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A reduced kinetic framework for predicting hydrogen auto-ignition and knock in spark-ignition engines

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ABSTRACT
Hydrogen-fuelled spark-ignition engines offer a promising pathway toward low-carbon power generation. However, the high reactivity of hydrogen–air mixtures increases the possibility of auto-ignition and knock. This poses challenges for stable engine operation. Rapid and reliable prediction of ignition limits under practical operating conditions remains essential for engine design and control. In this study, a zero-dimensional single-zone thermochemical model incorporating a reduced 17-step hydrogen oxidation mechanism is developed. This is to investigate auto-ignition behaviour under engine-relevant conditions. The model solves coupled conservation equations for mass, energy, and species evolution. Hence, this enables the prediction of in-cylinder thermodynamic histories and radical dynamics during compression. Auto-ignition onset is identified using a temperature rate-based criterion, providing a direct indicator of thermochemical runaway. Parametric analysis reveals that auto-ignition is not observed below a compression ratio of approximately 17. While lower engine speeds promote ignition due to increased residence time near top dead centre. A minimum knock propensity is identified near an equivalence ratio of approximately 1.6. This reflects the competing effects of mixture reactivity and thermal dilution. The results further highlight the dominant role of high-temperature chain-branching reactions in governing hydrogen ignition behaviour. This study demonstrates that the use of a reduced kinetic modelling within a simplified homogeneous framework can provide a computationally efficient and transparent tool for predicting hydrogen auto-ignition limits. The proposed approach offers practical value for rapid parametric assessment and preliminary design of hydrogen-fuelled spark-ignition engines.

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1.0 Introduction

The accurate prediction of combustion behaviour in reciprocating internal combustion engines requires the coupled treatment of fluid motion, heat transfer, and chemical reaction kinetics [1, 2]. In spark-ignition engines, this challenge becomes particularly critical when analysing end-gas auto-ignition, which is a phenomenon governed predominantly by chemical kinetic processes evolving over very short temporal scales. Although turbulence, flame propagation, and transport processes influence overall combustion development, the onset of auto-ignition is primarily controlled by the oxidation chemistry occurring in the unburned mixture ahead of the propagating flame front. Hydrogen, as a clean-burning fuel, requires a detailed understanding of its ignition behaviour, especially under practical engine conditions, to ensure safe and efficient utilisation.

Hydrogen is a unique fuel for internal combustion applications due to its exceptionally rapid reaction kinetics and short ignition delay times under high pressure and temperature conditions. Its low molecular weight, high diffusivity, wide flammability limits, and quick chain-branching reactions all contribute to ignition characteristics that are quite different from those of traditional hydrocarbon fuels. These properties

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increase the tendency of hydrogen–air mixtures to auto-ignite during high compression ratios or low engine speeds. With increasing interest in hydrogen-fuelled engines as part of global decarbonisation efforts, reliable prediction of ignition behaviour has become essential for improving efficiency while preventing abnormal combustion.

Chemical kinetic modelling is widely recognised as a physically grounded approach for predicting ignition delay, heat release behaviour, and species evolution during combustion. However, detailed chemical kinetic mechanisms typically involve dozens of reacting species and hundreds of elementary reactions. This makes their direct coupling with multidimensional engine simulations computationally demanding. Consequently, combustion modelling frequently involves a compromise between chemical fidelity and physical complexity. Here, either simplified chemistry is used in realistic flow simulations or detailed chemistry is retained within reduced physical descriptions [3, 4].

In the present study, this modelling trade-off is addressed by preserving chemically resolved reaction kinetics while simplifying the thermodynamic representation of the combustion chamber. The engine charge is modelled as a homogeneous single zone, enabling isolation of the chemical processes responsible for end-gas auto-ignition. This is done to remove any additional uncertainties introduced by spatial gradients or turbulence modelling. This approach is particularly suitable for studying ignition phenomena dominated by local chemical timescales rather than flame propagation effects.

A further objective of this work is to demonstrate that reduced kinetic modelling of hydrogen auto-ignition can be implemented within a transparent and accessible computational framework. By formulating the governing conservation equations together with the reduced reaction mechanism within a spreadsheet-based environment, the model provides numerical transparency and reproducibility. It also remains computationally efficient for parametric investigations. The resulting framework aims to bridge the gap between detailed combustion kinetics and practical engineering analysis of hydrogen-fuelled spark-ignition engines.

However, existing approaches often require either detailed chemical mechanisms with high computational cost or simplified models lacking chemical resolution. This study addresses this gap by developing a reduced kinetic modelling framework that preserves the essential chain-branching chemistry of hydrogen oxidation but also enabling computationally efficient prediction of auto-ignition behaviour under engine-relevant conditions.

Recent technology has made it possible for researchers to study how adding hydrogen to gasoline affects engine performance. By using computer simulations, we can understand what happens when different amounts of hydrogen are mixed with gasoline. This study uses these simulation tools to examine how a spark ignition engine performs when running on a mixture of hydrogen and gasoline. The goal is to find the best combination and engine settings that improve efficiency and reduces harmful emissions, especially NOx. The results could help design cleaner, more efficient engines that are better for our environment and health.

Hydrogen is a clean fuel that can help reduce harmful emissions from engines. However, when hydrogen burns, it creates very high temperatures, which leads to the production of nitrogen oxides (NOx). NOx is a harmful gas that causes air pollution and health problems. Though researchers have studied hydrogen as a fuel, there is still a need to find the best ways to use hydrogen in engines to reduce NOx emissions without losing performance. This study aims to solve this problem by using computer simulations to test different engine conditions. The goal is to find the best ways to use hydrogen to make engines cleaner and more efficient.

2.0 Modelling Framework and Methodology 2.1 Model Overview and Assumptions

Hydrogen auto-ignition in a spark-ignition engine is investigated using a zero-dimensional, single-zone thermochemical model representing the combustion chamber as a homogeneous control volume. At any instant of crank angle, thermodynamic properties, including temperature, pressure, and species concentrations, are assumed spatially uniform. This setup enables direct examination of the chemical kinetic processes governing ignition while also deliberately reducing uncertainties associated with multidimensional flow and turbulence modelling.

Although the single-zone assumption neglects spatial gradients in velocity, temperature, and composition, it remains well suited for analysing chemically controlled ignition phenomena. Here ignition onset is dominated by local thermochemical states rather than flame propagation dynamics. Similar homogeneous reactor formulations have been widely employed in knock prediction and ignition studies due to their transparency, robustness, and computational efficiency [5–9].

The working mixture is treated as a perfect gas under premixed conditions. Spark initiation is intentionally excluded so that ignition behaviour arises solely from spontaneous chemical reactions. Heat transfer between the gas and cylinder walls is incorporated through a lumped heat-loss formulation, while mass exchange with the surroundings is neglected, resulting in a closed thermodynamic system.

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2.2 Chemical Kinetic Mechanism

Hydrogen oxidation chemistry is described using a reduced 17-step elementary reaction mechanism originally proposed by Rafael and Sher [10]. The mechanism includes the principal species governing hydrogen ignition chemistry, namely H_2, O_2, H_2O, H, O, OH, HO_2, and H_2O_2 [11–13].

The selected mechanism retains the dominant radical production and chain-branching pathways responsible for thermal runaway during hydrogen oxidation. This is done to avoid the computational expense associated with detailed mechanisms containing hundreds of reactions. Previous investigations have shown that hydrogen ignition delay and knock behaviour are strongly influenced by these radical pathways, supporting the suitability of reduced mechanisms for auto-ignition analysis when appropriately validated [4, 12].

Adopting a reduced mechanism allows emphasis to remain on kinetic sensitivity and ignition behaviour rather than numerical stiffness associated with large reaction systems, consistent with the objectives of the present study.

2.3 Thermochemical and Physical Property Modelling

Reliable prediction of ignition behaviour requires accurate thermochemical properties. Thermodynamic data for all species are obtained from values consistent with the Active Thermochemical Tables (ATcT) framework. This provides internally consistent enthalpy, entropy, and specific heat data across wide temperature ranges [14].

Species-specific heats are treated as temperature-dependent while mixture properties are evaluated using instantaneous species compositions. The temperature in the cylinder is obtained from the equation of state for ideal gas using both

predicted pressure and mixture composition. Heat transfer between the working gas and cylinder walls is represented using a heat-loss term included in the energy conservation equation. Though simplified, this formulation captures the dominant thermal losses influencing ignition timing and provides a stable representation suitable for parametric analysis.

2.4 Engine Geometry and Operating Conditions

The thermodynamic model is based on the geometric characteristics of the single-cylinder Ricardo E6 spark-ignition variable-compression engine. The geometric parameters are:

In-Cylinder bore: 76.2 mm
In-Cylinder Stroke: 111.0 mm
Con rod length: 241.3 mm

Some parametric simulations are performed to evaluate the influence of operating conditions on hydrogen auto-ignition behaviour. The investigated parameters include:

Compression ratio (r_c)
Engine speed (N)
Air-fuel equivalence ratio (ϕ)

Unless otherwise specified, simulations are conducted under premixed conditions without spark initiation to ensure that ignition is governed purely by chemical kinetics.

2.5 Governing Equations

The temporal evolution of the in-cylinder thermodynamic state is determined from conservation relations applied to a closed control volume. The energy conservation equation is expressed as indicated in Equation 1.

$$dp/d\theta = (\gamma - 1)/V\{(\frac{dQ_{hr}}{d\theta} - \frac{dQ_{hl}}{d\theta}) - \frac{\gamma}{\gamma - 1}p\frac{dV}{d\theta}\} \quad (1)$$

Where p is the pressure, θ is the instantaneous crank position, γ is the specific heat ratio, V is the cylinder volume, Q_hr represents chemical heat release, and Q_hl denotes heat loss.

The mass conservation equation is expressed as indicated in Equation 2.

$$m(\theta + \Delta\theta) = M_m \cdot n_i(\theta + \Delta\theta) \quad (2)$$

Where m is the mass, M_m is the mixture molar mass, and n_i is the mole number of species i.

The ideal gas equation is expressed as indicated in Equation 3.

$$p(\theta + \Delta\theta)\, V(\theta + \Delta\theta) = n(\theta + \Delta\theta)\, R_u\, T(\theta + \Delta\theta) \quad (3)$$

Where p is the pressure, θ is the instantaneous crank position, V is the cylinder volume, n is the number of moles, R_u is the universal gas constant, and T is the temperature.

Species conservation equations are solved by accounting for each chemical species in the kinetic mechanism. This is achieved by enabling tracking of radical generation and consumption during the engine cycle based on time resolution. The mixture is assumed to obey ideal-gas behaviour throughout the simulation.

2.6 Auto-Ignition Criterion

Auto-ignition onset is identified using a temperature-rate criterion adapted from classical knock prediction approaches [3]. Ignition is detected when the rate of temperature rise increases rapidly relative to instantaneous temperature, indicating transition to thermochemical runaway [15–17]. A temperature-based indicator is adopted instead of pressure-based metrics because temperature responds directly to the exponential sensitivity of hydrogen oxidation kinetics. Computations are terminated once the ignition criterion is satisfied, representing the onset of uncontrolled ignition.

2.7 Numerical and Computational Implementation

The governing conservation equations and reaction kinetics are implemented within a spreadsheet-based computational framework using crank-angle–resolved time integration. Small crank-angle increments are employed to ensure numerical stability and adequate resolution of fast chemical timescales associated with hydrogen oxidation.

Separate computational modules are used for mixture preparation, reaction-rate evaluation, thermodynamic property calculation, heat-transfer modelling, and cycle integration. Some automated routines are employed for parametric simulations and post-processing. The transparent implementation enables direct inspection of intermediate variables, facilitating verification and reproducibility of the modelling procedure. Despite its well simplified structure, the framework captures the essential thermochemical processes governing hydrogen auto-ignition under engine-relevant operating conditions.

3.0 Results and Discussions

3.1 Thermodynamic Evolution Under Motoring, Normal Combustion and Auto-Ignition Conditions

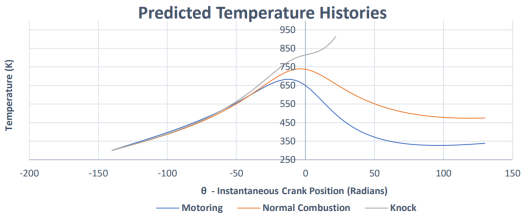

Figure 1: Predicted Temperature Histories

The predicted in-cylinder temperature histories under motoring, stoichiometric combustion, and knock-inducing conditions are compared in Figure 1. Distinct thermodynamic behaviours are observed, illustrating the transition from purely mechanical compression to chemically driven thermal runaway. Under motoring conditions ($\phi = 0$, $r_c = 14$, $N = 1000$ rpm), temperature evolution is governed solely by compression work and follows near-polytropic behaviour. The absence of chemical heat release confirms that the model correctly isolates thermodynamic compression effects and provides a consistent baseline for evaluating chemically induced temperature rise.

For stoichiometric hydrogen-air conditions ($\phi = 1$, $r_c = 14$), a rapid temperature increase occurs near Top Dead Centre (TDC). This results from exothermic chain-branching reactions characteristic of hydrogen oxidation. The dominant high-temperature branching pathway, $H + O_2 \rightarrow OH + O$, is widely recognised as the principal accelerator of ignition in hydrogen systems [1, 18]. The sharp thermal escalation predicted near TDC agrees with experimentally observed reductions in ignition delay at elevated compressed temperatures [12]. This shows that the reduced kinetic mechanism captures the essential ignition physics.

When the compression ratio, r_c, is increased to 17 (ϕ = 1, N = 1000 rpm), ignition occurs before TDC. The resulting steep temperature gradient reflects thermochemical runaway driven by exponential radical pool amplification. This behaviour highlights the strong temperature sensitivity of hydrogen ignition, arising from the Arrhenius dependence of chain-branching reactions [18, 19]. The predicted advance of ignition timing demonstrates the transition from controlled combustion to knock-like auto-ignition conditions.

3.2 Overview of Numerical Approach

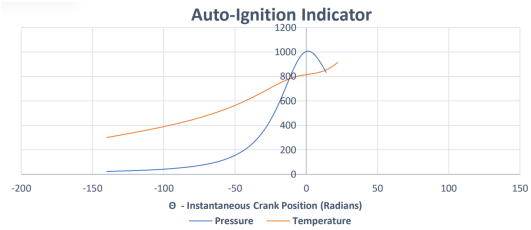

Figure 2: Auto-Ignition Indicator

Temperature evolution provides a clearer indicator of ignition onset than pressure, as illustrated in Figure 2. While pressure responds to both volumetric compression and chemical heat release, temperature directly reflects reaction-rate acceleration associated with radical growth. Hydrogen fuel reactivity and ignition are characterised by rapid escalation of $dT/d\theta$. This corresponds well to exponential increases in radical concentration driven by branching kinetics [1, 20]. The temperature-rate criterion adopted in this study identifies ignition when the rate of temperature rise increases sharply relative to instantaneous temperature. This obviously signals a transition to thermochemical runaway. This approach aligns with kinetic interpretations of ignition delay, where ignition is fundamentally governed by temperature sensitivity of reaction rates rather than macroscopic pressure changes [12]. The results demonstrate that temperature-based detection provides a physically meaningful indicator of knock onset for fast-reacting fuels such as hydrogen.

3.3 Parametric Influence on Auto-Ignitions

Parametric simulations based on the Ricardo E6 engine geometry were conducted to evaluate the influence of compression ratio, engine speed, and equivalence ratio on hydrogen fuel reactivity and ignition behaviour. The results highlight the competing roles of thermodynamic state and chemical timescales in determining knock propensity.

3.3.1 Compression Ratio Effect

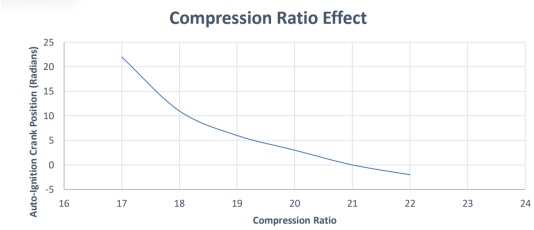

Figure 3: Auto-Ignition Indicator

In Figure 3, auto-ignition was predicted for compression ratios between 17 and 22 (ϕ = 1, N = 1000 rpm). Increasing compression ratio elevates end-gas temperature and pressure, hence reducing ignition delay through accelerated chain-branching reactions. The exponential reduction in ignition delay with temperature agrees with shock-tube and rapid-compression-machine measurements for hydrogen–air mixtures [12, 20].

The strong sensitivity observed reflects the dominance of the $H + O_2 \rightarrow OH + O$ reaction, which governs radical amplification at high temperatures ([18]). These results confirm that compression ratio primarily influences ignition through thermochemical state rather than flow effects within the single-zone framework.

3.3.2 Compression Ratio Effect

Hydrogen fuel reactivity and ignition were observed within a speed range of 700 – 850 rpm (r_c = 14, ϕ = 1), as shown in Figure 4. Lower engine speeds increase residence time near before peak compression. This allows sufficient accumulation of reactive radicals prior to expansion. This behaviour illustrates the fundamental competition between chemical reaction timescales and mechanical expansion timescales, a central concept in engine knock analysis [21].

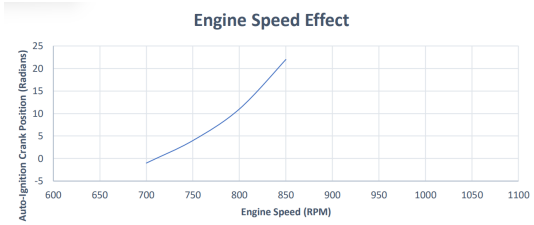

Figure 4: Engine Speed Effect

At higher speeds, reduced residence time limits radical growth before significant heat release occurs. Hence thereby suppresses auto-ignition. The results demonstrate that ignition behaviour depends not only on thermodynamic conditions but also on the temporal coupling between chemistry and piston motion.

3.3.3 Effect of Equivalence Ratio

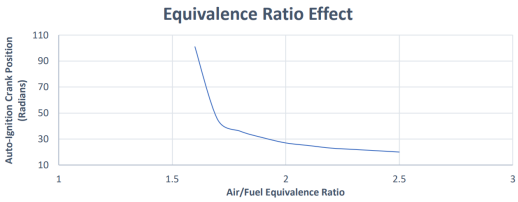

Figure 5: Equivalence Ratio Effect

As shown in Figure 5, auto-ignition occurred for equivalence ratios between 1.6 and 2.5 (r_c = 14, N = 1000 rpm). Rich mixtures increase H-atom availability and accelerate branching reactions. This leads to increased knock propensity. The strong dependence of ignition delay on mixture strength has been widely reported in hydrogen oxidation studies [1, 12].

Unlike heavier hydrocarbons, hydrogen ignition chemistry is dominated by high-temperature branching reactions rather than complex low-temperature oxidation pathways. Thus explaining monotonic increase in knock tendency with increasing equivalence ratio under the present operating conditions [19].

3.4 Species Evolution and Radical Pool Development

Generally, predicted species histories provide mechanistic

insight into ignition development.

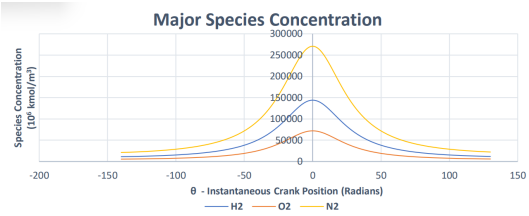

Figure 6: Major Species Concentration

Major species (H_2, O_2, N_2, H_2O) displayed in Figure 6, evolve consistently with expected combustion behaviour. Also rapid water formation occurs near TDC and coinciding with peak heat release. Nitrogen remains chemically inert and primarily acts as a thermal diluent. In Figure 7, minor radicals (H, O, OH) exhibit rapid growth immediately before ignition. Hence validating the dominance of chain-branching chemistry. The buildup and subsequent consumption of HO_2 and H_2O_2 indicate their function as intermediate radical reservoirs within hydrogen oxidation pathways [18]. At elevated temperatures, decomposition of H_2O_2 contributes to rapid radical multiplication, accelerating ignition [1].

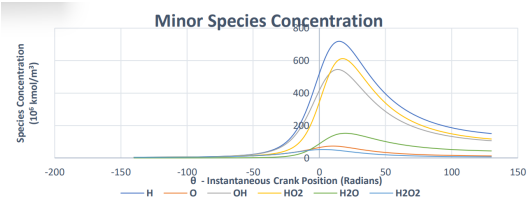

Figure 7: Minor Species Concentration

The observed radical pool amplification agrees with established hydrogen kinetic models. Thus confirming that auto-ignition in the present configuration is governed primarily by high-temperature branching reactions rather than low-temperature peroxy chemistry typical of heavier hydrocarbon fuels.

4.0 Conclusions

A zero-dimensional kinetic framework for analysing hydrogen fuel reactivity and ignition behaviour in a homogeneous spark-ignition engine has been developed using a reduced elementary reaction mechanism coupled with thermodynamic conservation equations. The combined solution of the energy equation, species conservation relations, and ideal-gas equation of state enabled prediction of in-cylinder thermodynamic evolution together with radical species dynamics governing ignition behaviour.

The results demonstrate that hydrogen auto-ignition under engine conditions is predominantly controlled by high-temperature chain-branching chemistry. Increasing compression ratio substantially reduces ignition delay by elevating end-gas temperature and accelerating radical amplification through the $H + O_2 \rightarrow OH + O$ reaction pathway. Engine speed was shown to influence ignition through time-scale competition between chemical kinetics and mechanical expansion, with lower speeds promoting knock due to increased residence time near peak compression. Increasing equivalence ratio enhances knock propensity by increasing reactive radical availability and strengthening branching kinetics.

The temperature-rate-based ignition criterion adopted in this study provides a physically consistent indicator of thermal runaway. Hence capturing ignition onset more directly than pressure-based metrics. Analysis of species evolution further confirms that ignition is governed by the rapid growth of H, O, and OH radicals, while HO_2 and H_2O_2 act as intermediate reservoir species preceding high-temperature decomposition and rapid heat release.

Beyond reproducing expected ignition trends, the present study demonstrates that chemically resolved analysis of hydrogen auto-ignition can be achieved within a computationally efficient homogeneous framework. The results emphasise the dominant role of chain-branching kinetics and chemical–mechanical time-scale interaction in hydrogen knock behaviour and provide a transparent modelling approach suitable for rapid parametric evaluation of hydrogen-fuelled spark-ignition engines.

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