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

Work package 3
Deliverable report 2

Optimized ammonia share in the fuel for a given injection strategy

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Contents

1 Introduction

1.1 Background

This report presents works carried out within the second deliverable (D3.2) of the third work package (WP3). It describes activities related to the application of the trained 0D stochastic reactor model (SRM) for the analysis of combustion and emissions formation from the engine operated with direct injection of ammonia and biodiesel, and varied fractions of ammonia in the total mass of fuel.

1.2 Specific objectives

The primary objective of the work assigned to D3.2 was the determination via 0D simulations the maximum ammonia energy share in the total fuel mass that the engine can tolerate without penalty in overall performance parameters and combustion stability; determination of the optimum fuel mixture composition. This work was projected as supporting the development work by the team at Silesian University of Technology (SUT) while retrofitting the baseline compression ignition (CI) engine to the operation with ammonia being directly injected into the cylinder. Similarly as in M3.2, the work here reported also aims to further assess the feasibility of using that SRM-based approach to simulate a CI engine ammonia and biodiesel being directly injected into the cylinder.

1.3 Scope of the work and report structure

After a brief introduction into the subject matter, along with the definition of the specific objective of the deliverable, chapter 2 of this report provides a reader with basic information about the reference engine, operating points and numerical model setup as well as with basic terms used for the description of the obtained results. Chapter 3 is the main part of the deliverable report. It presents results from the reference baseline 0D model. Then it discuses the extrapolated results for varied and constant engine loads. Finally chapter 4 summarizes the obtained results.

2 Reference engine model

2.1 Engine data and reference operating point

Simulations presented in this report refer to the same engine and experimental data as the ones described in the milestone report M3.2. Here, we briefly present them again for the completeness of the report whereas detailed information can be found in the reports by project partner from SUT who investigated the engine experimentally. The basic specification of the engine is given in Table 1. Table 2 summarizes operating conditions for four operating points described in the report M3.2. At these points the engine was operated at fixed start of injection (SOI) for biodiesel and varied SOI of ammonia.

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

Table 2: Engine operating points with direct ammonia and biodiesel injection.

OP	**1**	**2**	**3**	**4**
Engine speed (rpm)	1500	1500	1500	1500
IMEP (bar)	5.08	4.97	5.10	5.06
Phi (-)	0.43	0.41	0.40	0.41
AES (%)	26	26	25	29
SOI NH3 (deg aTDC)	-10	-14	-17	-20
SOI biodiesel (deg aTDC)	-17	-17	-17	-17

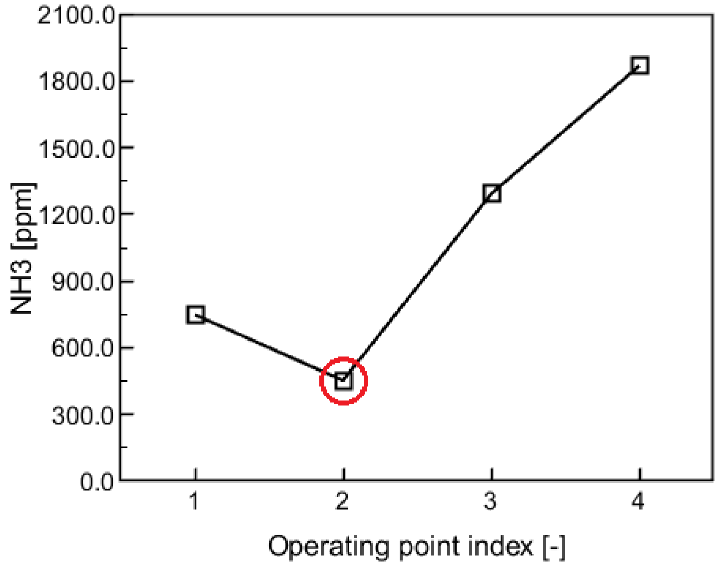

Figure 1: Measured concentration of ammonia in engine exhaust gasses for OPs in Table 2.

Out of four operating points presented in Table 2, OP2 was selected as basis for the analysis of the impact of increasing the ammonia energy share in the fuel on overall engine performance parameters and exhaust emissions. The OP2 was selected since st this point the lowest engine out ammonia was measured as shown in Figure 1.

2.2 Numerical model configuration

Simulations were carried out using the SRM from LOGEengine package that we used for the work reported in the milestone report M3.2 of WP3. Table 3 summaries parameters of the SRM that were used through the simulations and Table 4 lists the most important parameters of the $k-\epsilon$ turbulence model. These parameters were defined during model calibration that was conducted within the work described in the milestone report M3.2.

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

Table 4: Model constants in the calibrated $k-\epsilon$ turbulence model.

Parameter	$C_{\epsilon,1}$	$C_{\epsilon,2}$	C_{inj}	C_{τ}	$C_{k,init}$
Value	7.0	3.0	0.0529	9.448	11

2.3 Combustion metrics

Ammonia energy share (AES)

The share of ammonia in the total energy delivered with the fuel was calculated according to the formula that we used also in the deliverable report D3.1 of WP3.

$$AES\ [\%] = \frac{Y_{NH3} LHV_{NH3}}{Y_{NH3} LHV_{NH3} + Y_{MD} LHV_{MD}} \times 100. \tag{1}$$

Here, Y denotes mass fraction of NH_3 and methyldecanoate (MD), respectively. LHV stands for lower heating value (LHV) of NH_3 and MD, respectively.

Rate of heat release (RoHR)

The history of RoHR is used to quantify the combustion process. It provides the information about the ignition delay time, the start of combustion (SOC), the end of combustion (EOC) and the amount of heat transferred to the wall. Finally, it determines the total amount of the energy that is released during combustion. These parameters further complement the information obtained from the in-cylinder pressure data. RoHR is calculated from the in-cylinder pressure data (p), changes of the cylinder volume (V) and it depends on the in-cylinder mixture composition that is expressed by the ratio of specific heats (γ). The calculation of RoHR is carried out incrementally with time step defined by crank angle degree (φ).

$$RoHR\ [J/deg] = \frac{\gamma}{\gamma - 1} p \frac{dV}{d\varphi} + \frac{1}{\gamma - 1} V \frac{dp}{d\varphi}. \tag{2}$$

The RoHR history obtained from Eq. 2 is refereed to as the apparent rate of heat release that is a measure of the energy effectively absorbed by the working fluid; integrating Eq. 2 over the closed part of the engine cycle, one obtains cumulative heat release (CHR). By defining a crank angle (CA) corresponding to the point where on the CHR history 50% of the energy has been released, one obtains combustion center that is denoted by CA_{50} and is another parameter used for quantifying the combustion process.

Indicative thermal efficiency (ITE)

Indicated thermal efficiency (ITE) was calculated based as the ratio of the indicative work (W_i) and the energy delivered with the fuel that was calculated from known masses of ammonia (m_{NH3}) and MD, and their corresponding LHV values.

$$ITE\ [\%] = \frac{W_i}{m_{NH3} LHV_{NH3} + m_{MD} LHV_{MD}} \times 100. \tag{3}$$

3 Results

3.1 Baseline model calibration

Simulations pertaining to the analysis of the impact of increasing the ammonia energy share in the fuel on overall engine performance parameters and exhaust emissions were carried using as basis the the 0D model calibrated for OP2 from Table 2. The results of the calibration process are, for selected engine parameters, presented in Figure 2. As already discuss in the report M3.2, the obtained agreement between the simulated and the experimental data is satisfactory, and hence, can be used as basis for extrapolating the model results to different shares of ammonia in the total fuel mass.

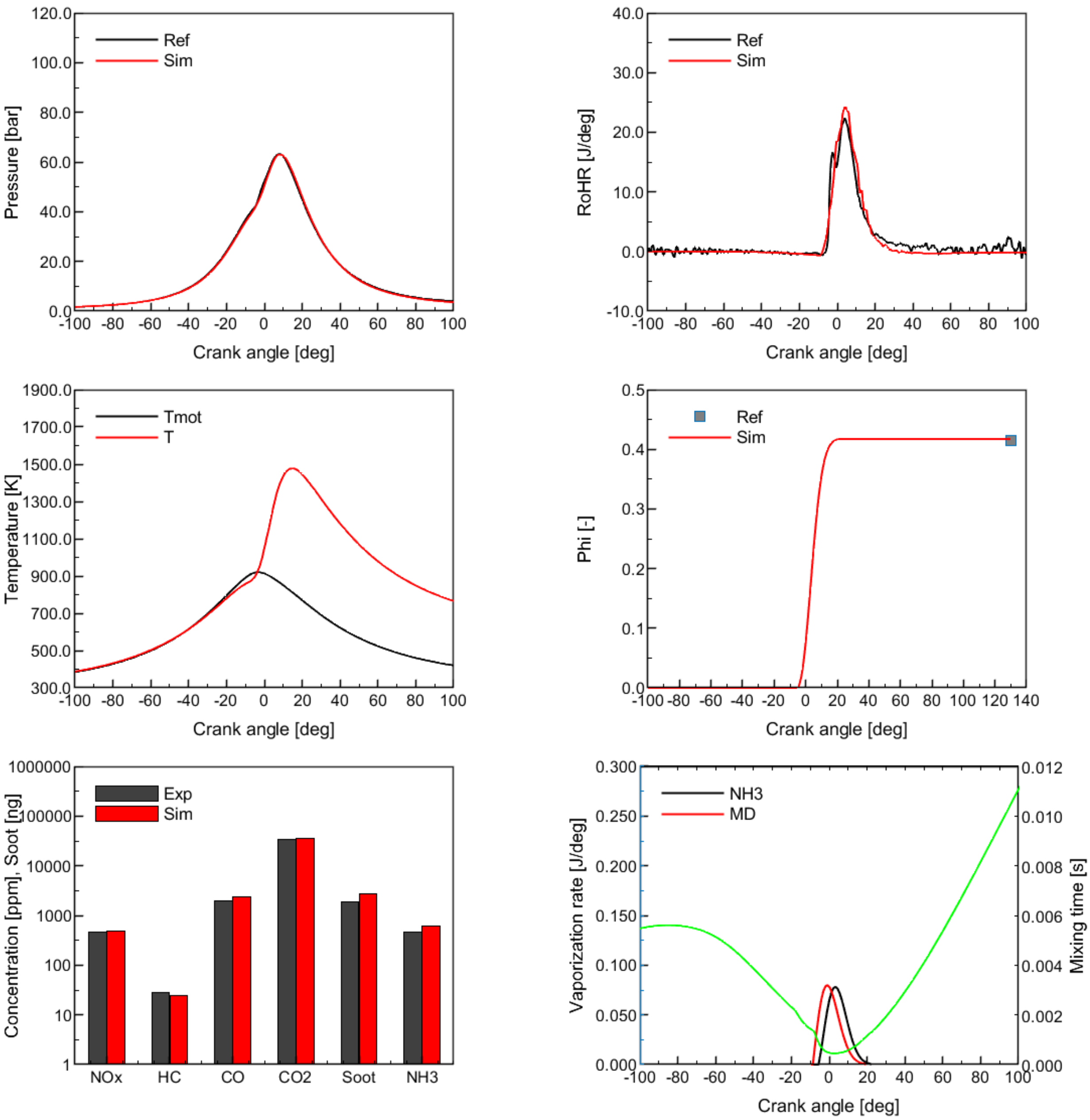

Figure 2: Selected engine in-cylinder performance parameters, exhaust emissions and operating conditions compared to their experimental counterparts for OP2.

Starting from the calibrated baseline model (AES=26%), simulations were carried out in two modes: 1) at fixed equivalence ratio (ϕ) and consequently varied load due different amount of ammonia in the fuel, and 2) at constant engine load that was due to the changes in total fuel mass and ϕ. These two modes are discussed in the next sections.

3.2 Results for varied engine load

The share of ammonia in the total fuel mass was increased gradually, and at the same time, the total mass of fuel and actual air fuel ratio were kept constant. In such a configuration, the energy delivered to the engine with the injected fuel varies due to the increased share of ammonia that has LHV lower than that of biodiesel. Results obtained in this configuration are refereed to as results for varied engine load.

Initially, the share of ammonia in the total fuel mass was increased gradually from 0% to 100%. However, the preliminary results showed that for operating points with above AES=56% the quality of combustion dramatically deteriorates and therefore we excluded these points from the analysis. The matrix of investigated operating points is presented in Table 5 and the obtained results are in Figure 5 and Figure 6.

Table 5: Matrix of operating points for simulating the impact of ammonia share at varied load. Operating condition No. 9 corresponds to the baseline model OP2 presented in Figure 2.

No.	NH3 [-]	MD [-]	$E_{in,tot}$ [MJ/kg]	$E_{in,NH3}$ [MJ/kg]	AES [%]
1	0	1	34.44	0	0
2	0.05	0.95	33.65	0.93	2.8
3	0.1	0.9	32.86	1.86	5.7
4	0.15	0.85	32.07	2.79	8.7
5	0.2	0.8	31.27	3.72	11.9
6	0.25	0.75	30.48	4.65	15.3
7	0.3	0.7	29.69	5.58	18.8
8	0.35	0.65	28.9	6.51	22.5
9	0.39	0.61	28.26	7.25	25.7
10	0.4	0.6	28.11	7.44	26.5
11	0.45	0.55	27.31	8.37	30.6
12	0.5	0.5	26.52	9.3	35.1
13	0.55	0.45	25.73	10.23	39.8
14	0.6	0.4	24.94	11.16	44.7
15	0.64	0.36	24.3	11.9	49
16	0.65	0.35	24.15	12.09	50.1
17	0.66	0.34	23.99	12.28	51.2
18	0.67	0.33	23.83	12.46	52.3
19	0.68	0.32	23.67	12.65	53.4
20	0.7	0.3	23.35	13.02	56

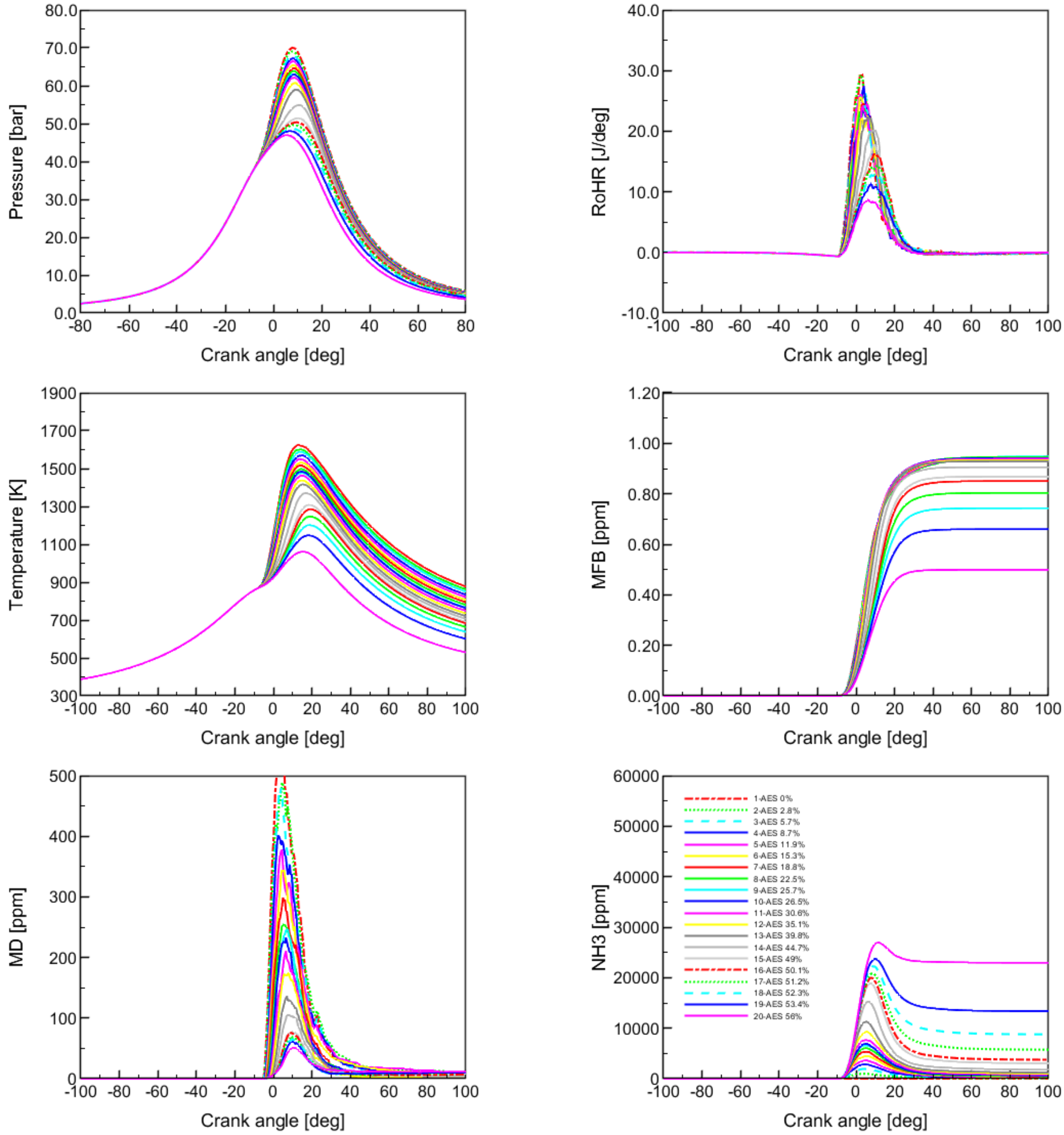

Figure 3: Selected, crank angle based, engine in-cylinder performance parameters for different ratio of ammonia and biodiesel that is represented by methyldecanoate (MD).

Figure 3 shows selected engine operating quantities as a function of crank angle. These results visualize how the increase of ammonia deteriorates the combustion process – more exhaust NH3 and MD, lower levels of MFB, in-cylinder pressure, temperature, and RoHR. These results are further supplemented by the results in Figure 4 that provides global engine in-cylinder performance parameter for the analyzed matrix of operating points. In this report as global results we understand these that describe through a single value engine in-cylinder processes that are crank angle dependent in an actual engine cycle. The global results are useful for determining the limiting value of AES, above which the engine operates less efficiently and with more engine out ammonia.

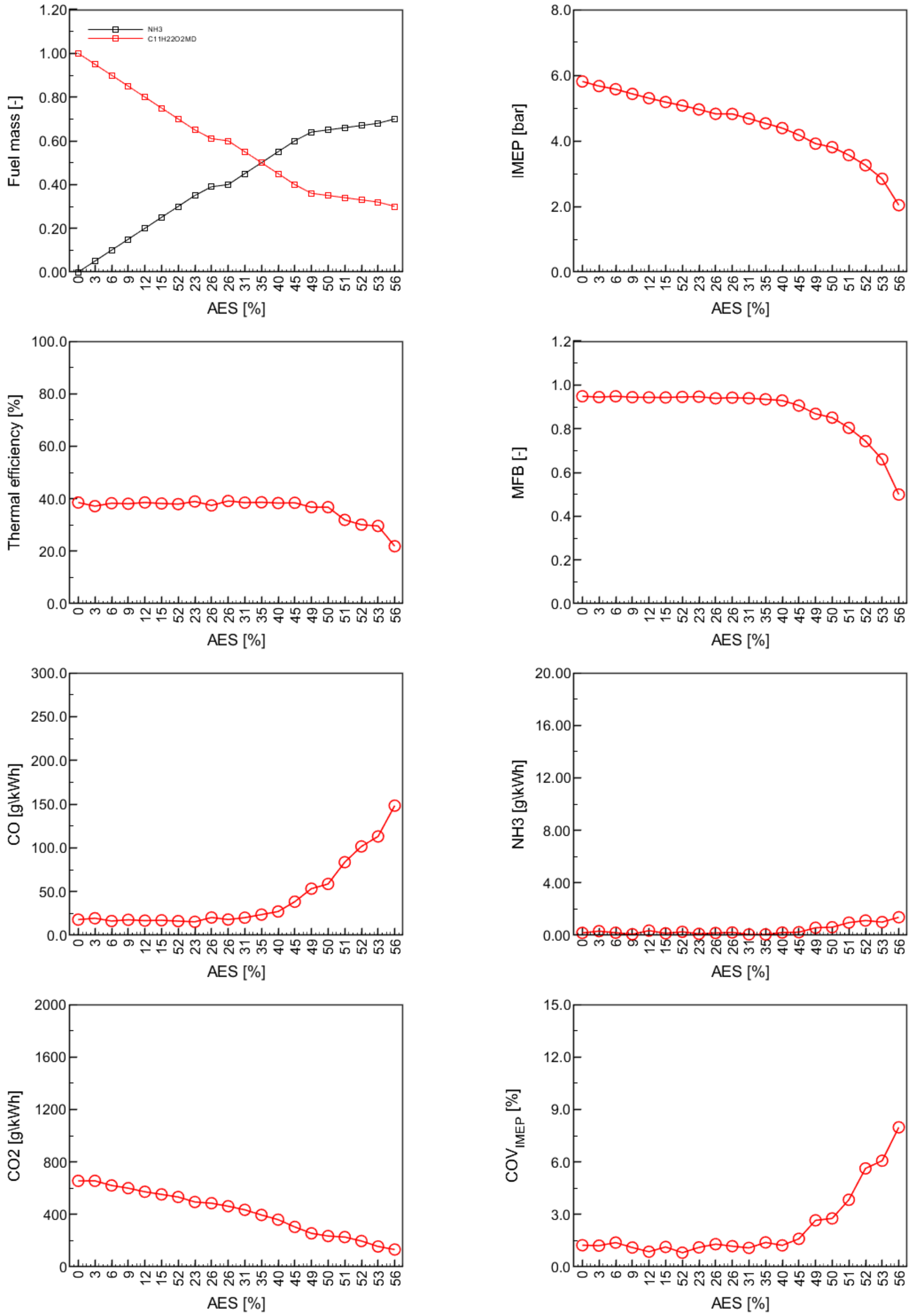

Figure 4: Selected global engine in-cylinder performance parameters for different ratio of ammonia and biodiesel.

From the results in Figure 3 and Figure 4, one can conclude that for the considered fuel injection strategy, AES=50% is the last point for which the thermal efficiency is at a level that is comparable to the points with AES<50%. After that point a decrease of ITE is observed that for AES=56% reaches almost 50% of that for the baseline point (AES=26%). For AES above 56% only a marginal amount of energy is released with extremely high engine out emissions and as mentioned earlier, these points were excluded from the analysis. Using ITE as a criterion, one can say that AES=50% is a limit for this operating point for stable and efficient operation. For AES above 50%, and up to 56%, the quality of combustion starts decreasing significantly.

3.3 Results for constant engine load

As results at constant engine load are referred those obtained with the same amount of energy delivered to the cylinder due to fuel injection, and for every investigated operating point. To maintain constant load for increased amount of ammonia, the mass of MD must have been increased to compensate for lower LHV of ammonia. This have led to also different lambda for every investigated operating point (Table 6). Calculations were carried out for AES between 0% and 100%. However, at operating points with AES above 57% the quality of combustion was extremely poor, with only a marginal amount of energy was released. Therefore we excluded these points from the analysis.

Table 6: Matrix of operating points for simulating the impact of ammonia share at fixed load.

No.	$E_{in,tot}$ [MJ/kg]	$E_{in,MD}$ [MJ/kg]	$E_{in,NH3}$ [MJ/kg]	AES [%]	Lambda [-]
1	28.26	21.01	7.25	26%	2.41
2	28.26	18.94	9.32	33%	2.435
3	28.26	17.22	11.04	39%	2.457
4	28.26	15.5	12.76	45%	2.479
5	28.26	13.78	14.48	51%	2.501
6	28.26	13.43	14.83	52%	2.506
7	28.26	13.27	14.99	53%	2.508
8	28.26	13.09	15.17	54%	2.51
9	28.26	12.74	15.52	55%	2.515
10	28.26	12.4	15.86	56%	2.519
11	28.26	12.05	16.21	57%	2.524

Results for the baseline fuel injection timings

Simulations of operating points listed in Table 6 were carried out with fuel injection timings the same as for the baseline point (OP2 in Table 2).

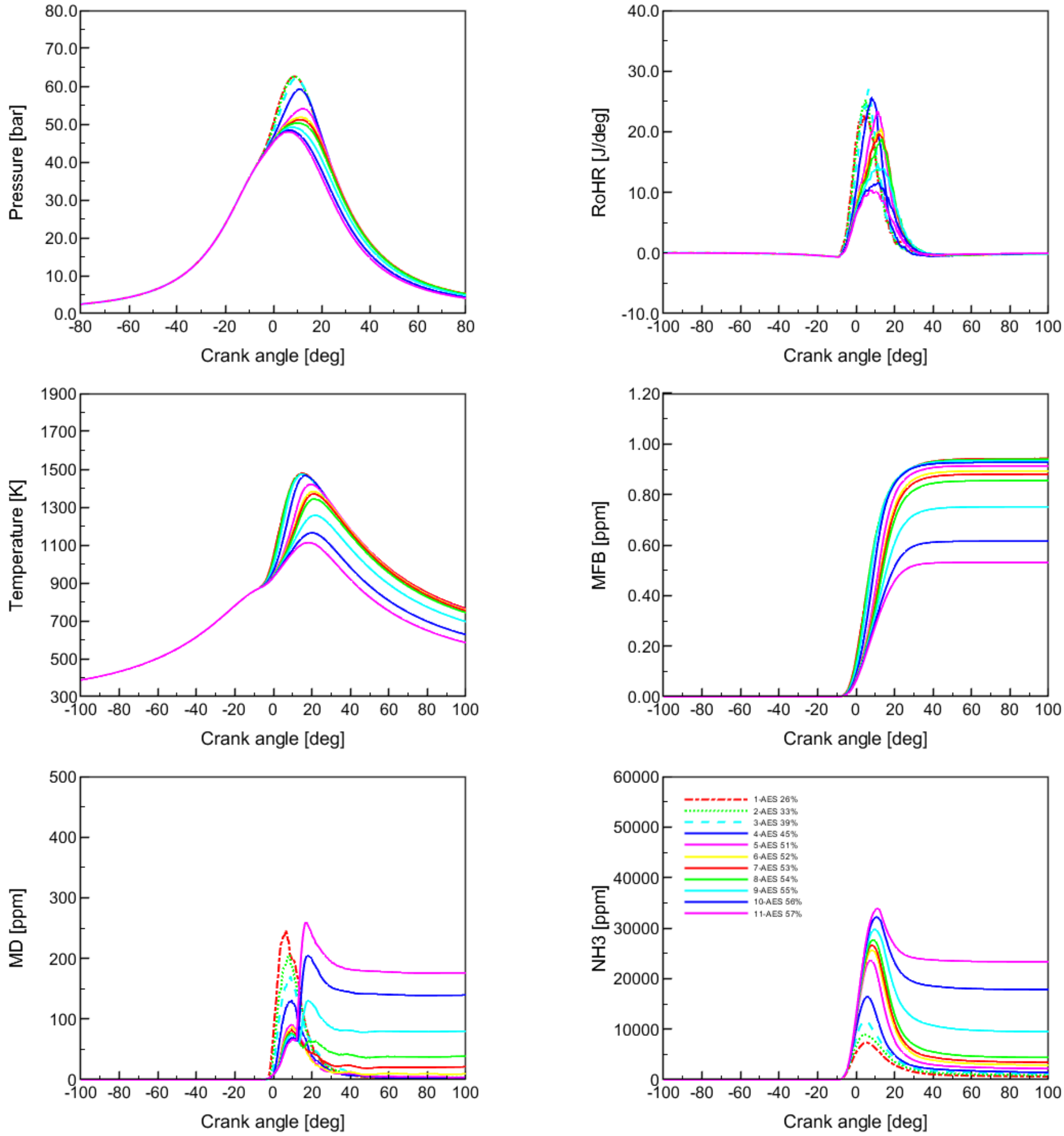

Figure 5: Selected, crank angle based, engine in-cylinder performance parameters for different ratio of ammonia and biodiesel that is represented by methyldecanoate (MD); fixed energy delivered to the cylinder due to fuel injection.

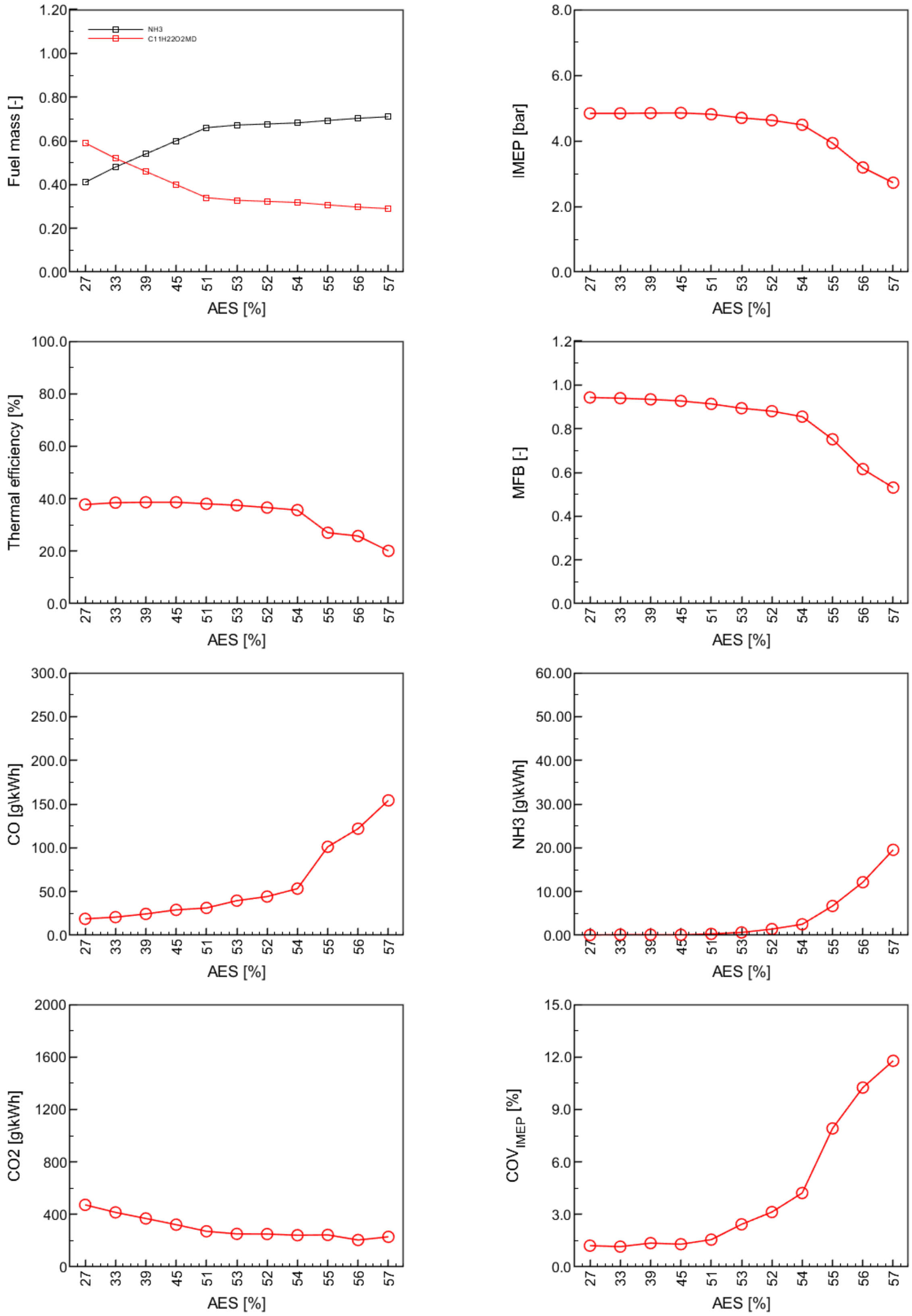

Figure 6: Selected global engine in-cylinder performance parameters for different ratio of ammonia and biodiesel; fixed energy delivered to the cylinder due to fuel injection.

The results in Figure 5 and Figure 6 are analyzed in the same manner as these in section 3. Up to AES=54% ITE is at a level that is comparable to the points with AES<54%. After that point, the ITE starts decreasing and for AES=57% the ITE drops down by almost factor 2. For AES above 57% only a marginal amount of energy was released these points were excluded from the analysis. For AES above 54% the ITE, MFB, IMEP decrease even though the energy input due to injected fuel remains unchanged (Table 6). This further indicates on deteriorating the quality of combustion for AES above 54%.

Results for the optimized fuel injection timings

Simulation results presented in the previous sub-section provide information about the limiting AES value (54%) above which the engine is operated less stable. In this section the operating point corresponding to AES=54% is further analyzed with respects to the obtained performance parameters when compared to the baseline results at AES=26%. The results for selected engine performance parameters, and for both AES values are compared in Figure 7.

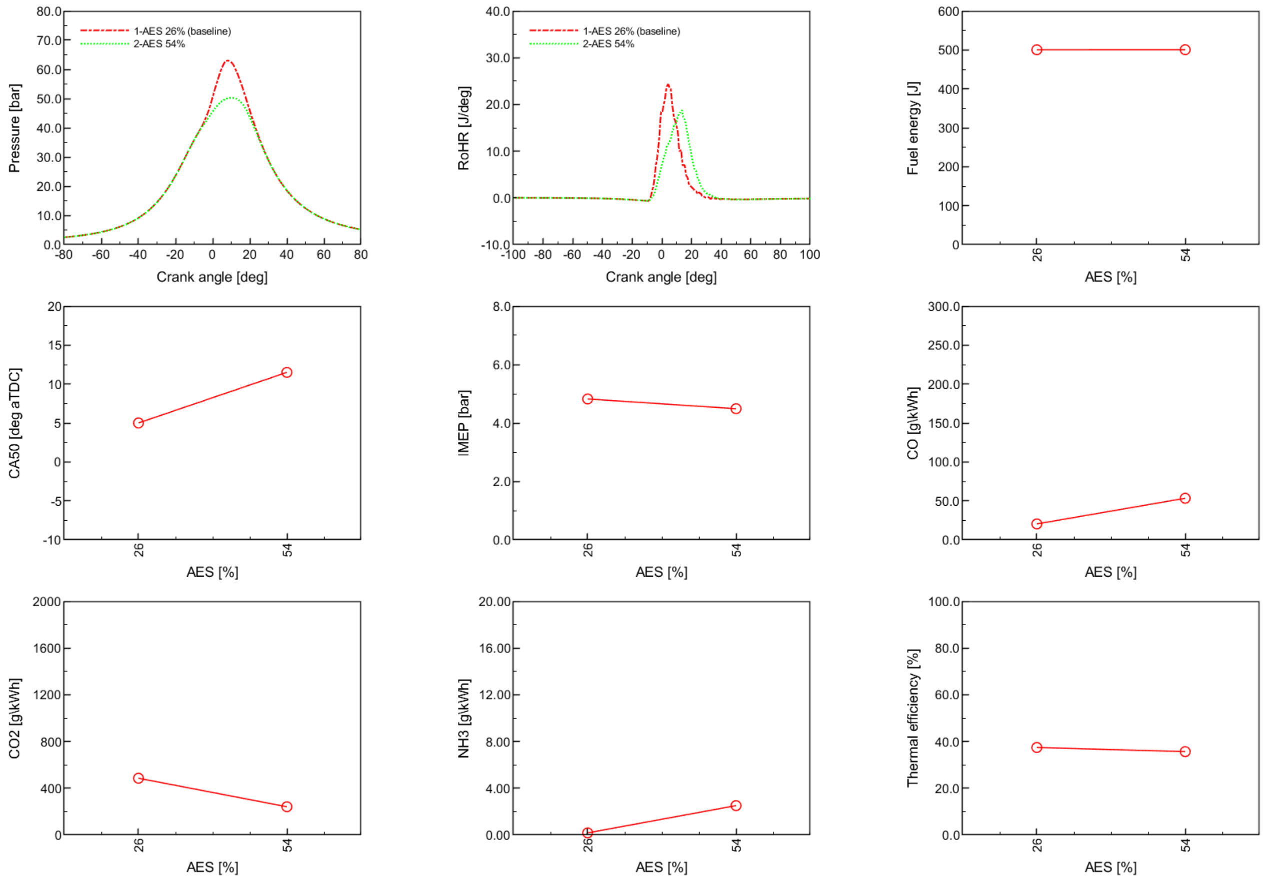

Figure 7: Selected global and instantaneous engine in-cylinder performance parameters for the baseline engine configuration with AES=26% compared to the results for AES=54%.

Increasing AES from the baseline value 26% to 54% have deteriorated engine performance parameters and exhaust emission even though that the energy delivered with the injected fuel was the same in both cases. The location of CA_{50} is delayed that results in lower IMEP. CO and NH3 emissions, expressed in the unit of g/kWh, increase that is due to lower IMEP, but indicates also less efficient combustion. The relative increase of NH3 can also be due to more ammonia in the fuel along with its less efficient burning. CO2 is reduced as the amount of biodiesel in the fuel is reduced, but it is also affected by less efficient combustion seen in an increase of CO emission.

From the results in Figure 7 it is expected that advancing the location of CA_{50}, which is delayed when compared to the baseline result (AES=26%) , could improve the results for AES=54%. The most effective and simplest way to advance CA_{50} is the advancing of SOI that was also selected in this work.

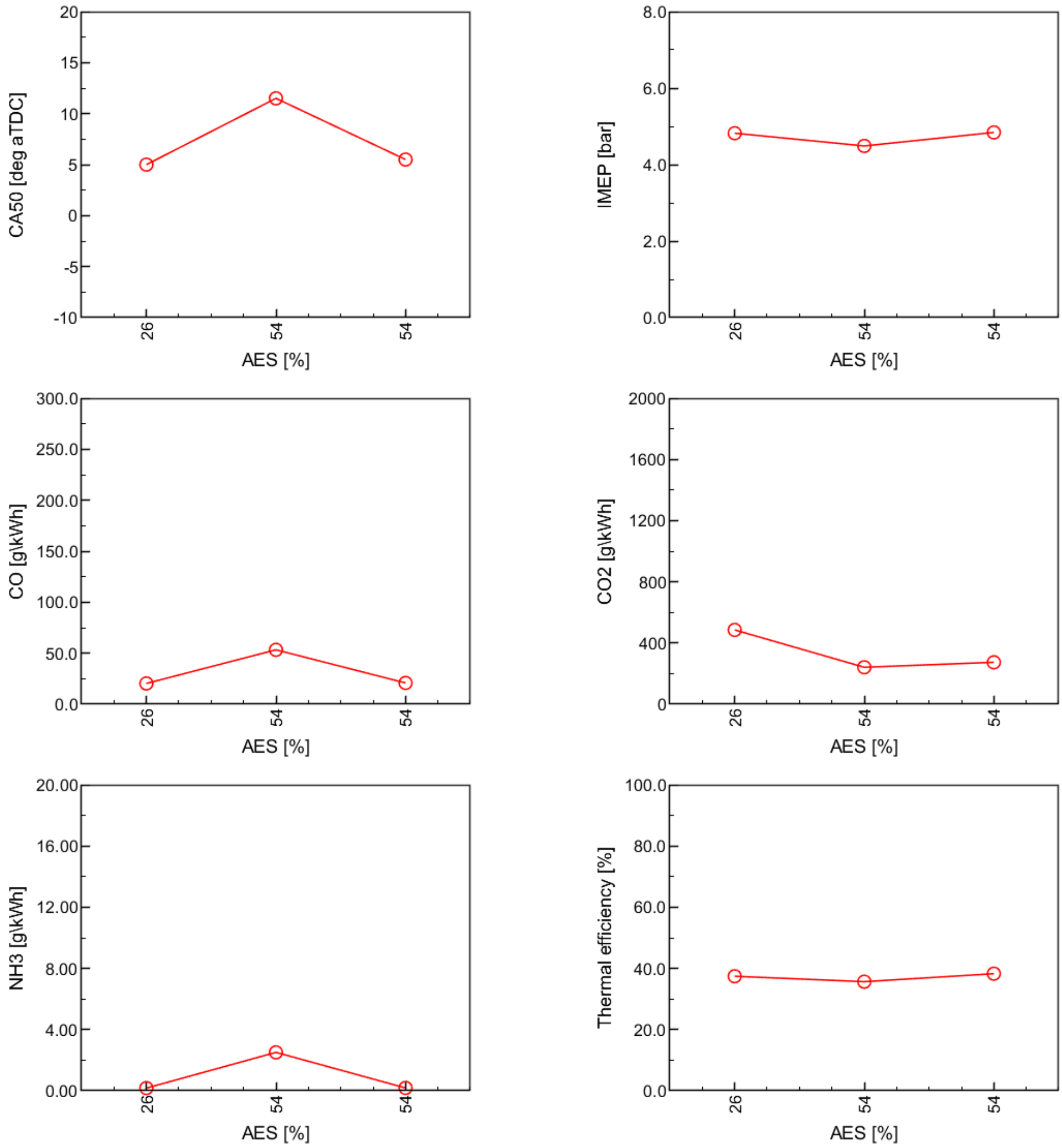

Figure 8: Selected global engine performance parameters for the baseline engine configuration with AES=26% compared to the results for AES=54% and AES=54% with SOI advanced by 4 CAD. Here, in plots in raw 1, 2 and 3 from the top the most right results correspond to AES=54% with SOI advanced by 4 CAD.

The SOI was gradually advanced for both ammonia and biodiesel. The rates of injection for both fuels remained unchanged. The advancing of SOI was carried out until the results, such as in-cylinder pressure, IMEP and CA_{50}, for AES=54% matched, with certain tolerance, the results for AES=26%. The match was obtained for SOI advanced by 4 CAD. The results for such optimized injection strategy and for instantaneous pressure, RoHR and temperature histories, along with relative difference for selected global paerformance parameters are presented in Figure 9. In turn Figure 8 contains remaining global performance parameters for these two cases.

Overall, when compare to the baseline results for AES=26%, the advancing of SOI by 4 CAD for AES=54%, while keeping the same IMEP for both cases, resulted in an increase of engine out NH3 and CO by 6% and 2.5%, respectively. The ITE increased by 2.5%, and CO2 was reduced by approximately 40%.

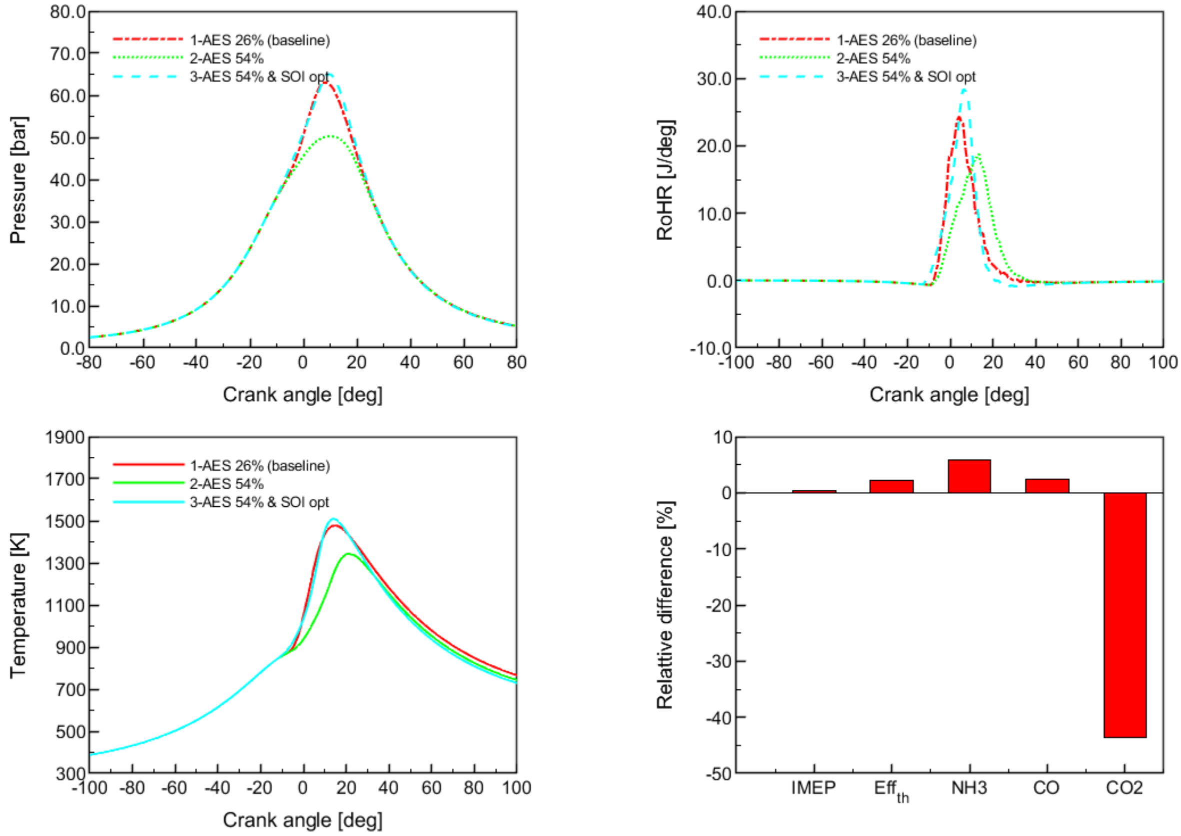

Figure 9: Engine in-cylinder pressure and RoHR histories for the baseline engine configuration with AES=26% compared to the results for AES=54% and AES=54% with SOI advanced by 4 CAD. The plot with relative difference compares results with AES=54% and optimized SOI to the baseline results with AES=26%.

4 Summary

The work conducted withing D3.2 concerned the determination the maximum ammonia energy share in the total fuel mass that the engine can tolerate without penalty in overall performance parameters and combustion stability. All calculations were carried out using the SRM presented in the report M3.2. The major achievements and results of the deliverable D3.2 can be summarized as follow.

- **Ammonia energy share at varied engine load**. For the considered fuel injection strategy, AES=50% is the last point for which the thermal efficiency is at a level that is comparable to the points with AES<50% and similar to the baseline point (AES=26%). Above AES=50% a decrease of ITE is observed that for AES=56% reaches almost 50% of that for the baseline point. The results indicate that AES=50% is a limit for this operating point for stable and efficient operation. For AES above 50%, the quality of combustion starts visibly decreasing.

- **Ammonia energy share for fixed engine load and baseline fuel injection strategy.** For AES=54% ITE is at a level that is comparable to the points with AES<54%. Thus AES=54% is considered as a limiting in this configuration. Then, the ITE starts decreasing, and for AES=57% it drops down by almost factor 2. For AES above 54% the ITE, MFB, IMEP decrease even though the energy input due to injected fuel remains unchanged. This further indicates on deteriorating impact of ammonia on combustion quality for AES above 54%.

- **Ammonia energy share for fixed engine load and optimized fuel injection timing.** By advancing the SOI of both ammonia and biodiesel the results obtained at fixed load (AES=54%) were further improved. Due to advancing SOI by 4 CAD the CA_{50} has been moved to the earlier part of the cycle. In consequence IMEP has been improved too that matches the one from the baseline operating point with AES=26%. At such a configuration (AES=54%, and advanced SOI) when comparing to the baseline results with AES=26%, engine out NH3 and CO, increased only by 6% and 2.5%, respectively. The ITE increased by 2.5%, and CO2 was reduced by approximately 40%.