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1. Introduction

Research into internal combustion engines (ICE) remains a fundamental research field because the need for cleaner and more efficient power production grows. Stricter emissions regulations and worldwide efforts to become carbon neutral make it an even more challenging task to develop robust numerical models with sound predictions of combustion behaviour and emissions performance when operating on conventional and alternative fuels. This research is regarding the development and implementation of a two-zone combustion model in MATLAB to model the combustion process and emissions of a Ford Gasoline Direct Injection (GDI) engine on alternative non-carbon-based fuel sources as alternative substitutes for gasoline.

A two-zone model of combustion divides the combustion chamber into an unburned gas zone and a burned gas zone and has better ability to predict in-cylinder thermodynamic environment and emissions development compared to one-zone models (Heywood, 1988). If applied using MATLAB, it can simulate how pressure inside the cylinder, temperature, burned mass fraction, and emissions such as NO_x, CO, and UHCs develop. The model will be validated with experimental data from a Ford GDI engine dataset to confirm the accuracy and predictive capability of the model. The model will also be used to extrapolate to verify the feasibility of other non-carbon fuels such as hydrogen and ammonia to investigate their impact on combustion efficiency emission reduction and engine performance.

Two-zone combustion model has been used extensively in ICE research since it is capable of separating burned and unburned gases, thus leading to more accurate heat release and emissions prediction. Two-zone models have also been used by previous studies to effectively apply to spark-ignition (SI) and compression-ignition (CI) engines and proved to be beneficial in the prediction of in-cylinder thermodynamics and pollutant formation (Jafari et al., 2018; Liu & Karim, 1999). The newer developments have included computer programs like MATLAB to increase model accuracy and speed of calculation.(Woschni, 1967; Zhang et al., 2021). The Ford GDI engine database is a suitable real-world application for the model's benchmarking to validate its applicability to subsequent analysis. The GDI engines have enjoyed widespread adoption due to enhanced fuel economy and reduced CO₂ emissions per engine compared to port fuel injection (PFI) engines (Zhao et al., 1999). But they also have negative higher NO_x and particulate matter (PM) emissions levels to achieve which more sophisticated modelling approaches are required to improve performance as well as keep the environmental impact at a low level (Xu et al., 2017).

With the automobile sector shifting its attention towards the use of renewable sources of energy, alternative fuels have continued to be a strong area of focus. Hydrogen and ammonia are specifically of high-potential non-carbon fuel sources that can reduce CO₂ emissions by a large amount but remain highly efficient. Hydrogen, for instance, has been studied extensively for application in SI engines with its fast-burning rate and carbon-free zero-emission characteristics (Verhelst & Wallner, 2009). Ammonia, though a weaker combustion quality agent, has also been proposed as a prospective contender for use in internal combustion engines when implemented within dual-fuel systems or combined with combustion promoters (Kumar & Yang, 2021). Their combustion characteristics, however, along with their emissions properties and future scope in GDI engines still needs to be examined. With the addition of these fuels to the two-zone MATLAB model, this research aims at their place as a prospective substitute for fossil fuel-based fuels. The study fits into sustainability objectives and international strategies for emission reduction, opening doors to the new generation of low-emission engine technology.

2. Industrial relevance

2.1 Understanding the Two-Zone Combustion Model and Its Importance

The two-zone combustion model is a crucial framework for analysing combustion in internal combustion engines (ICEs), dividing the cylinder into a burned zone and an unburned zone separated by a flame front, as seen in figure 1. This model helps engineers simulate and optimise engine performance, emissions, and efficiency, especially when using alternative fuels like hydrogen, ammonia, and synthetic e-fuels. By adjusting the model for each fuel's unique properties (flame speed, ignition characteristics, and air-fuel ratio), combustion can be fine-tuned before physical testing, offering insights into performance and emissions behaviour.

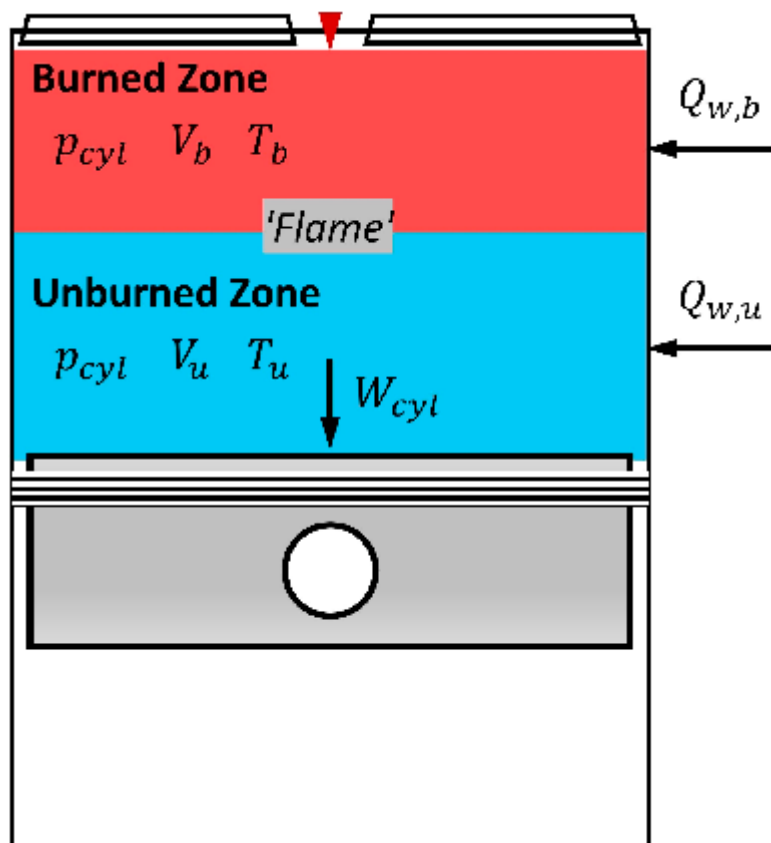


Figure 1 - Two zone combustion (Wang, Y. 2020)

In the two-zone model, the unburned zone contains the fuel/air mixture, while the burned zone contains combustion products. Both zones share the same pressure but have distinct volumes and temperatures. The model assumes uniform conditions within each zone, with no heat or mass transfer across the flame front. This approach allows engineers to predict the evolution of pressure, temperature, and burn fraction during the combustion cycle. The high temperature in the burned zone contributes to NO_x formation, while the unburned zone affects knocking and unburned hydrocarbon emissions. Despite simplifications, this model is highly useful for predicting combustion efficiency and pollutant formation, especially in simulations with varying fuels and engine conditions.

When applying the two-zone model to alternative fuels, key factors such as flame speed, fuel reactivity, and the air-fuel ratio are adjusted to reflect each fuel's unique combustion characteristics.

2.2 Hydrogen Properties

Hydrogen has a high flame speed (2.5–3.0 m/s), much faster than gasoline, leading to a rapid rise in the burned-zone mass fraction and a quicker heat release. Hydrogen's ability to sustain lean mixtures (from stoichiometric to extremely lean) also means the unburned zone is cooler, suppressing NO_x formation. However, hydrogen's low ignition energy and small quenching distance can lead to pre-ignition or backfire, requiring careful adjustment of ignition timing in the two-zone model. The model can also be used to optimise the combustion process by running lean to minimise NO_x emissions, which are controlled through aftertreatment systems.

2.3 Ammonia Properties

Ammonia has a low flame speed (~0.06–0.07 m/s), which makes its combustion slower and more gradual than hydrogen. The two-zone model can accommodate this slow burn by simulating a gradual growth in the burned-zone fraction. However, ammonia's high ignition energy (380–680 MJ) and poor flammability in spark-ignition mode make it difficult to ignite, requiring careful management of ignition timing and possibly the use of pilot fuels (like hydrogen or diesel) to accelerate combustion. The model can predict and optimise combustion parameters to reduce ammonia slip (Pearsall, T. C. Garabedian 1967) and minimise NO_x emissions, which can be further treated with catalytic systems.

2.4 Other alternatives fuels

e-Fuels, such as synthetic methane, methanol, and oxymethylene ethers (OMEs), are designed as drop-in replacements for conventional fuels. These fuels often allow for cleaner combustion due to their uniform composition and higher oxygen content, which reduces particulate

formation and NOx emissions. The two-zone model can be used to simulate their combustion behaviour, which is typically like traditional hydrocarbon fuels but with improvements in efficiency and lower emissions. The model can predict how e-fuels burn at different flame speeds, how they affect engine knock, and how their composition influences emissions.

2.5 Vehicles already using alternative fuels

Hydrogen-fuelled engines, such as those in Toyota's hydrogen-powered Corolla and BMW's Hydrogen 7 car, use two-zone modelling to predict cylinder pressures and optimise NOx emissions by running on lean mixtures. Porsche has also adopted e-fuels in their Supercup race cars (Porsche, 2024), finding improved emissions and performance, guided by combustion models.

3. Alternative to ICE and the challenges

The United Kingdom is committed to achieving net-zero greenhouse gas emissions by 2050, with a central component of this strategy being the transition to zero-emission vehicles (ZEVs) by 2035. The government plans to phase out the sale of new petrol and diesel cars by 2035, with a target of 22% of new car sales being ZEVs by 2024, rising to 80% by 2030 (Browne & Department for Transport, 2024). This ambitious policy includes ZEVs mandate requiring automakers to meet progressively higher ZEV sales quotas (commonslibrary.parliament.uk, 2024). While these policies aim to accelerate the adoption of electric vehicles (EVs), several critical challenges remain, including infrastructure limitations, energy supply concerns, and the environmental impact of battery production.

One of the most significant barriers to EV adoption is the need for substantial investment in charging infrastructure, particularly in rural and underserved areas. The UK's existing electrical grid may struggle to meet the increased demand for electricity driven by EV charging, and reliance on intermittent renewable energy sources like solar and wind raises concerns about grid stability (Browne & Department for Transport, 2024). The current electrical grid faces risks of instability, especially as EV adoption grows. For instance, each fully electric vehicle (FEV) typically requires between 40-60 kWh of battery capacity (Browne & Department for Transport, 2024), which could place additional strain on the network, particularly if the number of electric vehicles continues to rise in both private and commercial sectors, including heavy industries and freight transport.

In response to these challenges, the UK government has implemented several policies aimed at supporting EV adoption. The Plug-in Car Grant and the Electric Vehicle Home Charge Scheme provide financial support to consumers purchasing EVs and installing home charging points, helping to make EVs more affordable and accessible (Office for Zero Emission Vehicles, 2020). These incentives have led to a steady increase in EV sales, with battery electric vehicles (BEVs) representing 19.6% of the new car market in 2024 (S&P Global, 2024). Furthermore, there has been a shift toward lighter, more efficient battery packs to reduce costs and improve vehicle performance (ICCT, 2024).

However, concerns about the environmental impact of EV battery production continue to grow. The extraction of materials such as lithium, cobalt, and nickel, which are crucial for EV batteries, has significant environmental and geopolitical implications. Moreover, the recycling of lithium-ion batteries remains inefficient, which presents a major sustainability challenge (ICCT, 2024). Lifecycle emissions associated with the production of larger batteries, which are often used to improve vehicle range, can also be higher, undermining the environmental

benefits of BEVs. The increase in battery size leads to greater energy consumption and a reduction in overall vehicle efficiency, as larger batteries also add weight, further complicating efforts to reduce emissions in the transport sector (ICCT, 2024). Based on data from

While BEVs generally have lower operational costs, their higher upfront price compared to internal combustion engine (ICE) vehicles remains a significant economic barrier, even with government subsidies (National Grid, 2019). The break-even point for BEVs, in terms of total cost of ownership, depends on various factors such as battery longevity, charging rates, and electricity costs. Additionally, retrofitting existing ICE vehicles with alternative fuel capabilities, such as hydrogen or ammonia, may provide a more cost-effective solution, bypassing the need for large-scale infrastructure investments in charging networks (Wolfram & Lutsey, 2023).

Range anxiety is an issue faced by manufacturers and the government. Customers are wanting ranges similar to that of an ICE vehicle as suggested by the top 10 selling electric vehicles in the UK, as seen in figure 2.

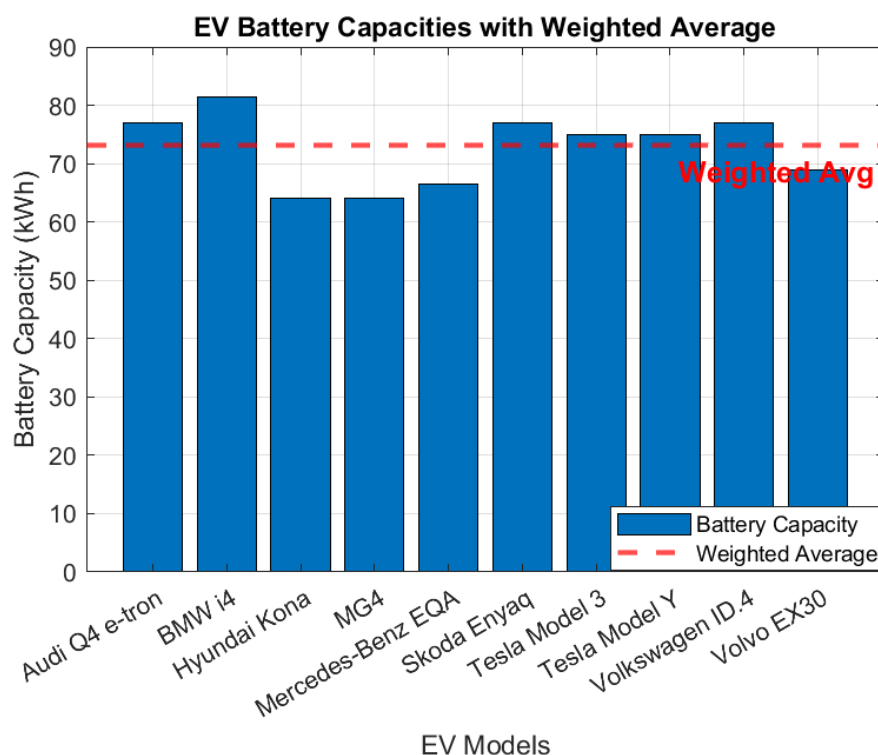


Figure 2 Weighted average battery capacity of UK EVs (2024). Data compiled from Electrifying.com (2024), Tesla (2024), Audi (2024), BMW (2024), MG (2024), Mercedes-Benz (2024), Škoda (2024), Hyundai (2024), Volvo (2024), and Volkswagen (2024)

4. Literature Review

Ammonia (NH_3) is becoming popular as a viable carbon-free fuel and hydrogen carrier for combustion processes from power production to transport. Nevertheless, ammonia is challenged with issues of engine or gas turbine utilization due to its low flame speed, high ignition energy, and potential creation of nitrogen oxides (NO_x) upon combustion. To overcome such, detailed understanding of ammonia combustion chemistry is important. The paper reviewed herein, "The combustion chemistry of ammonia and ammonia/hydrogen mixtures: A comprehensive chemical kinetic modelling study" by Yuxiang Zhu et al. (2024), seeks to develop and verify a detailed chemical kinetic model of ammonia and hydrogen/ammonia fuel mixtures. Here, we introduce the primary objectives and accomplishments of Zhu et al. (2024), address the significance of their findings to two-zone combustion modelling, place their two-zone approach (implicitly or explicitly) into context with other combustion models, and discuss the significance of their findings to combustion engineering. We also highlight any weaknesses of the research and the ways in which future research is perceived to be progressing by the authors.

4.1 Objectives and contributions of the paper

Zhu et al. (2024) set out to derive a comprehensive chemical kinetic mechanism for ammonia combustion, including ammonia-hydrogen blends, and to validate the mechanism against an extensive set of experimental data. The principal objectives were: (1) to update and extend existing ammonia reaction mechanisms with recent theoretical and experimental insight, (2) to verify the mechanism with new ignition and combustion data for NH_3/H_2 mixtures, and (3) to improve prediction of significant combustion characteristics (ignition delay times, flame speeds, and NO_x formation) for engine and gas turbine of interest conditions. This study is founded on previously developed kinetic models in the literature and incorporates significant improvements to accurately model the combustion characteristics of ammonia–hydrogen blends. For example, earlier mechanisms such as Singh et al. (2021) were focused on ammonia autoignition at specific conditions; Zhu et al. extend this by evaluating a broader temperature and pressure range and including hydrogen blending effects (Konnov, 2019; Kumar & Yang, 2021).

Among the key contributions of the paper are the development of a detailed reaction mechanism with novel rate constants for ammonia chemistry, founded on present quantum chemistry calculations and experiments. The mechanism encompasses low-, intermediate-, and high-temperature reaction pathways of ammonia, considering production and consumption of

intermediate species like NH_2 , NH , N_2H_4 , NO , and N_2O (Glarborg, 2018). Zhu et al. (2024) assembled data from shock tube experiments, flow reactors, and laminar flame speed measurements to test the accuracy of the model. For instance, ignition delay times measured in high-pressure shock tubes (5–30 bar, 1500–1900 K) for ammonia and NH_3/H_2 mixtures, and flame speeds and extinction limits in burner experiments, were used to test the mechanism across regimes (Okafor et al., 2018). By reproducing excellent agreement with these diverse datasets, the authors demonstrated their mechanism can reliably reproduce the reactivity of ammonia-containing fuel mixtures globally under a wide range of conditions. In the low-temperature high-pressure regime (applicable to motor engines), the model provides valuable insight into ignition propensity and NO_x formation mechanisms, which had previously been uncertain for ammonia fuels. In general, the contributions of the work are to report one of the most advanced and validated kinetic models for ammonia combustion that has been developed to date and an investigation of controlling reaction channels in ammonia/hydrogen flame chemistry.

Though Zhu et al. (2024) focus primarily on chemical kinetics, their findings have immediate consequences for two-zone combustion models of extensive use in engine simulations (Jafari et al., 2018). Two-zone combustion model divides the combustion chamber into an unburned zone (fresh fuel/air mixture) and a burned zone (products of combustion) to simulate flame propagation and heat release in internal combustion engines (Liu & Karim, 1999; Guzzella & Onder, 2010). They are based on utilizing the evolution of chamber pressure for inferring unmeasurable burn rates and other thermodynamic quantities (Hvězda, 2012; Jia et al., 2007). The Zhu et al.'s kinetic level of detail is embeddable in two-zone models in many ways:

Ignition Delay and Combustion Phasing: The model proposed by Zhu et al. (2024) is able to accurately predict ignition delay times for ammonia and NH_3/H_2 mixtures under various conditions. Two-zone engine models generally require input for ignition timing or delay in order to make premixed combustion calculations (Shapiro & Van Gerpen, 1989; Hall et al., 2012). With its provision of experimentally verified ignition delay data for a variety of fuel blends and conditions, the research enables more realistic prediction of the engine ignition timing under operation on ammonia or ammonia–hydrogen fuels. For instance, hydrogen addition (30% or 20% by volume in ammonia) is shown to lead to significant reduction of ignition delay and enhancement of mixture reactivity, which can be interpreted through a two-zone model when simulating an engine cycle (Ryu et al., 2014).

Burning Rate and Heat Release: Two-zone models typically need the laminar burning rate or burning velocity of the fuel to predict the rate at which the unburnt zone is consumed and

converted into burned products (Goodwin et al., 2017; Pitsch, 2006). Zhu et al.'s (2024) chemical kinetic model may also be used with simulation codes (e.g., Cantera) to predict NH_3/H_2 mixture laminar flame speeds at engine-like pressures and temperatures (Frigo & Gentili, 2013). The flame speeds can then be used to guide two-zone models through more accurate burn rates. Compared to ammonia, the flame velocities of ammonia–hydrogen blends are higher (hydrogen addition compensates for the slow burning of ammonia), and the model gives a quantification of this effect (Reiter & Kong, 2008). Adding such data allows a two-zone model to predict the augmented heat release rate with hydrogen addition and influence engine performance calculations (e.g., shorter combustion time and possibly increased peak pressure) (Turns, 2012).

Temperature and NO_x in Burned Zone: The complicated process traces the formation of NO_x (NO , NO_2) through a number of channels, among which is the thermal NO route and fuel-bound nitrogen pathways ($\text{NH} \rightarrow \text{N} \rightarrow \text{NO}$) (Westbrook & Dryer, 1981). Calculation of post-combustion NO_x in the burned zone is often included in two-zone models. With Zhu et al.'s (2024) mechanism, one can embed a NO_x formation sub-model into the two-zone framework, using the reaction rates for ammonia combustion chemistry validated (Verhelst & Sheppard, 2009).

Heat Release and Thermodynamic Properties: The two-zone model assumes that every zone is thermodynamically homogeneous. The detailed mechanism provides accurate thermodynamic data (specific heats, flame temperatures, etc.) for the burned gas resulting from ammonia/hydrogen combustion. Zhu et al.'s work, by correlating experimental pressure histories (via ignition delay and constant-volume reactor simulations), ensures that the energy release from the fuel is accurately described. In a two-zone model, this results in better estimates of the pressure rise and temperature in the burned zone as combustion progresses. I.e., tuning the two-zone model using the detailed kinetics can help guarantee that the prediction of cylinder pressure (and hence engine power and efficiency) for the model agrees with that which would be predicted by detailed chemistry under the same conditions.

It is also noteworthy that the paper itself does not explicitly model a two-zone engine model, but rather provides the fundamental kinetic data and insight which can be utilized in such models. The authors are engine combustion modelling practitioners (co-author Kelly Senecal is renowned for engine CFD), implying an intent to make the mechanism available in engine simulations. Briefly, the two-zone model is improved by Zhu et al.'s work through the better chemical foundation: the model is capable of using validated global reaction parameters

(ignition delay, burn rates, flame temperature) derived from detailed chemistry instead of empirical correlations only.

5. Methodology

The two-zone combustion modelling method involves splitting the combustion chamber into two sections, the burned and unburned zones. Unburned zone properties can be calculated and then used to calculate the burned zone parts. The following pages in this section will include calculations that will construct and calculate properties used to calculate the NO_x formation. Volumes and temperatures are the key components with temperature being especially important due to NO_x formation increasing exponentially with an increase in temperature (United States Environmental Protection Agency n.d). Applications such as Sage, Ansys ICE FORTE (Ansys-forte n.d), GT-POWER and Simcentre STAR-CCM+ (Papakostas, A.P. 2024), all have ability to model combustion cylinder conditions using a quasi-dimensional model. However, the time taken and resources required make these unsuitable options for this project.

MATLAB stands out for its flexibility, rapid prototyping capabilities, and ease of integration, making it superior for initial simulations and prototyping in combustion modelling compared to other software packages (Abbass, 2023). Its user-friendly environment, comprehensive libraries, and powerful visualisation tools allow researchers and engineers to quickly test and refine models, facilitating the exploration of various configurations and assumptions (Cisneros & Rojas, 2024). This approach is exemplified in studies where MATLAB has been utilised to model engine performance and combustion processes, highlighting its effectiveness in early-stage research and development (Yoon, 2022).

Within MATLAB, the two-zone combustion model will be developed by using crank angle, cylinder pressure, and fuel mass as the base components. The experimental data for those will be retrieved from PDFs from Ford for the 1.0L 3-cylinder EcoBoost engine. The start of combustion (SoC) and end of combustion (EoC) can be found from calculating the pressure added from combustion, which can be determined by the change in pressure per degree going positive and remaining positive, building towards 3-4 bar of pressure change per degree of crankshaft rotation (Blair, 2004). Knock can be indicated as knocking combustion can achieve 10-20 bar per degree of crankshaft rotation in severe cases (Meyer et al., 2012; Spencer & Roberts, 2009).

The whole project is based on the fundamentals of thermodynamics. The first law (Energy conservation) is used to determine the temperature, pressure and work done in each zone. The second law (Entropy & irreversibility) ensures that combustion efficiency and tracks entropy generation. Chemical equilibrium and reaction kinetics are used to model the burned zone species and heat release. Ideal gas law and state equations govern pressure and temperature relations in both zones. Mass conservation tracks fuel-air mixture evolution and mass burned.

The full list of equations that will be used for the two-zone combustion model, from start to beginning can be seen in Appendix B if more detailed information is required on the calculations.

6. Results collection & analysis

The key combustion parameters such as ignition delay (ID), burn duration, and heat release rate (HRR) provide information about the combustion characteristics of different fuels. Ignition delay, which is the time interval between the start of fuel injection and the initiation of combustion, is a function of fuel chemistry, octane number (for spark ignition), and in-cylinder conditions (Heywood, 2018). Ignition delay will also be ascertained and examined since a difference in these characteristics may potentially require modification of injection timing (Lapuerta et al., 2008). Similarly, burn duration and HRR affect engine efficiency and knocking tendencies. Fuels with a higher laminar flame speed, such as hydrogen, experience a higher combustion rate, leading to higher pressure rise rates, which can increase the engine knock tendency if not well controlled (Verhelst & Wallner, 2009). The cylinder pressure profile and mean gas temperature also provide data on the efficiency of how a fuel burns, with biofuels having a lower peak pressure due to their lower energy density (Hossain & Davies, 2013).

Fuels differ significantly in terms of equivalence ratio (Φ), flame speed, and laminar burning velocity, which influence the combustion process. The equivalence ratio influences the mixture strength and overall energy release, with alternative fuels often requiring different air-fuel ratios compared to gasoline. For instance, methanol also has a much lower stoichiometric air-fuel ratio of about 6.5:1 (Szabo, J. 2018) than gasoline at around 14.7:1 (Speight, J.G. 2011), enabling richer mixtures and lower combustion temperatures, which can help suppress knock (Stone, R 2012). Flame speed is another important parameter since fuels such as hydrogen have a much higher burning velocity than gasoline (Dong, C. et al. 2010), allowing for more effective combustion but with a higher pre-ignition risk (Verhelst et al., 2011). It is crucial to understand these properties to be able to optimise the ignition timing for stable combustion.

From the performance perspective, the parameters such as brake-specific fuel consumption (BSFC), indicated mean effective pressure (IMEP), and brake mean effective pressure (BMEP) provide useful information. Since alternative fuels have lower energy density than gasoline, BSFC is higher for fuels like ethanol and methanol, i.e., more fuel must be consumed to achieve the same power output (Kumar et al., 2013). However, gaseous fuels like compressed natural gas (CNG) have the tendency to have lower BSFC due to the higher-octane rating and lean-burn operation efficiency (Stone, 2012). Peak power and torque are also important since some alternative fuels have the tendency to limit power due to decreased volumetric efficiency or reduced flame speed (Turner, J. et al., 2011). In addition, exhaust gas temperature (EGT) can affect the performance of aftertreatment systems, with some fuels requiring special catalytic converters to handle different emissions profiles (Sharma & Soni, 2020).

One of the simplest distinctions between gasoline and alternative fuels is their energy density, which directly impacts engine design and efficiency. Alternative fuels such as ethanol and methanol have lower energy densities than gasoline, meaning that for the same volume of fuel, less energy is available for combustion (Balat & Balat, 2009). However, their higher-octane numbers allow higher compression ratios to be employed, which can increase thermal efficiency (Turner et al., 2011). Additionally, high latent heat of vaporisation fuels, such as ethanol, provide charge cooling benefits, reducing knock tendency and allowing volumetric efficiency to be improved (Stone, 2012). However, it also has the effect of cold-start performance becoming a problem, requiring additional fuel enrichment measures (Demirbas A, 2007).

The overall analysis will be done in MATLAB, directly comparing the above crucial points with a critical analysis being done, potentially independent variables will affect usefulness of the alternative fuels differently than all the variables put together.

7. Project Planning

Figure 3 Gantt chart is a graphical representation of the project activities, specifying when each task is scheduled to start and end. It is a valuable tool for tracking progress, providing a clear indication of whether the project is ahead or behind schedule. It also allows time modification of completed work, work in progress, and outstanding work. This flexibility ensures successful project management by allowing real-time updating and optimal resource utilisation.

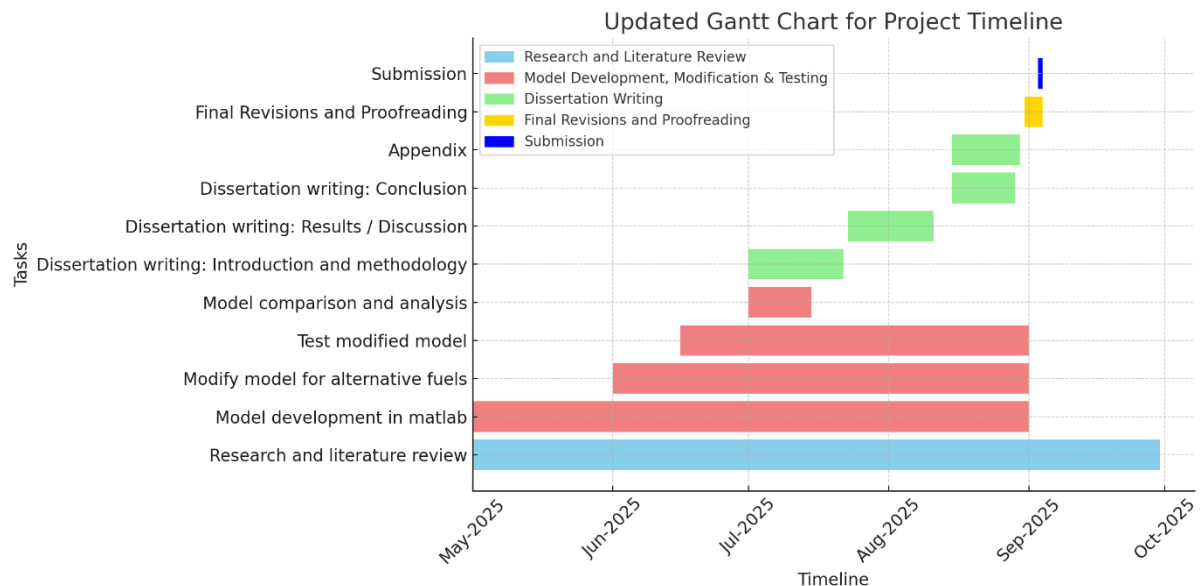


Figure 3 - Gantt chart project plan

8. Evaluation

This project proposal has outlined the development and implementation of a two-zone combustion model to analyse internal combustion engine (ICE) performance with conventional and alternative fuels. With increasing regulatory pressures and a global shift toward sustainable energy sources, the study aims to contribute to the optimization of ICEs by incorporating alternative non-carbon-based fuels such as hydrogen and ammonia. The research emphasizes the necessity of advanced modelling techniques to improve the accuracy of combustion simulations and emissions predictions (Heywood, 2018; Verhelst & Wallner, 2009). The industrial relevance of the project has been established through a detailed examination of current automotive trends and the challenges associated with transitioning away from fossil fuels (Kumar & Yang, 2021).

Literature review supports the application of a two-zone combustion model by demonstrating its ability to estimate thermodynamic conditions and emissions (Jafari et al., 2018; Liu & Karim, 1999). Moreover, the methodology section has set an initial foundation for developing and verifying the MATLAB-based model from experimental data of a Ford Gasoline Direct Injection (GDI) engine (Zhao et al., 1999). Despite the strengths of this research, several challenges and limitations are present.

The challenge of accurately modelling substitute fuels, the lack of experimental verification from real-world use, and the uncertainties of emissions behaviour need to be appropriately addressed. Furthermore, while the proposed timeline introduces structure, unforeseen technical problems may necessitate project planning revisions (Wolfram & Lutsey, 2023). In the long term, this study contributes to the overall efforts at reducing emissions and increasing engine efficiency. With the application of computational modelling, it seeks to supplement the theoretical combustion analysis by filling the gap towards experimental engine use. More improvement of the model, additional experimental verification, and investigation of other alternative fuels should be the areas of research in the future (Senecal, 2021; Zhu et al., 2024).

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Appendix A

Rank	Model	Units Sold	Battery Capacity (kWh)
1	Tesla Model Y	32,862	75
2	Audi Q4 e-tron	17,622	77
3	Tesla Model 3	17,425	75
4	MG4	15,651	64
5	BMW i4	12,953	81.5
6	Mercedes-Benz EQA	11,617	66.5
7	Skoda Enyaq	11,516	77
8	Hyundai Kona	10,858	64
9	Volvo EX30	9,931	69
10	Volkswagen ID.4	8,927	77

Appendix A Top 10 BEVs sales and Battery Capacities Data compiled from Electrifying.com (2024), Tesla (2024), Audi (2024), BMW (2024), MG (2024), Mercedes-Benz (2024), Škoda (2024), Hyundai (2024), Volvo (2024), and Volkswagen (2024).

Appendix B

Change in pressure Formula

$$\Delta P = P_2 - P_1 \cdot \left(\frac{V_1}{V_2}\right)^n$$

$$\text{Extra pressure from combustion} = \sum P_{soc \rightarrow eoc}$$

$$\text{MassFractionBurn} = \frac{\sum_{soc}^{eoc} \Delta P}{\sum P_{soc \rightarrow eoc}}$$

Calculating Fuel per cycle from kg/hr given in data:

$$\frac{n_{cylinder}}{\text{working strokes}}$$

$$\frac{3}{2} = 1.5$$

$$\div (60 \cdot RPM \cdot 1.5)$$

$$\frac{kg}{hour} \rightarrow \frac{kg}{cycle}$$

$$AFR = \frac{\text{Air mass}}{\text{Fuel mass}}$$

$$\lambda = \frac{AFR_{Actual}}{AFR_{Stoichiometric}}$$

$$\phi = \frac{1}{\lambda}$$

$$\text{Air Fuel mass ratio} = \frac{\text{Stoichiometric mass ratio} \cdot \text{Molecular mass of air}}{\text{Molecular mass of fuel}}$$

Ideal gas law

$$PV = RT$$

Gas constant calculation

$$R_i = R_u / m_i [=] J/kg \cdot K$$

First law of thermodynamics

$$\Delta U = Q - W$$

Zeroth Law

$$\bar{E} = E(N, V, T)$$

Arrhenius function

$$k = A \exp^{\frac{-E_a}{R_u T}}$$

Thermal efficiency

$$\eta_{otto} = 1 - \frac{1}{(V_1/V_2)^{\gamma-1}} = 1 - \frac{1}{cr^{\gamma-1}}$$

Polytropic index

$$n = \frac{-\Delta \log p}{\Delta \log V}$$

Heat release rate

$$HRR = \Delta H_c \cdot \dot{m}_f$$

Specific heats

$$\frac{\tilde{C}_{p,i}}{\tilde{R}} = a_{i1} + a_{21}T + a_{31}T^2 + a_{41}T^3 + a_{51}T^4$$

Fuel specific heat constant volume

$$\tilde{C}_p = 4.184(a_1 + a_2\theta + a_3\theta^2 + a_4\theta^3 + a_5\theta^{-2})$$

Average specific heat constant pressure

$$\tilde{C}_{p_{avg}} = \frac{\phi \tilde{C}_{p_{fuel}} + 12 \frac{1}{2} (\tilde{C}_{p_{O_2}} + 3.76 \tilde{C}_{p_{N_2}})}{\left(\phi + 12 \frac{1}{2} (4.76) \right)}$$

Average specific heat constant volume

$$\tilde{C}_{v_{avg}} = \tilde{C}_{p_{avg}} - 8314$$

Gamma

$$\gamma = \frac{\tilde{C}_{p_{avg}}}{\tilde{C}_{v_{avg}}}$$

$$Molecular\ mass = \frac{((\phi \cdot m_{C_8H_{18}}) + 12 \frac{1}{2} (m_{O_2} + (3.76 \cdot m_{N_2})))}{\left(\phi \cdot \left(12 \frac{1}{2} \cdot 4.76 \right) \right)}$$

Burned gas constant

$$R_b = \frac{R_u}{Mass\ burned}$$

Unburned gas constant

$$R_{unb} = \frac{R_u}{Molecular\ mass}$$

Unburned Temperature

$$T_{unb} = \frac{p \cdot V}{R_{unb} \cdot m_T}$$

Next unburned temperature

$$T_{2_{unb}} = T_{1_{unb}} \cdot \left(\frac{P_2}{P_1} \right)^{\frac{\gamma-1}{\gamma}}$$

Unburned volume

$$V_{unb} = \frac{((1 - MFB) \cdot m_T \cdot R_{unb} \cdot T_{unb})}{P \cdot 10^5}$$

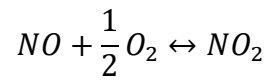
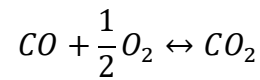
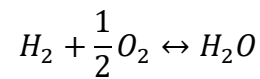
Burned volume

$$V_b = V_{cylinder} - V_{unb}$$

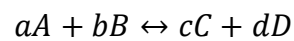
Burned temperature

$$T_b = \frac{p \cdot V_b}{MFB \cdot m \cdot R_b}$$

Dissociation



Equilibrium constants



$$\text{Forward reaction rate} = K_F [A]^a [B]^b$$

$$\text{Reverse reaction rate} = K_R [C]^c$$

Partial pressures

$$P_T = \sum \text{Partial pressures}$$

Partial pressure equilibrium constants

$$K_{CO_2} = \frac{n_1}{n_3 \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}}$$

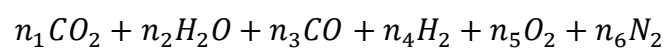
$$K_{H_2O} = \frac{n_2}{n_4 \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}}$$

N₂ and O₂ concentrations

Reactants

$$\varphi \cdot C_8H_{18} + 12 \frac{1}{2} (O_2 + 3.76 N_2)$$

Products



Guessing n_T

$$K_{CO2} = \frac{n_1}{n_3 \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}}$$

$$K_{H2O} = \frac{n_2}{n_4 \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}}$$

$$Carbon = 8\varphi = n_1 + n_3 \cdot \left(\frac{n_1}{n_3} + 1 \right)$$

$$Hydrogen = 18\varphi = 2n_2 + 2n_4$$

$$9\varphi = n_2 + n_4 = n_4 \cdot \left(\frac{n_2}{n_4} + 1 \right)$$

$$Oxygen = 25 = 2n_1 + n_2 + n_3 + 2n_5$$

$$Nitrogen = 47 = n_6$$

$$n_T = n_1 + n_2 + n_3 + n_4 + n_5 + n_6$$

$$\frac{n_1}{n_3} = K_{CO2} \cdot \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}$$

$$\frac{n_2}{n_4} = K_{H2O} \cdot \left(\frac{n_5}{n_T} \cdot p \right)^{\frac{1}{2}}$$

$$n_3 = \frac{8\varphi}{\left(\frac{n_1}{n_3} + 1 \right)}$$

$$n_1 = 8\varphi - n_3$$

$$n_4 = \frac{9 \varphi}{\left(\frac{n_2}{n_4} + 1\right)}$$

$$n_2 = 9 \varphi - n_4$$

$$n_5 = \frac{1}{2} (25 - 2n_1 - n_2 - n_3)$$

$$n_T = \frac{n_5}{n_5/n_T}$$

The concentrations for oxygen and nitrogen are calculated using the following equations

$$[O_2] = \alpha \frac{n_5 \cdot MFB}{V_b}$$

$$[N_2] = \alpha \frac{n_6 \cdot MFB}{V_b}$$

α is the multiplier calculated from

$$\alpha = \frac{\text{mass of fuel}}{(\varphi \cdot \text{molar mass of fuel})}$$

The probability of a NOx formation reaction is calculated with the following equation

$$\frac{\partial [C]}{\partial t} \propto [A][B] \exp\left(\frac{-EA}{R_u T}\right)$$

$$\frac{\partial [NO]}{\partial t} = 4.7 \cdot 10^{13} [N_2][O_2]^{\frac{1}{2}} \exp\left(\frac{-67837}{T}\right)$$

Converting NO from per unit time to Kmol per degree

$$\div (6 \cdot RPM)$$

$$\frac{\partial [NO]}{\partial t} \rightarrow \frac{\partial [NO]}{\partial \theta}$$

$$\cdot V_b$$

$$\frac{\partial[NO]}{\partial\theta} \rightarrow \frac{Kmol}{\theta}$$