points listed in Table 2;results based on SRM setup determined from calibrating OP3, OP6, OP12 and OP15.

3.3 Optimized engine performance map

Having verified the SRM in simulating in-cylinder performance parameters over sixteen operating points, the model can be applied to extrapolate engine performance parameters beyond the baseline conditions (see, previous section). Here, to demonstrate this capability, the modelling is applied for evaluating the possibility to reduce engine out CO2 by changing fuel injection strategy and enabling an increase of ammonia share in the fuel. The optimization was conducted using the engine-fuel co-optimization framework introduced in the report M3.3. The optimization strategy is outlined in Table 5.

Table 5: Overview of the optimization strategy.

No.	**Name**	**Type**	**Range**
1	dSOI	variable	$\pm 4[deg]$
2	dFF(NH3)	variable	$0 - 0.15[-]$
3	IMEP	constraint	$\pm 5\%$
4	CO2	target	reduction

In this table dSOI denotes the range within which the injection rates were varied from the reference value at each operating, dFF(NH3) denotes he range of increase of fuel fraction (FF) of NH3 from the reference value at each operating point. IMEP was constrained to $\pm$ 5% accuracy window from the reference value at each operating point. On one hand, such defined optimization task should give already some indications on possible improvements in engine performances. On the other hand by having IMEP as a constraint being close to the baseline results, it is prevented that the optimizer may search for a solution far from from the baseline data. This makes possible to evaluate the plausibility of the obtained results by their comparison to those existing baseline or experimental data. Such a possibility is an advantage at early application phase, and when there are no reference data available that would come from the same inputs as simulated/optimized ones. The results are presented in Figure 5 – Figure 8

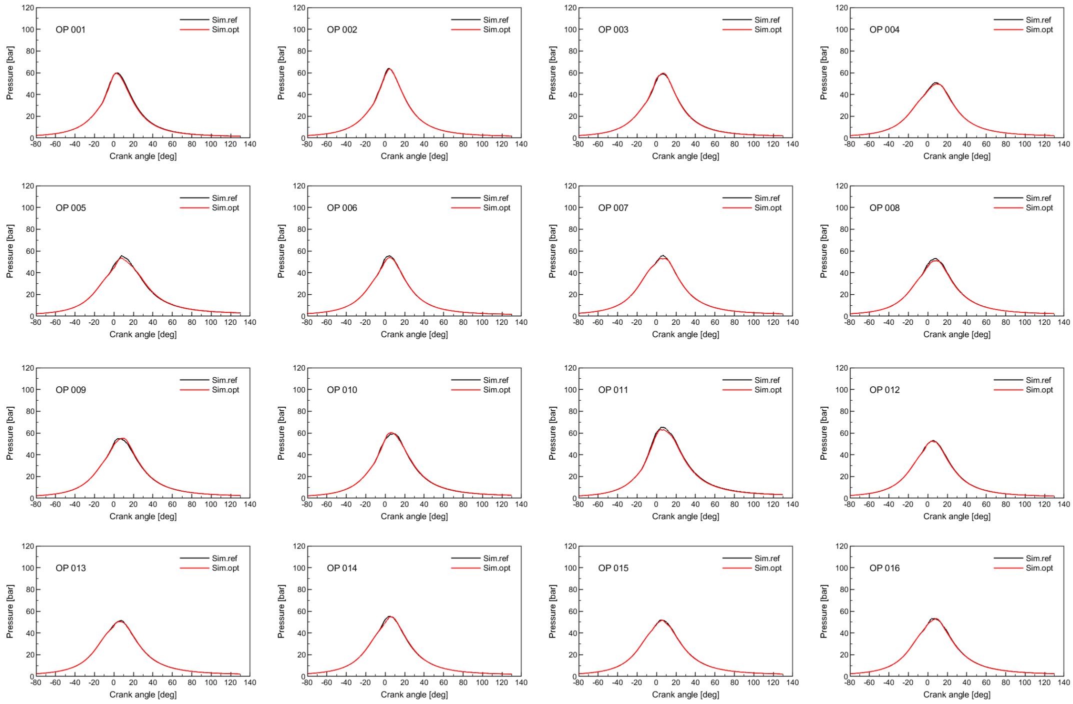

Figure 5: Comparison between the simulated baseline (ref.) and the simulated after optimization (opt.) in-cylinder pressure histories for operating points listed in Table 2

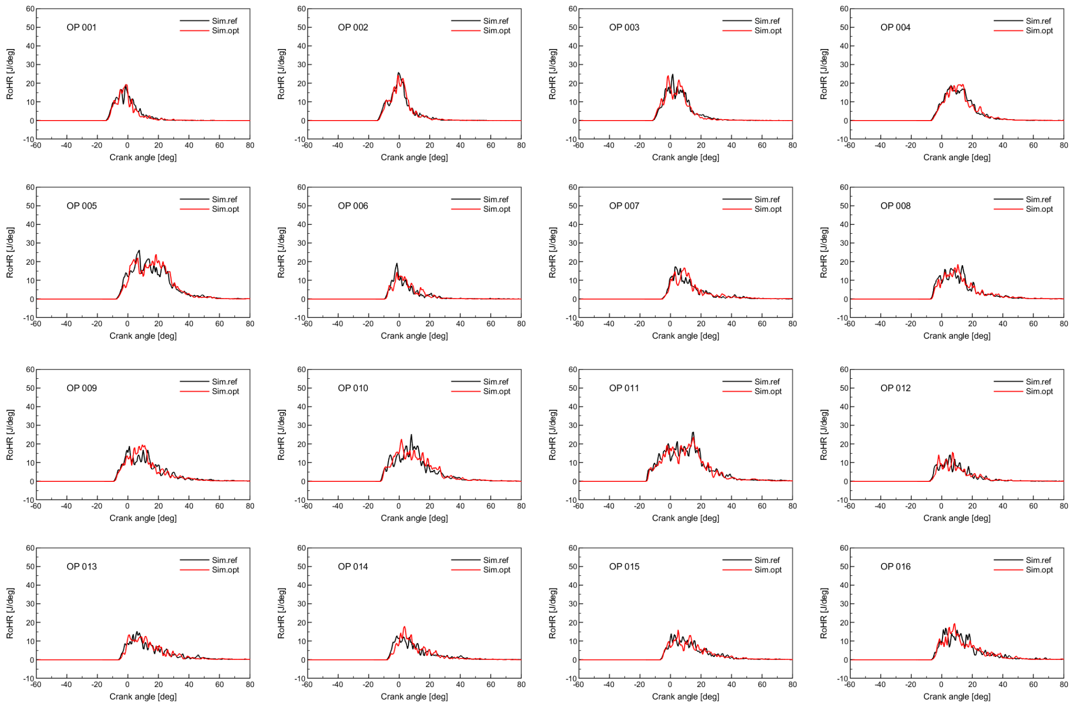

Figure 6: Comparison between the simulated baseline (ref.) and the simulated after optimization (opt.) RoHR histories for operating points listed in Table 2

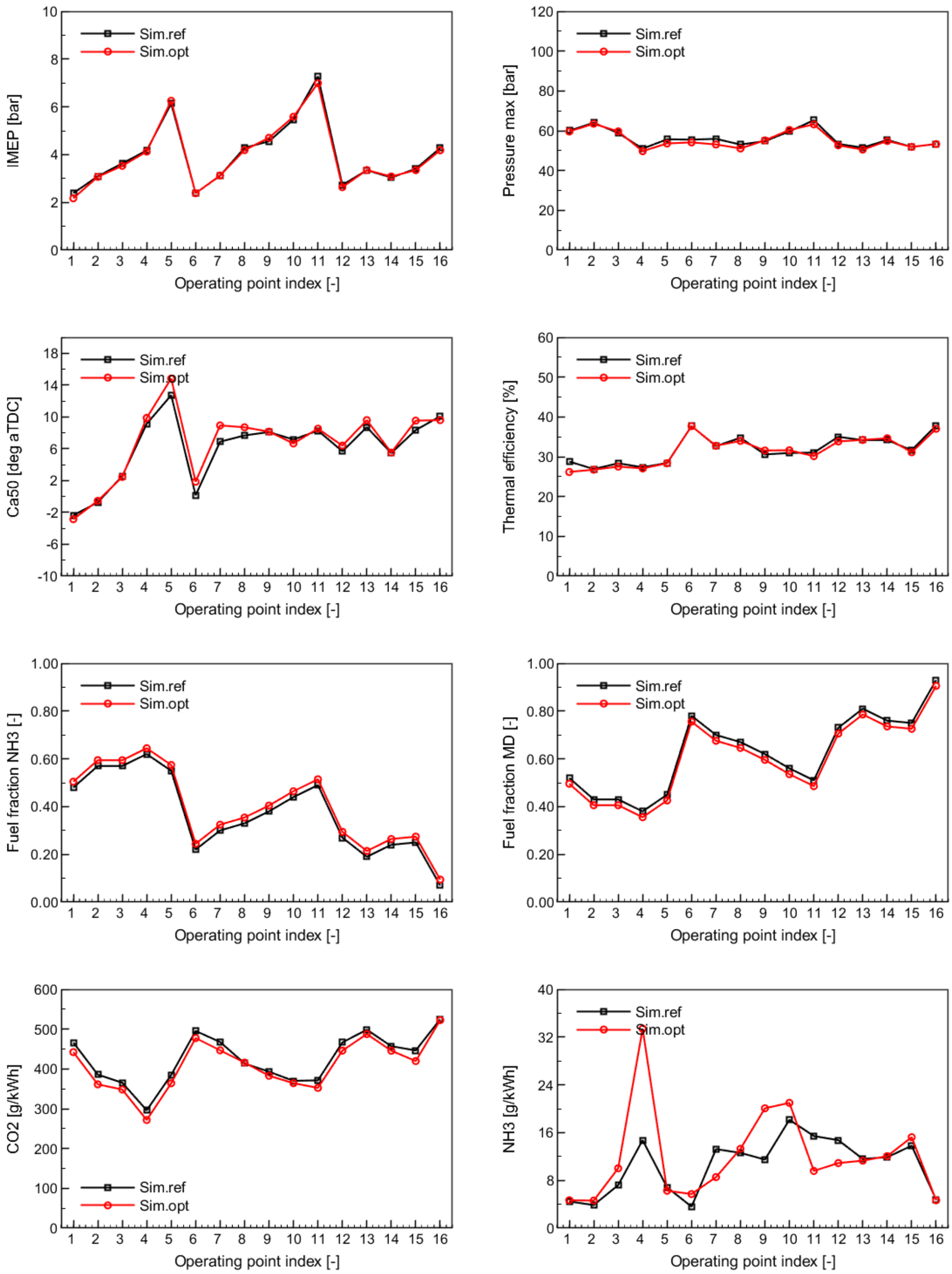

Figure 7: Comparison between the simulated baseline (ref.) and the simulated after optimization (opt.) for selected global engine performance parameters and exhaust emissions for operating points listed in Table 2

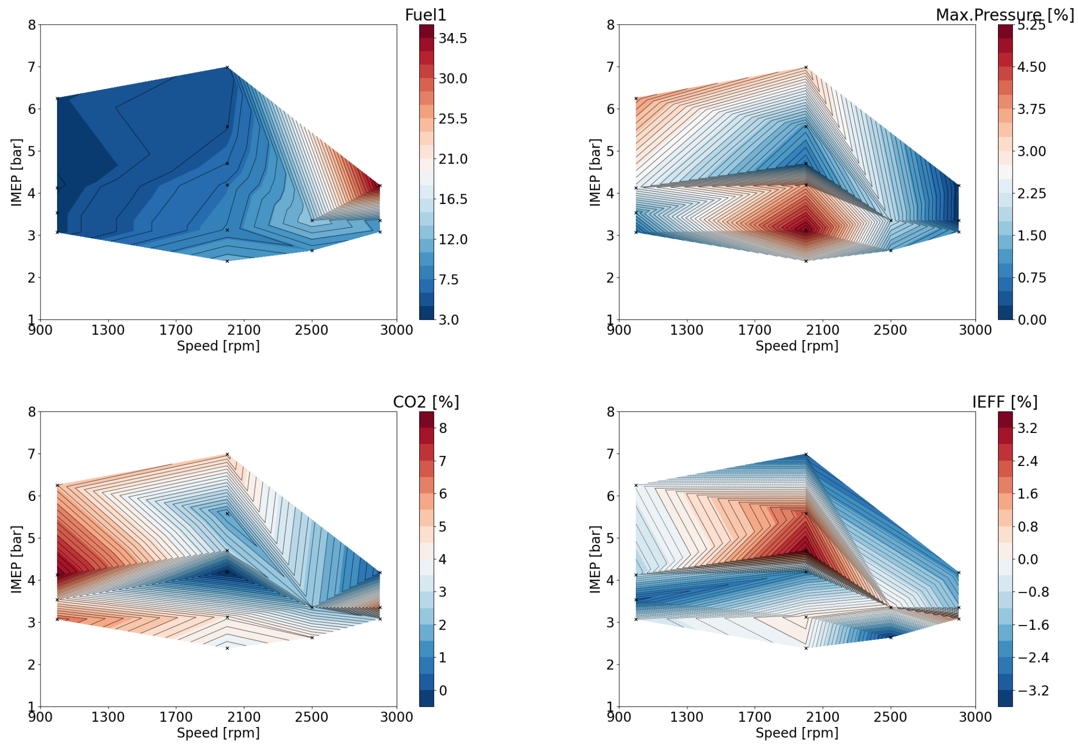

Figure 8: Difference maps (relative error %) between the simulated baseline (ref.) and the simulated after optimization (opt.) for selected global engine performance parameters and exhaust emissions for operating points listed in Table 2

4 Summary

This report presents a methodology for predicting engine performance parameters over wide range operating points based on a numerical model that was trained for a limited set of experimental data. The methodology is referred to as performance mapping and was applied to the engine with direct injection of ammonia and biodiesel. The methodology is of general purpose. It can be applied to differently formulated optimization tasks in the context of combustion engines and fuels used for their felling. Specifically in this report, the results obtained indicate on potential benefits of changing fuel injection timing and increasing ammonia share in the fuel for CO2 reduction, and for a given load conditions. By optimizing only the anchorage of start of fuel injection for both fuels, and without changing the the delay between them does not help significantly in reducing engine out CO2 (reduction between $1\% - 7\%$) for a given load condition determined by IMEP. In this specific case the reference data that were available for numerical campaigns came from and engine that was already preliminary optimized on the test bench for the use of ammonia and biodiesel. This partly explains why no significantly better results were obtained. However, when analyzing the experimental results versus the simulated results from the trained/optimized model the later ones show expected trends and hence, the optimized results and the co-simulations methodology are considered plausible. Definitive judgment of the obtained results and the robustness of the co-simulation procedure will only be possible if the optimized results could be compared to the measured ones from an engine that was operated according to the configuration given by numerical findings.

Norway grants

Definitions/Abbreviations

AES - Ammonia energy share
PM - Particulate matter
PSD - Particle size distribution
CFD - Computational fluid dynamics
SRM - Stochastic reactor model
PDF - Probablity density function
IEM - Exchange with the mean
EMST -Euclidean Minimum Spanning Tree
CN - Cetane number
LHV - Lower heating value
EGR - Exhaust gas recirculation
TDC - Top dead center
ATDC - After top dead center
CAD - Crank angle degree
SOI - Start of injection
EVO - Exhaust valve opening