

University of Wales Trinity Saint David

Wales Institute of Science & Art



Prifysgol Cymru
Y Drindod Dewi Sant
University of Wales
Trinity Saint David

CFD and Emissions Modelling

Student name: Aangan Nitinkumar Patel

Student ID number: 2511974

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Abstract

This report evaluates the combined use of Ricardo WAVE and ANSYS Forte for modelling combustion, spray development and emissions-related behaviour in a direct-injection internal combustion engine. The work responds to the requirement to investigate whether advanced liquid fuels and future low-carbon fuel strategies can remain technically feasible for ICE applications beyond 2035. WAVE was used as a fast one-dimensional system-level model to examine cylinder pressure and cycle behaviour, while ANSYS Forte was used to resolve in-cylinder fuel spray, vapour formation, temperature, pressure and heat-release behaviour. The results show that Forte captured the spatial development of fuel vapour mass fraction between -10 and 20 degrees crank angle, including wall impingement, local richness and subsequent mixing. The WAVE model predicted a higher-pressure magnitude than the Forte case, highlighting the influence of calibration and combustion-model assumptions. The main conclusion is that the combined workflow is valuable, but reliable fuel selection for future ICEs requires calibration against pressure data and careful treatment of fuel chemistry, heat transfer, mesh resolution and spray-wall interaction.

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1. Introduction

The role of the internal combustion engine is changing rather than disappearing. Electrification is expanding rapidly, but liquid and gaseous low-carbon fuels remain relevant for applications where energy density, infrastructure, duty cycle or cost make full battery operation difficult. For this reason, simulation tools are useful for investigating whether synthetic, bio-derived and non-carbon fuels can be used in future engines while controlling combustion quality and emissions.

The purpose of this report is to apply to Ricardo WAVE and ANSYS Forte to assess engine combustion behaviour. WAVE provides a rapid one-dimensional thermodynamic model suited to pressure, heat-release and cycle-level comparison. ANSYS Forte provides a higher-fidelity CFD description of spray penetration, evaporation, mixing and chemical heat release. This combination matches the assignment requirement to use both software environments and to judge the model critically rather than only presenting plots.

The study focuses on direct-injection combustion using gasoline-like 95 RON fuel behaviour as the base case. The main outputs are fuel vapour mass fraction, pressure, temperature and heat-release rate. These outputs are used to evaluate mixture preparation, combustion phasing and the limitations of the modelling approach. Direct-injection engines are highly sensitive to injection timing, spray-wall impingement, turbulence, heat transfer and fuel chemistry, so both global and local evidence are required before drawing conclusions about fuel suitability (Heywood, 2018; Zhao, 2010; Reitz and Duraisamy, 2015).

2. Literature and Modelling Rationale

Future ICE development depends on fuels that reduce lifecycle carbon while maintaining combustion stability and acceptable emissions. Bioethanol, methanol, synthetic gasoline and hydrogen-enriched blends are frequently discussed because they can reduce fossil carbon content, improve knock resistance or support renewable production routes. However, each fuel introduces different combustion, storage, safety and infrastructure challenges (Kalghatgi, 2018; Sileghem et al., 2014; Verhelst and Wallner, 2009). For liquid direct-injection engines, the first practical question is whether the fuel evaporates and mixes sufficiently before ignition. Poor mixture preparation produces locally rich zones, wall wetting, unburned hydrocarbons and particulate emissions (Zhao, 2010; Lefebvre and McDonell, 2017).

Two-zone combustion modelling remains useful because it gives a compact description of burned and unburned gas behaviour, pressure rise and apparent heat release (Heywood, 2018; Ferguson and Kirkpatrick, 2015). Its weakness is that it cannot directly resolve spray structures, wall films, flame kernel growth or local mixture stratification. CFD complements this by solving conservation equations for mass, momentum, energy and species transport, which are the governing basis of Forte reacting-flow simulations (ANSYS, 2024a; Versteeg and Malalasekera, 2007). Forte also enables Lagrangian spray parcel modelling, droplet evaporation and spray interaction with chamber boundaries.

The report therefore uses WAVE for cycle-level behaviour and Forte for local mixture formation. This is a deliberate compromise between computational cost and physical detail. A high-quality engineering judgement is not based on one plot alone; it requires comparing global pressure behaviour with local CFD evidence of mixture quality, and then explaining where the models agree, where they diverge and why.

3. Methodology

3.1 Ricardo WAVE model

The WAVE model was used to represent the one-dimensional engine system and produced cylinder pressure behaviour over crank angle. A two-zone combustion representation was adopted because it is computationally efficient and suitable for comparing pressure phasing and heat-release behaviour. The pressure and cycle outputs from WAVE were exported and compared with the Forte post-processing results. In this report, the WAVE output acts as the system-level benchmark rather than a fully independent experimental validation.

The operating speed was set to 2000 rpm, matching the provided 95 RON engine dataset. This speed was selected because it is low enough to make crank-angle-resolved interpretation clear while still representing a realistic light-duty operating point. The WAVE case was used to identify the expected pressure trend and to expose whether the CFD combustion case was under- or over-predicting combustion intensity.

3.2 ANSYS Forte model

The Forte case was built and run as a transient crank-angle simulation. The main CFD output selected for spatial analysis was fuel vapour mass fraction with spray parcel overlay. The chosen crank angles were -10, 0, 10 and 20 degrees CA. This sequence was selected because it captures pre-TDC injection development, mixture formation near TDC and post-TDC spreading. Thermodynamic outputs were exported from the Forte CSV files and used to plot pressure, temperature and chemical heat-release rate.

The combustion chemistry was represented using the ANSYS Model Fuel Library reduced gasoline (iso-octane surrogate) mechanism. This simplified chemistry approach allows efficient simulation of evaporation and heat release, although it was not fully calibrated against measured cylinder pressure data and therefore introduces uncertainty in absolute combustion intensity. The model employed standard Forte post-processing using EnSight visualisation. For consistency, the same camera angle, color scale and fuel vapour legend were maintained across the crank-angle sequence. This is important because changing the color scale between frames can create a false impression of mixture improvement or deterioration. The model setup was selected to balance computational cost with physical fidelity, with particular emphasis on resolving spray development and vapour formation while maintaining consistency with the 1D WAVE cycle simulation.

Table 1 summarizes the engine and simulation setup used for the report. It also shows the assumptions that should be considered when interpreting the results.

Table 1: Engine and simulation model setup

Parameter	Value	Description / justification
Engine type	Single-cylinder, four-stroke SI engine	Representative research model for coupled 1D and CFD analysis.
Bore	86 mm	Taken from engine summary data.

Displacement volume	499.56 cm ³	Confirms an approximately 0.5-liter single cylinder.
Compression ratio	7.37:1	Relatively low value: limits peak compression temperature and pressure.
Engine speed	2000 rpm	Matches the 95 RON reference operating condition used for comparison.
Fuel type	Gasoline, 95 RON model fuel	Consistent with the supplied Bosch/Fox GTDI reference data.
Injection strategy	Direct injection	Required for spray and vapour mass fraction analysis.
Injection timing	Approximately -10 degrees CA BTDC	Based on the CFD visualisation sequence and near-TDC spray development.
Ignition / combustion	Simplified, not fully calibrated	Explains lower Forte pressure and temperature relative to WAVE/reference data.
Turbulence model	RANS k-epsilon type closure	Standard practical Forte approach for engine CFD.
Spray model	Lagrangian parcels with KH-RT type breakup	Appropriate for high-pressure liquid spray representation.
Evaporation / wall interaction	Droplet evaporation and spray-wall impingement enabled	Needed to represent vapour formation and wall wetting risk.
Mesh type	Sector mesh with local refinement	Reduces computational cost while retaining spray-region resolution.
Chemistry model	ANSYS Model Fuel Library reduced mechanism	Computationally efficient chemistry representation.
Outputs exported	Pressure, temperature, HRR, fuel vapour mass fraction	Used for validation, interpretation and emissions-risk discussion.

3.3 Validation and uncertainty approach

Validation was treated as a critical comparison rather than a claim of exact agreement. The pressure trace, temperature trend and heat-release rate were compared qualitatively against WAVE outputs and expected engine combustion behaviour. The model was judged on whether it reproduced correct phasing, sensible trends and physically interpretable spray and vapour development. This is appropriate because CFD predictions in engines are sensitive to mesh, turbulence closure, spray breakup, wall temperature, chemistry mechanism and timestep resolution (Pope, 2000; Versteeg and Malalasekera, 2007).

No full mesh independence study was completed within the available time. This is a limitation, but it is preferable to state it clearly rather than imply false certainty. The numerical results are therefore used mainly to support trend interpretation, model critique and future refinement

4. Results and Discussion

4.1 Fuel vapour formation and spray development

Figure 1 shows the Forte fuel vapour mass fraction and spray parcel evolution from -10 to 20 degrees CA. At -10 degrees CA, liquid spray is visible with vapour concentrated close to the wall-impingement and injector region. At 0 degrees CA, the vapour-rich zone becomes stronger, indicating accelerated evaporation close to TDC where gas temperature and pressure are higher. By 10- and 20-degrees CA, the vapour field spreads further into the chamber, and the gradients become less localised. This progression suggests improved mixture preparation after the initial injection and impingement phase.

The figure is valuable because it reveals physics that a one-dimensional model cannot show. WAVE may predict pressure and heat release, but it cannot identify wall wetting, spray asymmetry or local rich mixture pockets. These local features are critical for emissions because rich zones and wall films promote incomplete combustion and unburned hydrocarbon formation (Zhao, 2010; Lefebvre and McDonell, 2017). The CFD result therefore supports the argument that direct-injection fuel selection must consider evaporation characteristics, not only calorific value.

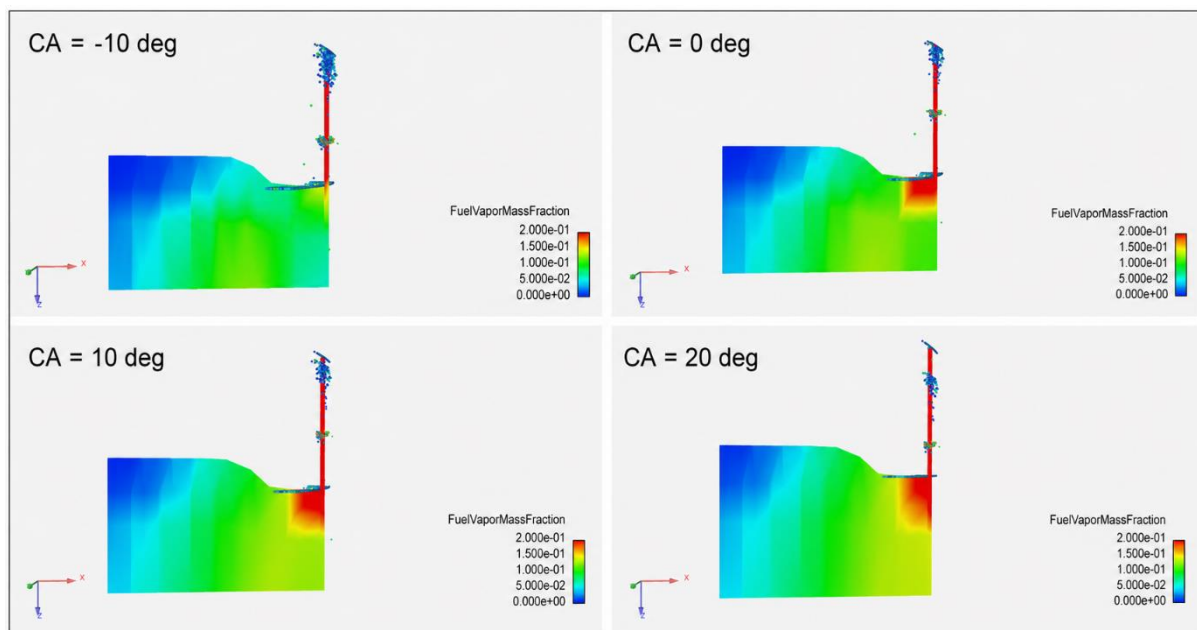


Figure 1: Fuel vapour mass fraction with spray overlay at -10, 0, 10 and 20 degrees CA from ANSYS Forte.

4.2 Forte pressure, temperature and heat-release behaviour

The Forte pressure trace in Figure 2 increases during compression and reaches its maximum close to TDC before reducing during expansion. This trend is physically credible because the pressure rise follows piston compression and heat addition. The peak pressure from the engine summary was approximately 1.40 MPa, which is lower than expected for a strongly combusting SI engine and lower than the WAVE pressure level. This indicates that the CFD

case is either under-releasing chemical energy or using assumptions that reduce combustion intensity.

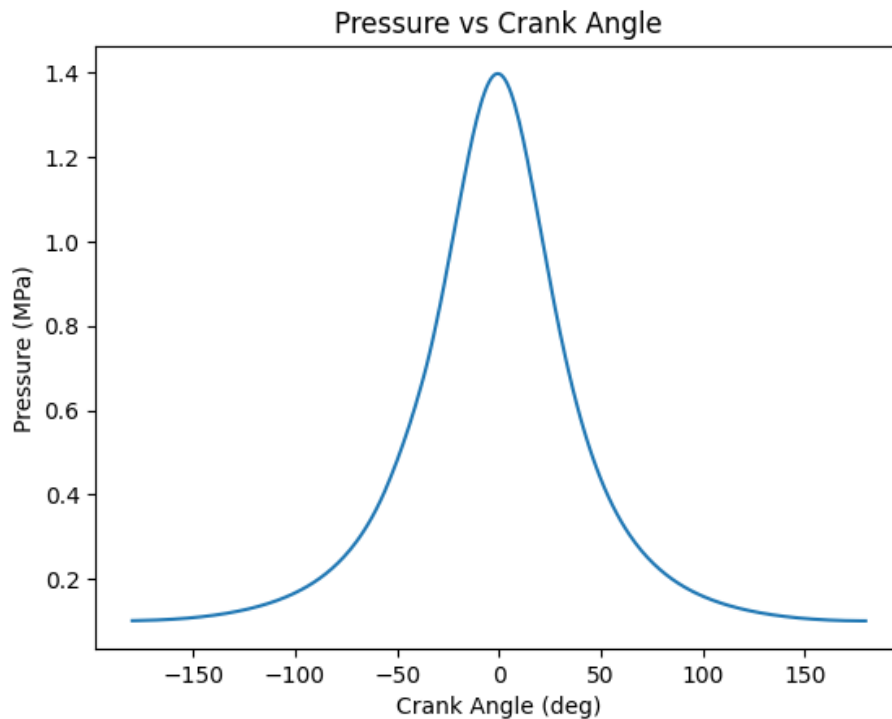


Figure 2: ANSYS Forte cylinder pressure vs crank angle.

The temperature result in Figure 3 follows the same overall combustion-cycle pattern. The temperature increases toward TDC and then decreases during expansion. The reported maximum temperature of approximately 639 K is much lower than normally expected for a fully developed combustion event. This should not be ignored; it is evidence that the case is more representative of spray and mixture formation than a fully calibrated reactive combustion event.

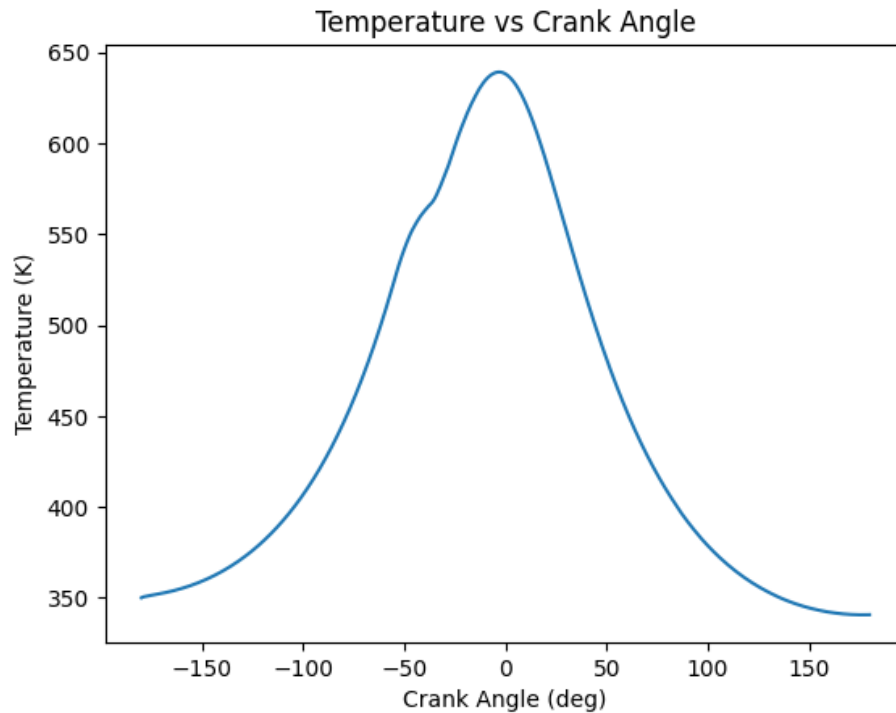


Figure 3: ANSYS Forte averaged cylinder temperature vs crank angle.

The heat-release-rate curve in Figure 4 contains a sharp peak close to TDC. This indicates rapid localised energy release or numerical stiffness in the ignition and chemistry representation. A narrow HRR peak can be produced by limited timestep resolution, overly abrupt combustion onset or simplified chemistry. Therefore, the HRR result is useful for identifying combustion phasing, but it should not be over-interpreted as a fully validated burn-rate prediction.

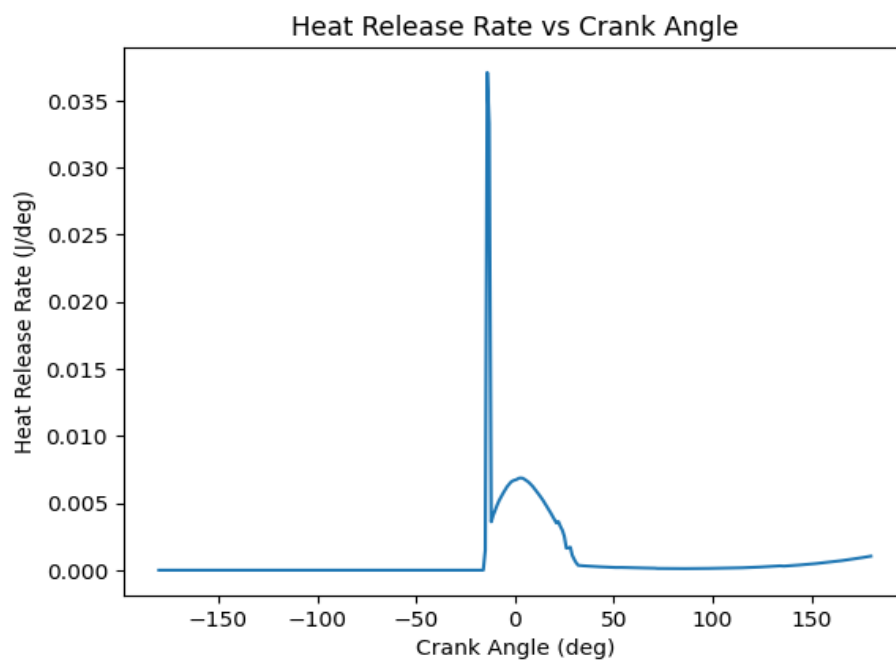


Figure 4: ANSYS Forte chemical heat-release rate vs crank angle.

4.3 WAVE comparison

The WAVE pressure result in Figure 5 predicts a much higher-pressure level than the Forte pressure trace. This is not simply an error; it reflects the different modelling philosophies. WAVE uses a calibrated cycle model and can impose combustion behaviour through heat-release parameters. Forte resolves local spray and thermal processes, but the result depends more strongly on mesh, chemistry, spray and boundary-condition choices.

Figure 6 shows the reference cylinder pressure dataset. Compared with Figure 2, the WAVE and reference pressure traces are closer to a fully combusting engine cycle, while the Forte case appears conservative in combustion intensity. The difference is a useful finding because it identifies the next model-improvement step: the Forte chemistry and combustion setup should be calibrated using cylinder pressure, start of combustion and heat-release rate.

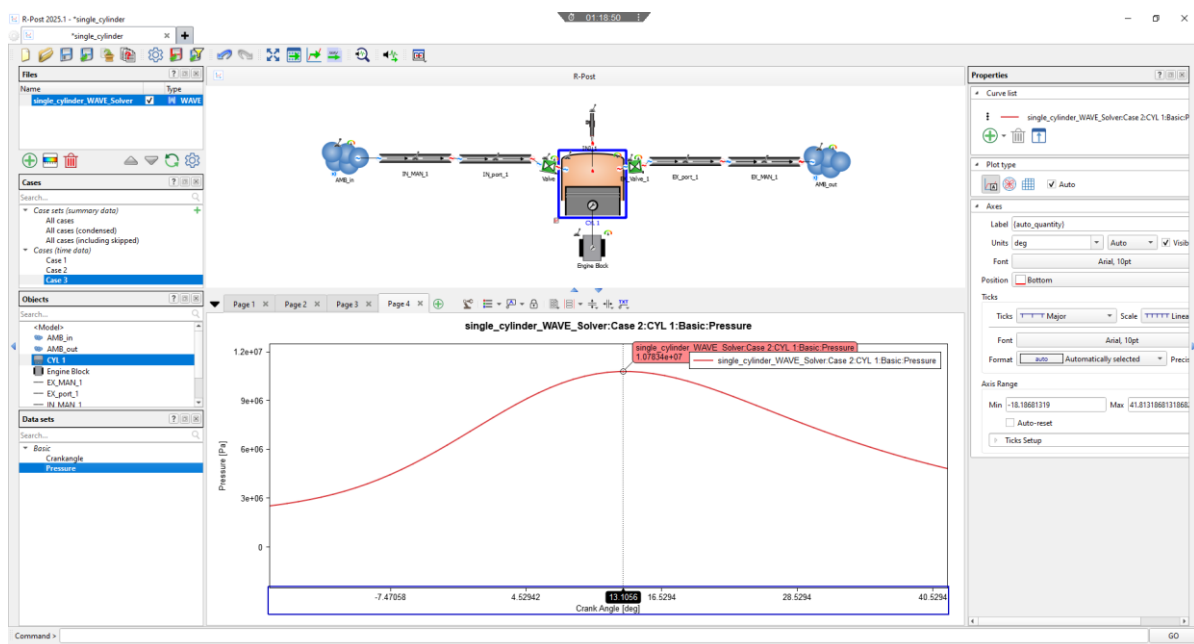


Figure 5: Ricardo WAVE pressure output used in comparison with the Forte case.

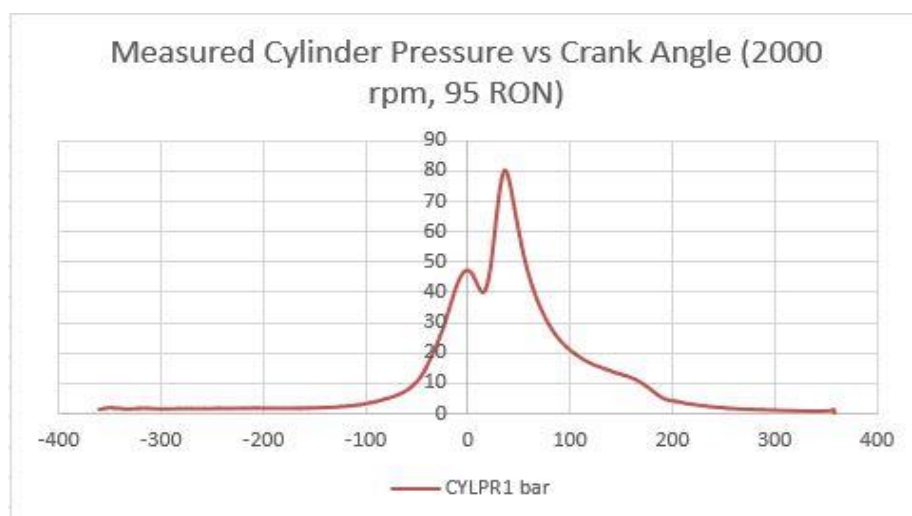


Figure 6: Measured/reference WAVE cylinder pressure trace at 2000 rpm and 95 RON.

4.4 Emissions implications

The emissions values in the Forte summary should be interpreted cautiously. The file reported zero soot, zero NO_x and zero CO at EVO, but a large UHC/VOC quantity. These values are not treated here as fully validated emissions predictions because the pressure and temperature fields were not yet calibrated to the WAVE/reference pressure level. Instead, the emissions discussion is based on risk indicators: local fuel vapour richness, spray-wall impingement and incomplete combustion potential.

NO_x formation is strongly temperature dependent, so an under-predicted temperature field may artificially suppress NO_x. Similarly, a poorly burned or weakly ignited case may exaggerate UHC because fuel remains unoxidized. The CFD plots in Figure 1 therefore provide the most reliable qualitative emissions evidence: wall-adjacent rich vapour and spray impingement are consistent with higher UHC and particulate risk in a real direct-injection engine, unless injection timing, targeting and wall temperature are improved (Glassman, Yetter and Glumac, 2014; Turns, 2013).

5. Critical evaluation and model refinement

The negative indicated work and low combustion efficiency reported in the engine summary were interpreted as diagnostic indicators rather than final performance results. These trends suggest that the Forte simulation is not yet fully calibrated for predictive combustion analysis. Instead, the model is best understood as a controlled CFD study of spray evaporation and mixture formation. This interpretation strengthens the analysis by avoiding overstatement of numerical results and by using discrepancies between WAVE, reference data and CFD predictions to define a clear calibration pathway. This distinction is essential when interpreting CFD results for future fuel feasibility, where both accuracy and model limitations must be considered.

A key strength of the study is the combined use of WAVE and Forte. The WAVE model provides reliable global pressure behaviour, while Forte captures local spray and vapour development. This combined approach reflects practical engine-development methodology, where both thermodynamic performance and mixture preparation are critical.

However, the main limitation is the quantitative gap between WAVE and Forte pressure magnitude, which prevents the CFD results from being considered fully validated. This discrepancy is likely due to simplified chemistry, insufficient combustion calibration, mesh limitations near the spray region, and uncertainties in wall heat-transfer assumptions. In addition, the absence of mesh and timestep sensitivity analysis limits confidence in numerical accuracy. As a result, the findings should be interpreted as qualitatively correct but not yet grid independent.

A further limitation is the presence of a sharp HRR spike, which indicates unrealistic combustion behaviour, as physically accurate heat release should occur over a finite duration.

Future work should focus on staged model refinement, including validation of non-reacting spray behaviour, calibration of ignition timing and heat-release profiles using pressure data, and mesh/timestep sensitivity studies. Once calibrated, emissions indicators such as CO, NO_x and UHC can be assessed with greater confidence.

6. Fuel and 2035 feasibility discussion

The results indicate that direct-injection engines remain technically feasible with suitable fuel selection, but the fuel must support rapid evaporation, stable ignition and low emissions. Gasoline-like fuels are convenient because of volatility and established combustion behaviour, while alcohol fuels can improve knock resistance but may change cold-start and evaporation behaviour. Hydrogen offers zero carbon at the point of use, but storage, pre-ignition and NO_x control remain major barriers (Verhelst and Wallner, 2009). Synthetic fuels could be attractive where existing liquid-fuel infrastructure is valuable, but their climate benefit depends strongly on production pathway and renewable electricity availability (Kalghatgi, 2018).

The Forte vapour results suggest that mixture preparation is a major design constraint. If an alternative fuel produces excessive wall wetting or slow evaporation, it may increase hydrocarbon and particulate emissions even if its lifecycle carbon is favourable. Therefore, future ICE feasibility should be judged using both combustion performance and fuel-production sustainability. A credible 2035 strategy would combine high knock resistance, low lifecycle carbon intensity, calibrated injection targeting, exhaust aftertreatment and robust combustion validation.

Table 2: Comparison of Candidate Future Fuels for ICE Applications

Fuel Type	Category	Key Advantages	Key Limitations
Gasoline (95 RON)	Fossil carbon-based	High energy density, well-established combustion behaviour	High CO ₂ emissions, fossil origin
Ethanol (Biofuel)	Bio-based	Renewable, high octane, reduces net CO ₂	Lower energy density, cold-start issues
Synthetic e-fuel	Synthetic carbon-based	Compatible with existing engines, low lifecycle CO ₂ (if renewable)	High production cost, energy intensive
Hydrogen	Non-carbon fuel	Zero CO ₂ at point of use, fast combustion	Storage challenges, NO _x formation risk

The comparison highlights that while non-carbon fuels such as hydrogen offer zero tailpipe CO₂ emissions, practical implementation challenges remain, whereas synthetic and bio-based fuels provide a more immediate pathway through compatibility with existing engine architectures.

7. Conclusion

This work successfully applied Ricardo WAVE and ANSYS Forte to investigate combustion and spray behaviour in an internal combustion engine model. The Forte results captured physically meaningful fuel vapour development across crank angle, showing local rich regions near injection followed by improved mixing after TDC. The pressure, temperature and HRR plots demonstrated correct cycle trends, although the temperature and pressure magnitudes indicate that the CFD combustion model is not yet fully calibrated.

The comparison with WAVE showed that the system-level model predicts stronger combustion behaviour than the CFD case. This difference is valuable because it identifies where model refinement is needed: chemistry selection, heat-release calibration, spray-wall interaction, mesh sensitivity and timestep control. Overall, the combined WAVE/Forte workflow is appropriate for assessing future ICE fuel strategies, but robust conclusions about 2035-ready fuels require calibrated combustion and emissions validation.

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