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CFD and Emissions Modelling

Alternative Fuels & Combustion Modelling (ACHA7002)

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Abstract

This report evaluates whether a representative Mazda-based 2.0 L naturally aspirated spark-ignition engine can be adapted for ethanol-containing fuels using a combined ANSYS Forte and Ricardo WAVE workflow. Gasoline, E50 and E100 were compared using the same base engine geometry. Forte thermo outputs were post-processed to obtain CA50 and 10-90% burn duration, which were then used to define the Wiebe combustion model in WAVE. This provided a one-way link from detailed in-cylinder combustion behaviour to full-engine performance prediction. The final Forte-phased WAVE results showed that gasoline and E50 produced very similar peak power, 110.1 kW and 110.5 kW respectively, while E100 reduced peak power to 106.6 kW. A 2 deg CA50-advance sensitivity improved E100 to 107.6 kW and E50 to 111.2 kW, confirming that ethanol operation is strongly dependent on combustion phasing. The study therefore supports E50 as the most practical of the tested fuels for maintaining performance, while E100 would require further ignition and combustion optimisation. The work is relevant to future Euro 7 and post-2035 regulation because low-carbon liquid fuels may retain a limited role where tailpipe CO₂ flexibility and pollutant-emissions compliance are both required.

1 Introduction

The future role of internal combustion engines is being reshaped by climate policy, tailpipe pollutant limits and the practical difficulty of replacing all vehicle applications with battery-electric systems in the same time frame. The European Union's current direction is no longer simply a fixed ban on all combustion engines; the Commission's automotive package describes a 2035 framework in which manufacturers would meet a 90% tailpipe CO₂ reduction target, with the remaining 10% compensated through low-carbon steel, e-fuels or biofuels (European Commission, 2025a; European Commission, 2025b). In parallel, Euro 7 applies to new light-duty vehicle types from 29 November 2026 and adds a broader compliance framework including exhaust and non-exhaust emissions (European Union, 2024).

This regulatory context makes alternative-fuel combustion modelling relevant. The aim of this work is to assess the feasibility of gasoline, E50 and E100 operation in a representative 2.0 L inline-four SI engine using WAVE for engine-system modelling and Forte for combustion phasing support. The objectives are to establish a stable gasoline baseline, create fuel-specific E50 and E100 cases, transfer Forte-derived CA50 and burn-duration data into WAVE, and compare the resulting power, torque, fuel-consumption and emissions-related trends. The analysis is not intended to certify a production vehicle; it is a simulation-based feasibility assessment of whether ethanol substitution can maintain useful performance while giving a route towards lower fossil-carbon operation.

2 Literature and technical justification

A 2.0 L inline-four spark-ignition architecture was selected because it represents a common passenger-car engine size and provides a manageable modelling platform. This also follows standard SI-engine modelling practice, where geometry, operating point, fuelling and burn-rate assumptions are separated so that each modelling change remains traceable (Stone, 2012; Heywood, 2018). Modern SI engines are strongly affected by fuel octane quality, laminar flame speed, latent heat of vaporisation and knock resistance. High-octane fuels can allow more favourable combustion phasing and improved efficiency when the engine calibration is optimised (Davies et al., 2011; Leone et al., 2018). Alcohol fuels are therefore technically attractive because they generally have high octane number and charge-cooling potential. Sileghem et al. (2015) showed that alcohol fuels in a production DISI engine can produce favourable combustion and efficiency behaviour compared with gasoline, although the result depends strongly on the calibration strategy.

Ethanol was selected instead of a non-carbon fuel because it is a realistic transitional liquid fuel. It is already compatible with blending infrastructure at low and medium concentrations, and neat ethanol represents the upper limit of alcohol substitution for this study. Previous ethanol-fuel reviews also identify ethanol-gasoline blends as relevant to SI engines and to regulated and unregulated exhaust-emissions behaviour (Bielaczyc et al., 2016). E50 provides an intermediate case that tests whether a major reduction in gasoline fraction can be achieved without the full fuelling, cold-start and volumetric-energy penalties of E100. E100 is useful as a stress case because its lower stoichiometric air-fuel ratio and different combustion behaviour require a much larger change to the fuel system and ignition strategy. This makes the gasoline-E50-E100 sequence suitable for identifying whether performance changes are caused simply by fuel-energy input or by combustion phasing. Recent work on mid- to high-alcohol blends also shows that blend performance and emissions depend strongly on stoichiometry, ignition calibration and fuel-delivery strategy (Turner et al., 2020).

3 Methodology

The WAVE model was based on a Mazda-derived 2.0 L inline-four naturally aspirated spark-ignition engine. The same engine geometry, valve system and speed points were retained for all fuels so that the comparison isolated fuel and combustion effects. Gasoline used the supplied gasoline fuel file. E100 used the ethanol fuel file. E50 was generated from the supplied gasoline and ethanol fuel-property files using a 50/50 blend ratio. The fuel-air ratio was corrected for each fuel before comparison: E50 used an AFRAT value of 0.0834, corresponding to its approximately 12.0 stoichiometric AFR, while E100 used approximately 0.111, corresponding to ethanol stoichiometry near 9.0. This avoided the misleading lean operation that occurred when ethanol-containing fuels were initially run using gasoline fuelling.

Method workflow: one-way transfer from Forte combustion phasing to WAVE engine-system comparison.

Fuel files -> Forte combustion cases -> Thermo export -> CA50/burn-duration extraction -> WAVE Wiebe input -> WAVE performance and emissions comparison

The study combined in-cylinder combustion analysis in Forte with 1D engine-system simulation in WAVE. Forte was used to obtain fuel-dependent combustion phasing, while WAVE evaluated full-engine performance over the speed range. Rather than claiming a direct CFD-to-1D solver coupling, the workflow used a one-way transfer of combustion phasing. Forte thermo exports were processed to obtain CA10, CA50, CA90, 10-90% burn duration, peak pressure and peak-pressure crank angle. Additional Forte cases at 7000 and 7200 rpm were completed for all three fuels, so the high-speed WAVE inputs were based on direct Forte data rather than extrapolation. Intermediate WAVE points between measured Forte speeds were obtained by interpolation only. In WAVE, the cylinder combustion submodel was the SI Wiebe model. The Forte CA50 values were entered as the WAVE location of 50% burn point, and the Forte 10-90% burn duration values were entered as the WAVE combustion duration. The Wiebe exponent and Woschni heat-transfer model were retained to avoid introducing uncontrolled calibration changes.

The main outputs assessed were power, torque, lambda, volumetric efficiency, brake specific fuel consumption, exhaust temperature and hydrocarbons. Forte was used mainly for combustion phasing, while WAVE was used for the full-engine comparison. Forte thermo files did not provide usable CO or NOx outputs. WAVE NOx-related outputs were checked separately, but the values remained effectively zero and were therefore treated only as an appendix check rather than a validated quantitative emissions result. Some WAVE points did not fully meet the solver convergence flag, but neighbouring values were smooth and the fuel-air ratios and combustion inputs were consistent, so they were retained for comparative analysis.

Table 1. Fuel and model setup

Fuel case	Fuel file / definition	AFR control	Combustion phasing
Gasoline	gasoline.fue	Gasoline AFRAT; lambda approx. 0.978	Forte CA50 and 10-90% burn duration
E50	E50_clean_from_gasoline_ethanol.fue, generated from gasoline.fue + ethanol.fue at 50/50 blend	AFRAT = 0.0834; lambda approx. 1.000	Forte CA50 and 10-90% burn duration
E100	ethanol.fue	AFRAT approx. 0.111; lambda approx. 1.007	Forte CA50 and 10-90% burn duration

The table demonstrates the controlled parameterisation used to avoid comparing fuels at incorrect fuel-air ratios.

3.1 Controlled parameter strategy

A further modelling decision was to avoid tuning several variables simultaneously. The final WAVE cases changed only the fuel definition, AFRAT value, CA50 table and burn-duration table. Geometry, valve timing, heat transfer and Wiebe exponent were fixed. This was important for traceability because if E100 lost output, the cause could be linked to fuel requirement and combustion phasing rather than an unrelated manifold or valve change. After the main comparison, E50 and E100 refinement cases were run by advancing the CA50 table

by 2 deg while retaining the same fuel, AFRAT and burn duration. This tested whether the ethanol cases were recoverable through phasing optimisation rather than wider engine redesign.

3.2 Rationale for Forte-to-WAVE transfer

This distinction is important for a high-level interpretation of the results. A fuel can look attractive in a constant-volume or single-speed combustion study but fail at engine-system level because of air handling, fuelling demand or poor combustion phasing over the speed range. Conversely, a WAVE-only fuel-file change can hide the combustion penalty by using an unrealistically generic burn model. Combining Forte phasing with WAVE speed sweeps therefore gives a more balanced assessment than either tool alone, while still remaining within a manageable computational workload.

4 Results and discussion

The Forte-phased WAVE results demonstrate that correcting both the fuel-air ratio and combustion phasing materially changes the interpretation of the fuel comparison. When only the fuel file was changed, the ethanol cases could appear weak simply because they were being fuelled at a gasoline-like AFR. After the AFRAT correction and the Forte-derived Wiebe inputs were applied, gasoline and E50 produced almost identical peak output, while E100 showed a modest penalty.

The figures and tables in the following section should therefore be read as comparative evidence. The absolute power numbers depend on the representative Mazda-based model and the assumed combustion model, but the relative trend between the three fuels is the key output. This is also why lambda is reported with every case: without proving comparable fuel-air control, the performance comparison would not be valid.

4.1 Performance

Gasoline produced a peak power of 110.1 kW at 6500 rpm and a peak torque of 181.9 Nm at 5250 rpm. E50 produced the highest peak power, 110.5 kW at 6500 rpm, and a peak torque of 181.5 Nm at 5000 rpm. The difference between gasoline and E50 is small enough that it should not be over-interpreted as a decisive performance gain, but it does show that a 50% ethanol blend can retain gasoline-level output in this model. E100 produced 106.6 kW at 6500 rpm and 175.3 Nm at 5000 rpm. This is not a severe failure, but it is a clear reduction relative to the other two fuels.

The performance trend is consistent with the combustion phasing data. Forte predicted later CA50 and longer burn duration as ethanol content increased. When those values were imposed in WAVE, E100's pressure release occurred later in the expansion process, reducing the useful work extracted from combustion. The direct 7000 and 7200 rpm Forte runs strengthened this interpretation: at 7200 rpm the imposed CA50 increased from about 15.1 deg for gasoline to 20.1 deg for E50 and 23.1 deg for E100, matching the larger high-speed power drop for ethanol-rich operation. A 2 deg CA50-advance sensitivity was therefore applied to E50 and E100. E100 peak power increased from 106.6 to 107.6 kW and peak torque increased from 175.3 to 177.2 Nm. E50 peak power increased from 110.5 to 111.2 kW and peak torque increased from 181.5 to 183.1 Nm, although the high-speed 7000-7200 rpm

region reduced. This suggests that ethanol-rich operation requires speed-dependent ignition optimisation rather than a simple fixed advance across the full speed range. Table 2. Final Forte-phased WAVE peak results

Fuel	Peak power	Peak torque	Lambda control
Gasoline	110.1 kW @ 6500 rpm	181.9 Nm @ 5250 rpm	approx. 0.978
E50	110.5 kW @ 6500 rpm	181.5 Nm @ 5000 rpm	approx. 1.000
E100	106.6 kW @ 6500 rpm	175.3 Nm @ 5000 rpm	approx. 1.007

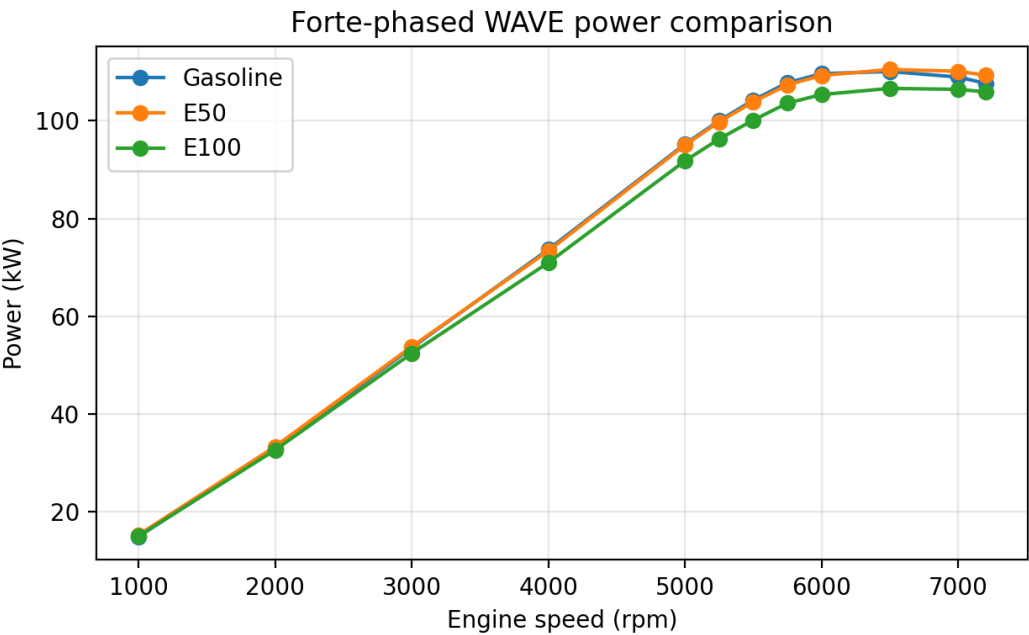


Figure 1. Power versus engine speed for the Forte-phased WAVE cases.

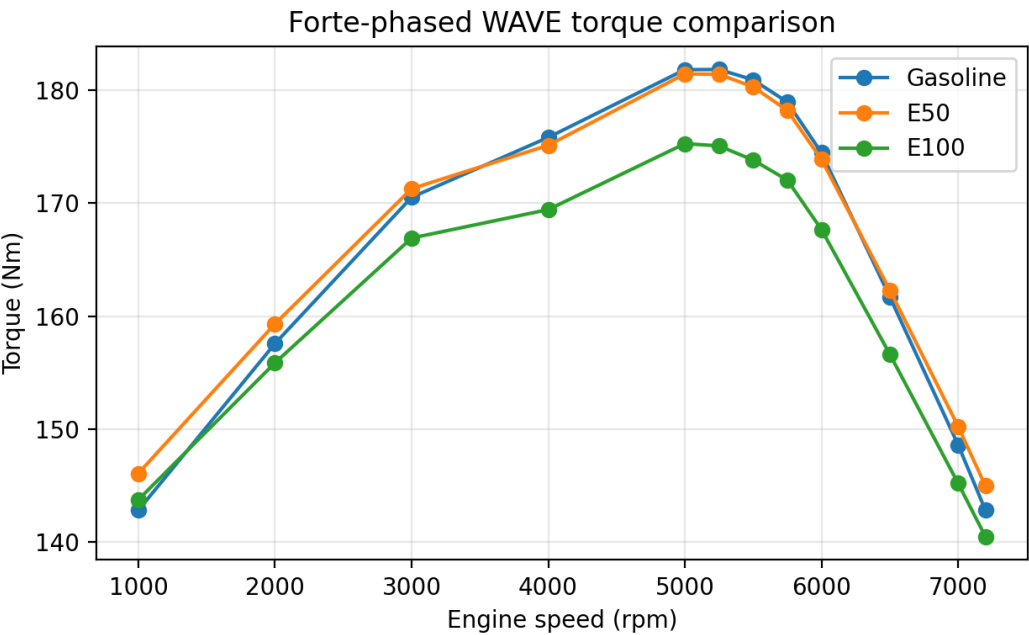


Figure 2. Torque versus engine speed for the Forte-phased WAVE cases.

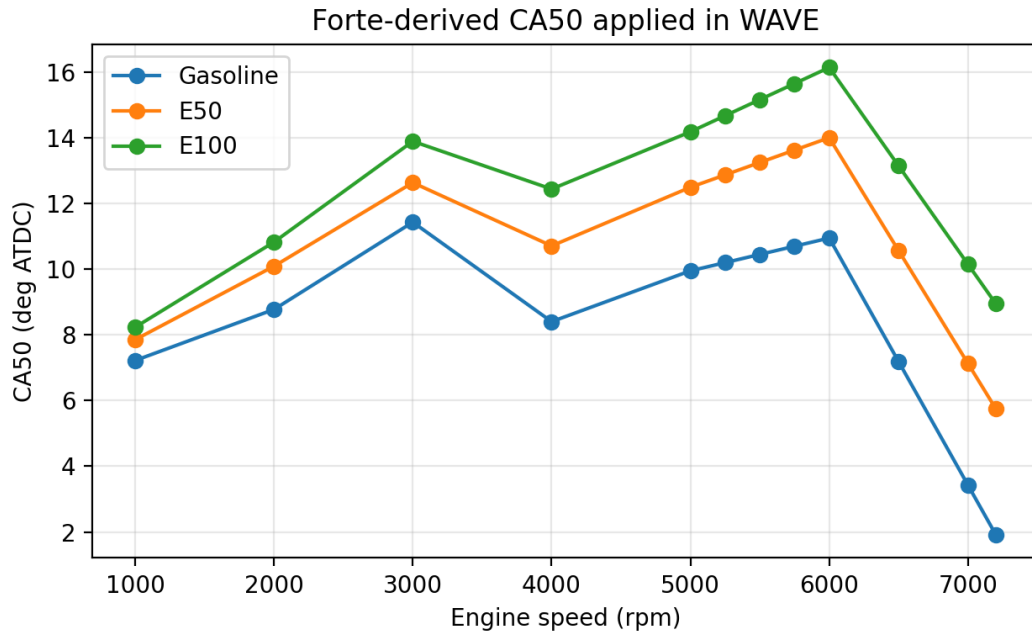


Figure 3. Forte-derived CA50 imposed in the WAVE Wiebe model.

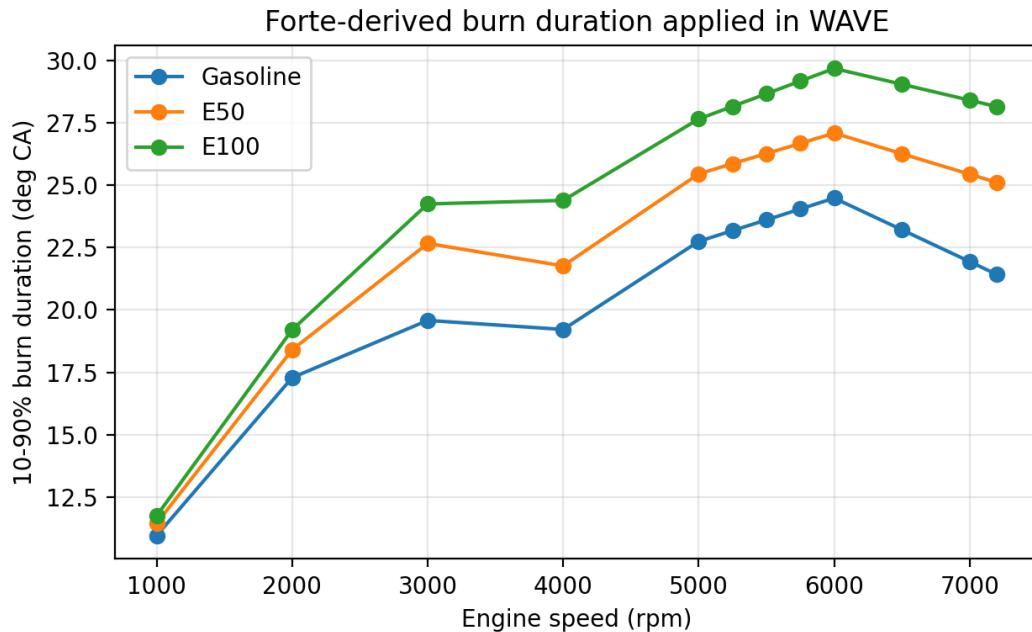


Figure 4. Forte-derived 10-90% burn duration imposed in WAVE.

4.2 Fuel consumption and emissions-related behaviour

BSFC increased with ethanol content because more fuel mass is required to produce the same energy input. This is expected from the lower heating value and lower stoichiometric AFR of ethanol. In regulatory terms this does not automatically mean worse climate impact, because tailpipe CO₂ and lifecycle CO₂ are not the same. Ethanol can reduce fossil-carbon dependence only if produced from genuinely low-carbon feedstocks and certified supply chains. Therefore, the result should be interpreted as a tank-to-wheel performance model, not a full well-to-wheel carbon assessment.

The emissions analysis is limited because the available Forte thermo files did not give usable CO or NO_x data. WAVE HC and exhaust-temperature trends were therefore used as qualitative indicators, not proof of emissions compliance. WAVE NO_x-related outputs were also checked, including engine-out NO_x concentration and brake-specific NO_x, but the reported values remained effectively zero across the speed range. These outputs were not considered physically reliable because the active NO_x formation chemistry could not be validated for the SI Wiebe setup used in this study. A high-confidence Euro 7 assessment would require validated CO, THC, NMHC, NO_x, PN and catalyst light-off modelling.

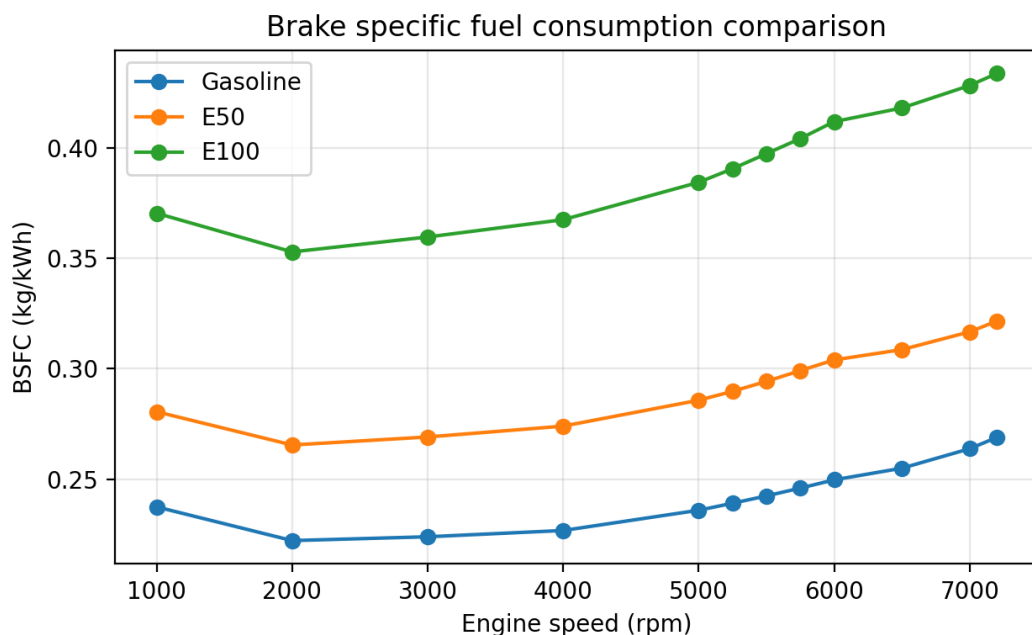


Figure 5. BSFC trend showing the fuel-mass penalty of higher ethanol content.

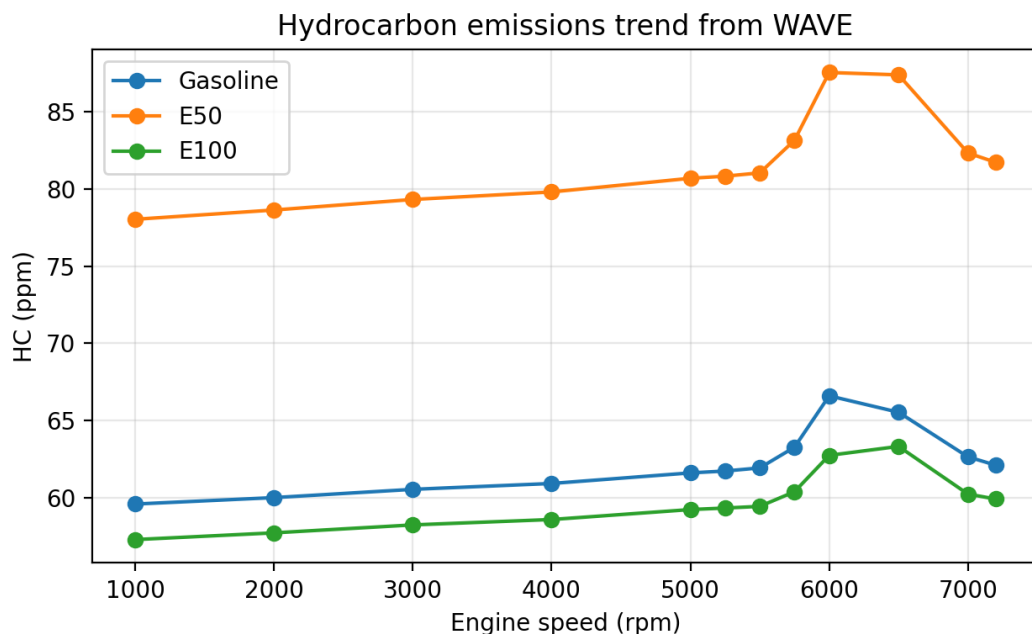


Figure 6. WAVE hydrocarbon trend used as the available emissions indicator.

5 Regulatory relevance, limitations and future work

The results have direct relevance to the new EU and possible UK regulatory direction. Euro 7 is not only concerned with whether a vehicle uses gasoline, ethanol or another fuel; it requires robust pollutant control over a wider durability and compliance framework. At the same time, the EU's proposed post-2035 flexibility for a residual 10% tailpipe emissions allowance, compensated by low-carbon materials or renewable fuels, creates a narrow but meaningful space for highly efficient combustion engines using certified low-carbon fuels. The UK consultation on Euro 7 means similar pollutant requirements may also become relevant for British type approval. Therefore, E50 is only attractive if it preserves drivability while remaining compatible with aftertreatment. This study supports E50 more strongly than E100 because it maintained performance with less calibration penalty.

The main limitations are model fidelity and emissions completeness. WAVE's Wiebe model is a single-zone representation and cannot reproduce local mixture preparation, flame propagation, wall quenching or cycle-to-cycle variation in the same way as a detailed CFD model. The Forte model was used as a closed-cycle combustion support case rather than a complete gas-exchange model, although the additional 7000 and 7200 rpm runs improved confidence in the high-speed WAVE inputs. The E50 fuel file was generated by blending supplied gasoline and ethanol properties, so it should be treated as a representative fuel definition rather than a certified commercial fuel. A further practical limitation is material compatibility. Higher ethanol blends can be more demanding on fuel-system materials because ethanol is hygroscopic and may promote corrosion or seal degradation if unsuitable metals, elastomers or storage conditions are used (Davis, 2017). Therefore, the favourable E50 performance result should not be interpreted as a direct production recommendation without checking ethanol-compatible fuel lines, seals, injectors, pump components and long-term durability. In addition, several WAVE points did not fully converge, although the overall trends remained physically consistent. Future work should optimise spark timing as a speed-dependent map rather than using a uniform CA50 advance, and should activate a full emissions, aftertreatment and durability workflow before making any compliance or production claim.

6 Conclusion

The combined Forte-WAVE workflow produced a technically credible comparison of gasoline, E50 and E100 in a representative Mazda-based 2.0 L SI engine. The strongest result is that E50 preserved gasoline-level performance once fuel-air ratio and Forte-derived combustion phasing were correctly applied. Gasoline reached 110.1 kW and 181.9 Nm, while E50 reached 110.5 kW and 181.5 Nm. E100 remained usable but fell to 106.6 kW and 175.3 Nm because Forte predicted later CA50 and longer burn duration, which reduced effective

expansion work in WAVE. The CA50-advance sensitivity improved E50 to 111.2 kW and 183.1 Nm and improved E100 to 107.6 kW and 177.2 Nm, supporting the conclusion that ethanol operation needs careful speed-dependent ignition phasing rather than only a fuel-file change.

For the assignment proposal, E50 is therefore the preferred fuel specification. It gives most of the potential fossil-gasoline displacement while avoiding the larger calibration penalty seen with E100. The result also connects clearly to future regulation. If the EU moves towards a 90% tailpipe CO₂ reduction framework with a residual allowance linked to e-fuels, biofuels or other low-carbon compensations, and if the UK follows Euro 7-style pollutant control, then combustion engines will only remain credible where low-carbon fuels are combined with strong emissions control. The study also highlights that performance feasibility is not the same as emissions compliance, since quantitative NO_x prediction, aftertreatment modelling and material durability assessment were outside the validated scope of the present work. The modelling here does not prove Euro 7 compliance, but it identifies E50 operation as the most feasible direction for further development, especially if the next stage includes ignition optimisation, catalyst modelling, validated CO, NO_x and particulate outputs, and ethanol-compatible fuel-system durability checks.

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Appendix A. WAVE model layout

Figure A1 shows the WAVE system-level layout used for the Mazda-based 2.0 L inline-four spark-ignition engine. The same engine layout was retained for the gasoline, E50 and E100 cases so that the study isolated fuel definition, fuelling control and combustion phasing rather than geometry changes.

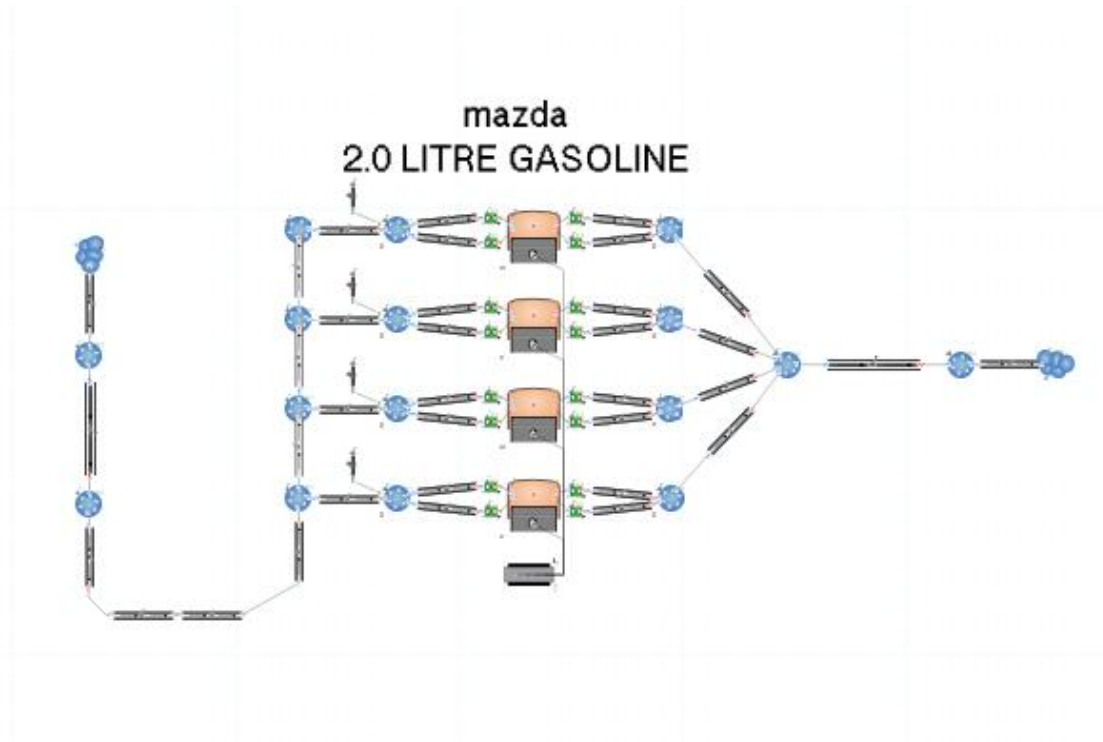


Figure A1. Ricardo WAVE layout of the representative Mazda-based 2.0 L inline-four SI engine model.

Appendix B. WAVE combustion model setup

Figure B1 shows the WAVE SI Wiebe combustion model used to apply the Forte-derived combustion phasing. The THB50 table defines the location of 50% burn point, while the BDUR table defines the 10-90% combustion duration.

Edit

Cylinder: 401

Label

Settings

Usage

Comments

Properties

Location of 50% burn point

Combustion duration

Exponent in Wiebe function

Profile control

Burn fraction at completion

Plot curve

Figure B1. WAVE SI Wiebe combustion settings used for Forte-derived CA50 and burn-duration input.

Appendix C. Forte closed-cycle combustion setup

Figure C1 shows the ANSYS Forte closed-cycle spark-ignition setup used to generate the combustion-phasing data. The spark-ignition model and boundary-motion preview were used to define speed- and fuel-dependent combustion behaviour before transferring CA50 and burn duration to WAVE.

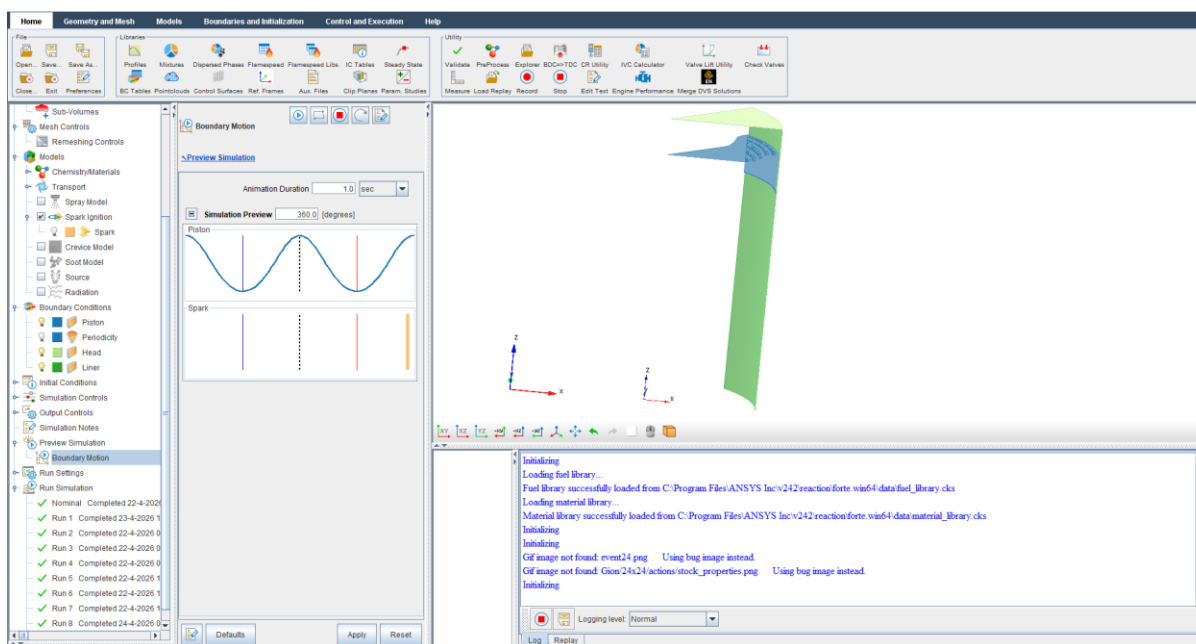


Figure C1. ANSYS Forte closed-cycle spark-ignition setup used to obtain combustion phasing outputs.

Appendix D. Indicative WAVE NOx output check

The WAVE solver output was checked for engine-out NOx values because NOx can be included as an emissions output in WAVE. For the Forte-phased 7000 rpm cases, the solver output reported zero NOx for gasoline, E50 and E100.

Fuel	Speed	WAVE NOx	NOx as NO2	BSNOx	Comment
Gasoline	7000 rpm	0.000 ppm	0.000 g/hr	0.000 g/kWh	WAVE solver output checked
E50	7000 rpm	0.000 ppm	0.000 g/hr	0.000 g/kWh	WAVE solver output checked
E100	7000 rpm	0.000 ppm	0.000 g/hr	0.000 g/kWh	WAVE solver output checked

The zero NOx result confirms that the WAVE emissions section was checked, but no reliable NOx trend between fuels could be established from the available model outputs. These results were therefore not used to support any fuel ranking. NOx was excluded from the main fuel comparison and treated only as a supplementary emissions-output check.