INTERNATIONAL JOURNAL OF PROGRESSIVE RESEARCH IN ENGINEERING MANAGEMENT AND SCIENCE (IJPREMS)
(Int Peer Reviewed Journal)
Vol. 05, Issue 10, October 2025, pp : 1316-1326

www.ijprems.com
editor@ijprems.com

e-ISSN : 2583-1062
Impact Factor : 7.001

COMPUTATIONAL MODELLING OF N-DODECANE COMBUSTION KINETICS USING CANTERA: MECHANISM SELECTION, IGNITION SIMULATION, AND REACTION PATHWAY ANALYSIS

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DOI: https://www.doi.org/10.58257/IJPREMS44401

ABSTRACT

The advancement of computational combustion modelling has been driven by the rise of open-source frameworks and detailed chemical-kinetic mechanisms. This study develops a Cantera-based internal combustion engine simulation for n-dodecane—a surrogate for diesel and jet fuels—using a detailed reaction mechanism (*nDodecane_Reitz.yaml*). The model integrates full thermodynamic, kinematic, and kinetic coupling under realistic engine conditions (compression ratio = 20, speed = 3000 rpm). A comparative mechanism review identifies *gri30.yaml* for methane/natural gas, *h2o2.yaml* for hydrogen, and *nDodecane_Reitz.yaml* for diesel-type fuels. The reactor network incorporates intake, injection, and exhaust dynamics, with adaptive integration for precision. Results include pressure–temperature evolution, P–V and T–S diagrams, heat-release and work-rate synchronization, and transient species concentrations. Integral quantities release, work, efficiency, and emissions (CO, NOx)quantify global performance. The model demonstrates accurate reproduction of combustion phasing, energy conversion, and emission trends, establishing a robust computational foundation for multi-fuel and hydrogen transition studies in compression-ignition engines.

1. INTRODUCTION

The advancement of computational combustion modelling has been strongly influenced by the development of open-source tools and detailed chemical-kinetic databases. The foundation of such modelling lies in the Cantera software suite, initially described in the *Cantera C++ User's Guide* by Goodwin (1), which introduced a modular approach for simulating thermochemical processes. The Cantera Developers (2) later released comprehensive documentation expanding its Python interface, making it accessible to both researchers and students. Educational institutions such as Brigham Young University (3) and the Skill-Lync (4) online platform have contributed by providing training workshops and structured courses demonstrating Cantera's application in combustion analysis. Likewise, Cerfacs (5) has played a pivotal role in integrating Cantera within its open-source CFD frameworks for high-fidelity turbulent combustion simulations.

The scientific robustness of Cantera was further validated by Goodwin et al. (6), who presented an in-depth discussion of its object-oriented architecture for simulating kinetics, thermodynamics, and transport processes in reacting systems. Supporting theoretical work by Kee, Coltrin, and Glarborg (7) provided essential insights into chemically reacting flow behaviour, establishing a direct theoretical link between chemical kinetics and fluid mechanics that underpins Cantera's core solver.

Fundamental combustion science continues to be guided by cornerstone references such as Turns (8) and Law (9), which describe ignition, flame propagation, and pollutant formation in hydrocarbon and hydrogen systems. Complementary perspectives were provided by Glassman, Yetter, and Glumac (10), emphasizing practical and experimental aspects, and by Poinsot and Veynante (11), who explored theoretical and numerical aspects of turbulent flame modeling. Classical texts by Williams (12) and Heywood (13) remain critical in understanding detailed reaction kinetics and engine-specific thermodynamic behavior, respectively.

Broader thermodynamic and fluid-mechanical coupling is extensively treated in Çengel and Ghajar (14), while Warnatz, Maas, and Dibble (15) focused on modeling combustion processes through advanced simulation and reaction mechanism analysis. Further contributions by Bowman et al. (16) detailed kinetic modeling for various fuels, providing key datasets for mechanism validation.

The emerging shift toward low-carbon fuels and hydrogen technology is supported by global research and open-access databases. IRENA (17) outlined the role of hydrogen as a sustainable energy vector, while LLNL (18) maintains one of the most comprehensive online combustion mechanism repositories. The University of California, San Diego (19) and University of Galway (20) have produced validated chemical-kinetic mechanisms—such as the San Diego, NUIGMech, and AramcoMech models—that form the backbone of modern combustion simulations for hydrogen, ammonia, and hydrocarbon systems. The Smith et al. (21) GRI-Mech 3.0 mechanism remains the benchmark for

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methane and natural gas combustion, and LibreTexts Chemistry (22) provides open educational resources that reinforce the understanding of fundamental combustion reaction principles.

Collectively, these studies represent the multidisciplinary foundation of modern combustion research, combining classical thermochemical theory with computational advances to enable accurate simulation of hydrogen, natural gas, and hydrocarbon combustion systems within Cantera and related frameworks.

2. METHODOLOGY

Combustion Mechanisms

The selection of chemical-kinetic mechanisms in Cantera determines the accuracy and relevance of combustion simulations for different fuels. Each mechanism represents a collection of chemical reactions, rate coefficients, and thermodynamic data that describe how a particular fuel reacts with air or oxygen under various conditions. For engine and gas turbine modeling, the mechanism must balance detail and computational efficiency-capturing ignition delay, flame speed, and pollutant formation accurately.

For natural gas combustion, mechanisms from the GRI-Mech family are preferred. The standard GRI-Mech 3.0 mechanism (gri30.yaml) includes detailed methane, ethane, carbon monoxide, and hydrogen reactions, validated extensively for gas turbines, burners, and internal combustion engines. Its high-temperature variant (gri30_highT.yaml) is suitable for environments above 2000 K , such as afterburners or reheat systems.

For hydrogen combustion, the h202.yaml mechanism provides a compact but precise description of hydrogen-oxygen kinetics, covering ignition, flame propagation, and radical species formation over a wide temperature range. The ohn.yaml mechanism can supplement it when nitrogen-oxide (NOx) formation or hydroxyl-hydrogen-nitrogen interactions are studied,

For liquid-fuel or diesel-type combustion, nDodecane_Reitz.yaml is the recommended mechanism. It models n-dodecane ($C_{12}H_{25}$), a common surrogate for diesel and jet fuels, and includes detailed oxidation pathways, intermediate species, and soot precursors. This mechanism is widely used for spray, ignition, and emission analysis in compression-ignition engine studies.

The following table summarizes the most appropriate mechanisms for natural gas, hydrogen, and n dodecane combustion:

Table 1: The combustion Mechanisms used for Natural gas, Hydrogen and Dodecane

Fuel Type	Mechanism File	Main Components Modelled	Typical Application
Natural Gas (methane-based) could be used for hydrogen.	gri30.yaml	Methane, ethane, CO, H_2, and NOx chemistry	Gas turbines, internal combustion engines, premixed and diffusion flames
Hydrogen	h202.yaml	Hydrogen and oxygen reactions, radical formation (H, O, OH)	Hydrogen engines, gas turbines, and flame propagation studies
Diesel surrogate (ndodecane)	nDodecane_Reitz.yaml	n -Dodecane oxidation and decomposition chemistry	Diesel and jet-fuel engine modelling. spray ignition, and emission analysis

In summary, gri30.yaml is ideal for natural gas and hydrogen together for engine application, h2o2.yaml for hydrogen, and nDodecane_Reitz.yaml for diesel-type fuels such as n-dodecane. The careful selection of these mechanisms ensures that each simulation accurately reflects the chemical and physical processes governing combustion performance, ignition behaviour, and emission formation.

The gri30.yaml mechanism can be effectively used for both natural gas and hydrogen–air combustion systems. It includes detailed chemical pathways for methane (CH_4), ethane (C_2H_6), carbon monoxide (CO), hydrogen (H_2), and key radicals such as OH, O, and HO_2. Because hydrogen is already included as one of the participating species, the mechanism accurately captures the oxidation behaviour of mixed fuels containing hydrogen-enriched natural gas. This

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makes it suitable for modelling hydrogen–methane blends, often referred to as H₂–NG hybrid fuels, which are increasingly studied for low-emission gas turbines and retrofitted internal combustion engines.

Engine Simulation Input Parameters

The present simulation employs the nDodecane_Reitz.yaml reaction mechanism to represent the detailed chemical kinetics of n-dodecane ($C_{12}H_{26}$), a common diesel surrogate fuel, within an internal combustion (IC) engine model. The mechanism is loaded under the gas-phase configuration nDodecane_IG, ensuring ideal gas assumptions for thermodynamic and transport properties. The stoichiometric oxidizer-to-fuel mixture is based on standard air composition, expressed as:

Air: $O_2: 1,\ N_2: 3.76$

Fuel: $C_{12}H_{26}: 1$

The engine operates at a speed of 3000 revolutions per minute (rpm), equivalent to a cyclic frequency $f = \frac{3000}{60} = 50\ s^{-1}$. The displaced cylinder volume is set to $V_H - 0.5 \times 10^{-3}$ m^3, and the compression ratio is $\varepsilon = 20$. The piston diameter is $d_p = 0.083$ m, defining the geometric basis for volume variation during compression and expansion strokes according to the relation:

$$V(\theta) = V_c + \frac{V_H}{2}\left(1 - \cos\theta + \frac{1}{r_c}\left(1 - \sqrt{1 - r_c^2 \sin^2\theta}\right)\right)$$

where V_c is the clearance volume and r_c is the crank-to-connecting-rod ratio. The inlet (turbocharged) conditions are defined by an intake temperature $T_{\text{inlet}} = 300$ K and an intake pressure $p_{\text{inlet}} = 1.3 \times 10^5$ Pa. The outlet (exhaust) pressure is slightly lower at $p_{\text{ontlet}} = 1.2 \times 10^5$ Pa, representing typical turbocharger backpressure effects. The injected n-Dodecane fuel is treated as a gaseous phase, with an injection temperature of $T_{\text{injector}} = 300$ K, injection pressure $p_{\text{injector}} = 1.6 \times 10^8$ Pa, and composition consistent with the defined fuel mixture.

Ambient boundary conditions correspond to $T_{\text{ambient}} = 300$ K and $p_{\text{ambient}} = 1.0 \times 10^5$ Pa, assuming quiescent air identical in composition to the intake mixture. The valve dynamics are parameterized by empirical friction coefficients $C_v = 1.0 \times 10^{-6}$ and timing angles (in radians) defining the valve opening and closing periods:

Inlet Open: $\theta_{\text{IO}} = -18°$

Inlet Close: $\theta_{\text{IC}} = 198°$

Outlet Open: $\theta_{\text{EO}} = 522°$

Outlet Close: $\theta_{\text{EC}} = 18°$

Fuel injection occurs over a short duration between $350°$ and $365°$ crank angles, corresponding to $\theta_{\text{inj , oppen}}$ =350 and $\theta_{\text{inj,close}}$ =365, with an injected fuel mass of $m_{\text{fuel}} - 3.2 \times 10^{-5}$ kg.

The numerical solver advances the engine cycle over eight revolutions, ensuring sufficient transient convergence and cyclic stability. Adaptive integration is employed with a maximum temperature step of $\Delta T_{\max} - 20$ K and stringent error tolerances of rtol -10^{-12} and atol -10^{-16}, ensuring numerical accuracy during the rapid combustion phase.

Overall, these input parameters define a high-compression, single-cylinder engine operating on n-dodecane fuel, suitable for comparative simulations with alternative mechanisms such as gri30.yaml (methane/natural gas), h2o2.yaml (hydrogen), facilitating multi-fuel combustion analysis under consistent thermodynamic conditions.

Configuration of Engine Operating Parameters and Functional Models

The cylinder geometry and crankshaft kinematics define the fundamental relationships governing piston motion and instantaneous cylinder volume in an internal combustion engine. The clearance volume V_{0T}, which is the minimum volume at top dead center (TDC), is determined from the known displaced volume V_H and compression ratio ε as

$$V_{0T} = \frac{V_H}{\varepsilon - 1}$$

where $V_H - 0.5 \times 10^{-3}$ m^3 (displaced volume per cycle) and $\varepsilon = 20$ (compression ratio). This yields a clearance volume of approximately $V_{0T} = 2.63 \times 10^{-5}$ m^3. The piston cross-sectional area is given by

$$A_p - \frac{\pi d_p^2}{4}$$

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where $d_p = 0.083$ m is the piston diameter, resulting in $A_p = 5.41 \times 10^{-3}$ m^2. The stroke length, representing the total piston travel between TDC and bottom dead center (BDC), follows from the displaced volume-area relationship:

$$L_s = \frac{V_H}{A_p} - 9.24 \times 10^{-2} \text{ m}$$

or approximately 92.4 mm , typical of high-speed diesel engines. The crank angle $\theta(t)$ defines the instantaneous angular position of the crankshaft as a function of time:

The crank angle, denoted as $\theta(t)$, defines the instantaneous angular position of the crankshaft as a function of time and is expressed as

$$\theta(t) = (2\pi f t) \text{mod} 4\pi$$

where f is the engine rotational speed (in revolutions per second). The term mod (modulus) ensures periodicity, meaning that the angle resets to zero after every 4π radians (two full revolutions or $720°$). This captures the complete four-stroke cycle of an internal combustion engine - intake, compression, power, and exhaust. For an engine speed of

$$f = 50 \text{ s}^{-1} (3000 \text{rpm})$$

the function $\theta(t)$ increases continuously with time, but is wrapped back to a range between 0 and 4π radians, ensuring that the motion repeats exactly every two revolutions.

The piston velocity $u_p(t)$ is modelled as a sinusoidal function to represent the approximate simple harmonic motion of the piston along the cylinder axis:

$$u_p(t) = -\frac{L_s}{2}(2\pi f) \sin[\theta(t)]$$

where L_s is the stroke length and f is the engine frequency. The negative sign indicates that the piston moves downward (from top dead center to bottom dead center) during the expansion stroke.

The maximum piston velocity occurs at mid-stroke, corresponding to crank angles $\theta = \pi/2$ and $\theta = 3\pi/2$, where the sine function attains its maximum value. Hence, the peak velocity is given by

$$u_{p,\max} = \pi f L_s$$

Substituting $f = 50 \text{ s}^{-1}$ and $L_s - 0.0924$ m, we obtain

$$u_{p,\max} = \pi(50)(0.0924) = 14.5 \text{ m/s}$$

This relationship quantifies the dynamic coupling between crankshaft rotation and piston motion, defining how the instantaneous volume $V(t)$, piston velocity $u_p(t)$, and the corresponding work rate evolves throughout the engine cycle. These expressions form the kinematic foundation for the zero-dimensional Cantera-based combustion simulation, linking the engine's geometric configuration with its thermodynamic behaviour.

Development of the Reactor Network Framework

The reactor network defines the thermodynamic domain and boundary interactions of the single-cylinder engine model in Cantera. The simulation begins by loading the chemical kinetic mechanism and defining the thermodynamic phase through

gas = ct.Solution(reaction_mechanism, phase_name) where the reaction mechanism (nDodecane_Reitz.yaml) specifies all species and elementary reactions, and the phase name (n Dodecane_/G) identifies the ideal-gas configuration. The working fluid inside the cylinder is initialized at inlet conditions ($T_{\text{inlet}}, p_{\text{inlet}}, X_{\text{air}}$), and the IdealGasReactor object represents the combustion chamber with an initial volume equal to the clearance volume V_{0T} :

$$\boldsymbol{T = T_{\text{inlet}}, p = p_{\text{inlet}}, X = O_2: 1,\ N_2: 3.76}$$
$$\boldsymbol{V_{\text{cyl}} = V_{0T}}$$

An inlet reservoir supplies fresh air to the cylinder through a valve that opens and closes according to crank angle. The valve's behaviour is controlled by a time-dependent logical function:

$$f_{\text{in}}(t) - \begin{cases} 1, & \text{if } (\theta(t) = \theta_{\text{open,in}}) \text{mod} 4\pi < \Delta\theta_{\text{in}} \\ 0, & \text{otherwise} \end{cases}$$

where $\theta_{\text{open, in}}$ and $\theta_{\text{close, in}}$ define the intake valve timing, and $\Delta\theta_{\text{in}} = \theta_{\text{close, in}} - \theta_{\text{open, in}}$. The valve flow coefficient $C_{v,\text{ in}} - 1 \times 10^{-6}$ governs the mass flow rate.

The injector is defined as a gaseous reservoir at high pressure and temperature ($p_{\text{inj}} = 1.6 \times 10^8$ Pa, $T_{\text{inj}} - 300$ K). It is connected to the cylinder via a mass flow controller (MFC), which specifies the instantaneous fuel injection rate:

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$$\dot{m}_f = \frac{m_{\text{inj}}}{t_{\text{open}}}, t_{\text{open}} = \frac{\theta_{\text{close,inj}} - \theta_{\text{open,inj}}}{2\pi f}$$

Fuel enters the chamber only during the crank-angle window between $350°$ and $365°$, determined by the injector's time function, identical in form to the intake valve expression.

The exhaust reservoir maintains a backpressure of $p_{\text{out}} = 1.2 \times 10^5$ Pa and is connected through an outlet valve defined by

$$f_{\text{out}}(t) = \begin{cases} 1, & \text{if } (\theta(t) - \theta_{\text{open,out}}) \bmod 4\pi < \Delta\theta_{\text{out}} \\ 0, & \text{otherwise} \end{cases}$$

with the same coefficient $C_{v,\text{ out}} - 1 \times 10^{-6}$.

The piston is modeled as a moving wall separating the cylinder from an external ambient reservoir. Its instantaneous velocity follows

$$u_p(t) = -\frac{L_s}{2}(2\pi f)\sin[\theta(t)]$$

and its surface area equals the piston head area $A_p = \pi d_p^2/4$. This moving boundary continuously updates the reactor volume according to crank position, coupling mechanical motion with in-cylinder thermodynamics.

The entire configuration-cylinder, valves, injector, and walls-is assembled into a reactor network using sim - ct.ReactorNet([cyl])

Numerical tolerances are imposed to maintain precision:

$$\textbf{rtol} = \mathbf{10^{-12}},\ \textbf{atol} = \mathbf{10^{-16}}, \mathbf{\Delta T_{max} = 20\ K}$$

where $\Delta T_{\max}$ limits the allowable temperature change per integration step. This reactor network framework ensures realistic mass and energy transfer across all system boundaries, forming the physical basis for simulating n-Dodecane combustion in the zero-dimensional Cantera engine model.

Execution of the Numerical Simulation

The simulation phase advances the coupled thermochemical and mechanical equations of the engine model over time, recording the instantaneous evolution of all key state variables. **A Cantera** SolutionArray is first created to store the transient results of the reactor, containing thermodynamic properties along with additional parameters such as time, crank angle, cylinder volume, gas mass, inlet and outlet mass flows, and the rate of work transfer: ***states - ct.SolutionArray(cyl.thermo,extra*** $= (t, ca, V, m, \dot{m}_{in}, \dot{m}_{out}, \dot{W}_v))$

Table 2: The parameters of the solution Array

Symbol	Name	Description	Units	Physical Meaning / Role in Simulation
t	Time	Simulation time corresponding to each crank-angle increment.	s (seconds)	Represents the progression of the engine cycle in real time. Each time step corresponds to one degree of crank rotation.
ca	Crank Angle	Instantaneous angular position of the crankshaft, calculated as $\theta(t) = 2\pi f t \bmod 4\pi$.	rad	Defines piston position and cycle phase (intake, compression, power, exhaust). Ensures the cycle repeats every $720°$.
V	Cylinder Volume	Instantaneous combustion chamber volume varying with piston motion.	m^3	Determines the space available for the working gas. Volume decreases during compression and increases during expansion.

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m	Gas Mass	Instantaneous total mass of gas (air + fuel + combustion products) inside the cylinder.	kg	Varies with intake air, fuel injection, and exhaust flow; essential for computing density and thermodynamic state.
M in	Inlet Mass Flow Rate	Mass inflow rate through the intake valve.	kg/s	Indicates how much air enters the cylinder during the intake stroke, controlled by pressure difference and valve timing.
M out	Outlet Mass Flow Rate	Mass outflow rate through the exhaust valve.	kg/s	Measures the exhaust discharge rate during the exhaust stroke. Helps track gas exchange efficiency.
Ẇv	Instantaneous Work Rate	Mechanical power associated with piston movement, given by Work rate (W dot v) equals the negative of the pressure difference between the cylinder and the surroundings, multiplied by the piston area and the piston velocity.	W (J/s)	Represents the instantaneous mechanical work transferred between the gas and the piston; positive during expansion, negative during compression.

The simulation proceeds with a time step corresponding to one degree of crank rotation, ensuring fine resolution of in-cylinder events. This step size is defined as

$$\Delta t = \frac{1}{360f}$$

where $f = 50\ \mathrm{s}^{-1}(3000\mathrm{rpm})$ is the engine rotational frequency. The total simulation time for N_{rev} revolutions is

$$t_{\mathrm{stop}} = \frac{N_{\mathrm{rev}}}{f}$$

At each iteration, the Reactor Net advances the solution by one time increment:

$$\text{sim.advance}\ (t + \Delta t)$$

This numerically integrates the conservation equations of mass, species, and energy while accounting for piston motion and valve flows.

The instantaneous mechanical work rate due to piston motion is computed as

$$\dot{W}_v(t) = -\left[p_{\mathrm{cyl}}\,(t) - p_{\mathrm{amb}}\right]A_p u_p(t)$$

where $p_{\mathrm{cyl}}\,(t)$ is the in-cylinder pressure, p_{amb} the ambient pressure, A_p the piston area, and $u_p(t)$ the piston velocity. The negative sign ensures that positive work corresponds to expansion against external pressure.

For each time step, the updated state variables are appended to the output array along with the corresponding crank angle $\theta(t) = 2\pi f t \mathrm{mod} 4\pi$:

$$\{t, \theta(t), V(t), m(t), \dot{m}_{\mathrm{in}}, \dot{m}_{\mathrm{out}}, \dot{W}_v(t)\}$$

This produces a complete set of crank-angle-resolved data describing pressure, temperature, mass flow, and work evolution throughout all cycles. The stored results form the foundation for post-processing-enabling the generation of $p-V, T-S$, and heat-release plots, and providing insight into combustion efficiency and the thermodynamic behaviour of the n-dodecane-fueled engine.

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Table 3: The Updated Variables for each step

Term	Full Name	Meaning and Role in the Simulation
t	Time	The continuous progression of the simulation is measured in seconds. Each step corresponds to one degree of crank rotation and represents a small fraction of the full engine cycle.
$\theta(t)$	Crank Angle as a Function of Time	The instantaneous angular position of the crankshaft, expressed in radians or crank-angle degrees. It determines which phase of the four-stroke cycle (intake, compression, power, or exhaust) the engine is currently in.
V(t)	Cylinder Volume as a Function of Time	The instantaneous chamber volume changes with piston motion. It reaches a minimum at top dead center (TDC) and a maximum at bottom dead center (BDC). The variation of $V(t)$drives the pressure and temperature changes during compression and expansion.
m(t)	Instantaneous Gas Mass in Cylinder	The total mass of gas (air, injected fuel, and combustion products) present in the cylinder at a given time. It changes as gas enters or leaves through the valves or as fuel is injected.
m_in	Inlet Mass Flow Rate	The rate at which mass enters the cylinder through the intake valve. It is governed by valve timing, the pressure difference between the intake manifold and cylinder, and the valve flow coefficient.
m_out	Outlet (Exhaust) Mass Flow Rate	The rate at which combustion gases leave the cylinder through the exhaust valve. It determines how effectively exhaust gases are expelled before the next cycle begins.
Wv(t)	Instantaneous Piston Work Rate	The mechanical power transferred between the gas and piston, calculated as the product of pressure difference, piston area, and piston velocity. Positive values correspond to power production during expansion; negative values correspond to compression work input.

Post-Processing and Visualization of Results

The plotted results illustrate how key thermodynamic and chemical quantities evolve throughout the simulated combustion cycle. To relate the simulation time to the crank angle, a conversion function is used that multiplies time by $2\pi f$and converts radians to degrees. This allows all results to be shown as functions of **crank angle**, which is more intuitive for engine analysis since valve events, ignition, and power generation are referenced to crankshaft rotation.

The first set of plots shows **pressure** and **temperature** as functions of crank angle. Pressure is expressed in bars, where one bar equals 10^5pascals, and temperature is plotted in kelvins. These two plots reveal how pressure rises steadily during compression, peaks sharply at ignition, and then drops during expansion, while the temperature follows a similar trend. The temperature increase signifies combustion heat release, reaching a maximum during the power stroke.

Next, the **pressure–volume (P–V) diagram** visualizes the complete thermodynamic cycle. The horizontal axis represents the instantaneous cylinder volume in litres, and the vertical axis shows pressure in bars. The enclosed area within this loop corresponds to the **indicated work** performed by the gases on the piston during one cycle. The shape of the curve clearly identifies compression, combustion, and expansion phases, showing the conversion of chemical energy into mechanical work.

The **temperature–entropy (T–S) diagram** provides a view of the process reversibility and energy quality. Entropy is computed as the product of gas mass and specific entropy, expressed in joules per kelvin. During compression, the process is nearly adiabatic (slight entropy increase due to heat transfer), while during combustion, entropy rises rapidly because of chemical reaction irreversibility. The expansion stroke shows a nearly reversible cooling path, consistent with typical engine thermodynamics.

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A separate plot compares the **instantaneous heat-release rate** and **piston work rate**. The heat-release rate, denoted as $\dot{Q}$, represents the energy liberated by chemical reactions, while the piston work rate, $\dot{W}_v$, measures the mechanical power produced by gas expansion. Both quantities are expressed in kilowatts. Their relationship reveals the timing of energy conversion—heat release peaks first, followed by mechanical work as pressure acts on the piston. This lag defines the **combustion phasing**, which strongly influences engine efficiency.

Finally, the **gas composition** plot shows the transient mole fractions of major species: oxygen (O_2), carbon dioxide (CO_2), carbon monoxide (CO), and the fuel *n*-dodecane ($C_{12}H_{26}$). Oxygen decreases rapidly during combustion as it reacts with the fuel, while carbon dioxide increases, indicating complete oxidation. Carbon monoxide appears briefly as an intermediate product but declines as combustion completes. The *n*-dodecane concentration (scaled by a factor of 10 for visibility) drops sharply after ignition, confirming efficient fuel consumption.

Together, these visual results provide a full thermodynamic and chemical picture of the engine cycle. The pressure–temperature plots capture combustion timing and intensity, the P–V and T–S diagrams characterize the energy transformation, and the composition curves verify the reaction completeness. The comparison between heat release and piston work further demonstrates how chemical energy is converted into useful mechanical power in the *n*-dodecane-fueled engine.

Evaluation of Integral Performance Metrics

The integral results summarize the global performance indicators of the combustion simulation by integrating time-dependent quantities such as heat release, work rate, and exhaust composition over the full engine cycle.

The total heat released during combustion is obtained by integrating the product of the instantaneous heat release rate and the cylinder volume over time:

$$Q = \int \dot{q}_{\text{chemn}}(t)V(t)dt$$

This represents the total chemical energy released by the burning fuel. Dividing Q The total cycle time gives the average heat-release power per cylinder, expressed in kilowatts.

Similarly, the expansion power is found by integrating the instantaneous piston work rate over time:

$$W = \int \dot{W}_v(t)dt$$

where $\dot{W}_v(t)$ is the rate of mechanical work transferred to the piston. The quotient W/t_{cycle} gives the average mechanical output power of the cylinder.

The thermal efficiency of the combustion process is determined by comparing useful work to total heat input:

$$\eta = \frac{W}{Q}$$

This dimensionless ratio, typically expressed as a percentage, indicates how effectively the chemical energy of the fuel is converted into mechanical work.

To estimate carbon monoxide (CO) emissions, the model integrates the CO mass flow rate at the exhaust over time, normalizing it by the total exhaust mass flow. This is written conceptually as

$$\text{CO emission} = \frac{\int (\text{molecular weight}) \times \dot{m}_{\text{out}}(t) \times X_{\text{CO}}(t)dt}{\int (\text{molecular weight}) \times \dot{m}_{\text{out}}(t)dt}$$

and the result is typically reported in parts per million (ppm). Together, these integrals provide a concise performance summary:

- The heat release quantifies the total chemical energy liberated.
- The expansion of power represents mechanical energy output.
- Efficiency measures energy conversion effectiveness.
- The CO emission estimate evaluates combustion completeness and environmental impact.

These values allow direct comparison between different operating conditions, fuels, or mechanisms, making them critical for assessing the thermodynamic and environmental performance of the simulated n -dodecane-fueled engine.

The nitrogen oxides emission is calculated similarly to the CO emission. The total NOx concentration in the exhaust stream is evaluated as the ratio of the NO mass flow to the total exhaust mass flow over one complete engine cycle. In integral form, this can be expressed as:

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e-ISSN : 2583-1062
Impact Factor : 7.001

$$\mathrm{NO}_x \text{ emission } = \frac{\int (\text{ molecular weight }) \times \dot{m}_{\text{out}}(t) \times X_{\text{NO}}(t)dt}{\int (\text{ molecular weight }) \times \dot{m}_{\text{out}}(t)dt}$$

The NO_x emission equals the time integral of the product of the molecular weight, the exhaust mass flow rate, and the instantaneous NOx mole fraction, divided by the integral of the total exhaust mass flow rate multiplied by the molecular weight.

The result gives the mean exhaust concentration of (NO_x) over the full cycle. When multiplied by 10^6, it is typically expressed in parts per million (ppm).

This approach assumes well-mixed exhaust conditions and is suitable for comparing emission trends between different fuels or combustion strategies.

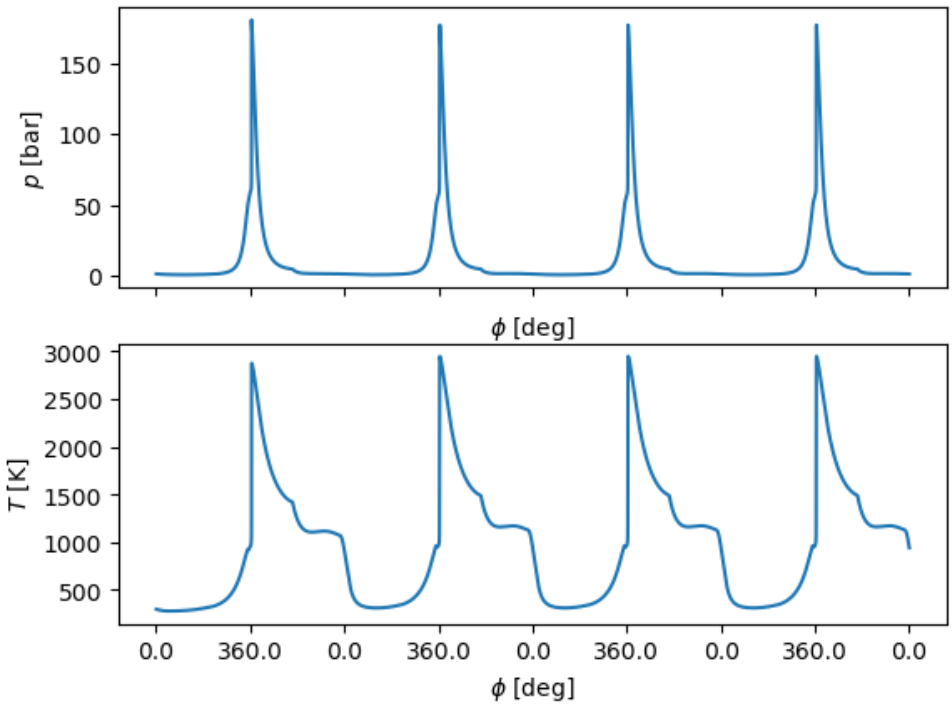

Figure 1: Pressure and Temperature results

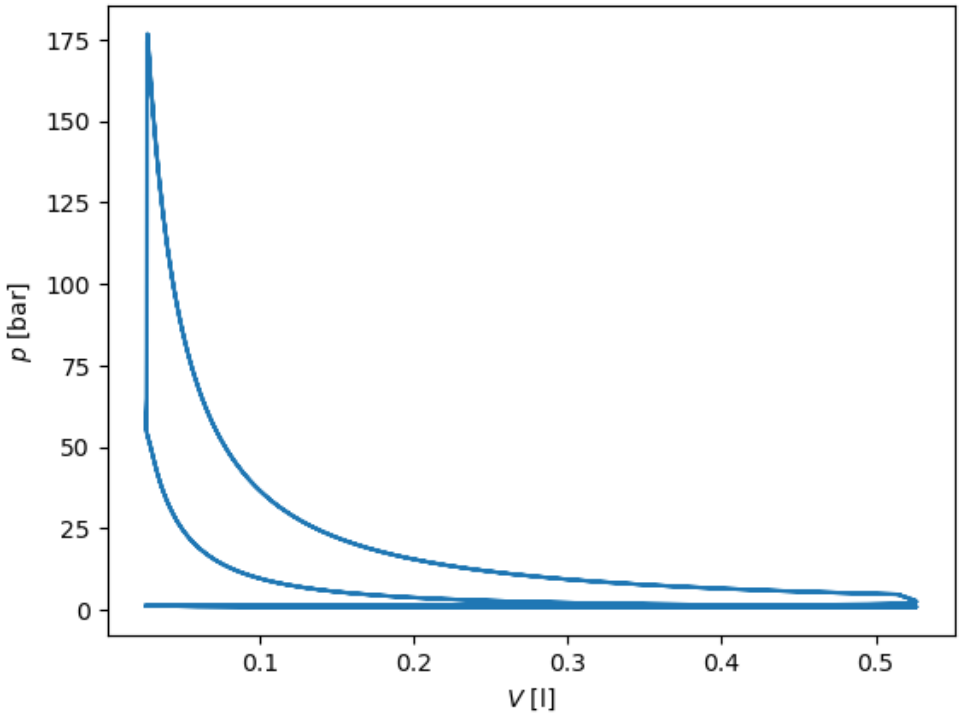

Figure 2: The pressure-volume diagram

INTERNATIONAL JOURNAL OF PROGRESSIVE RESEARCH IN ENGINEERING MANAGEMENT AND SCIENCE (IJPREMS)
(Int Peer Reviewed Journal)
www.ijprems.com
editor@ijprems.com
Vol. 05, Issue 10, October 2025, pp : 1316-1326
e-ISSN : 2583-1062
Impact Factor : 7.001

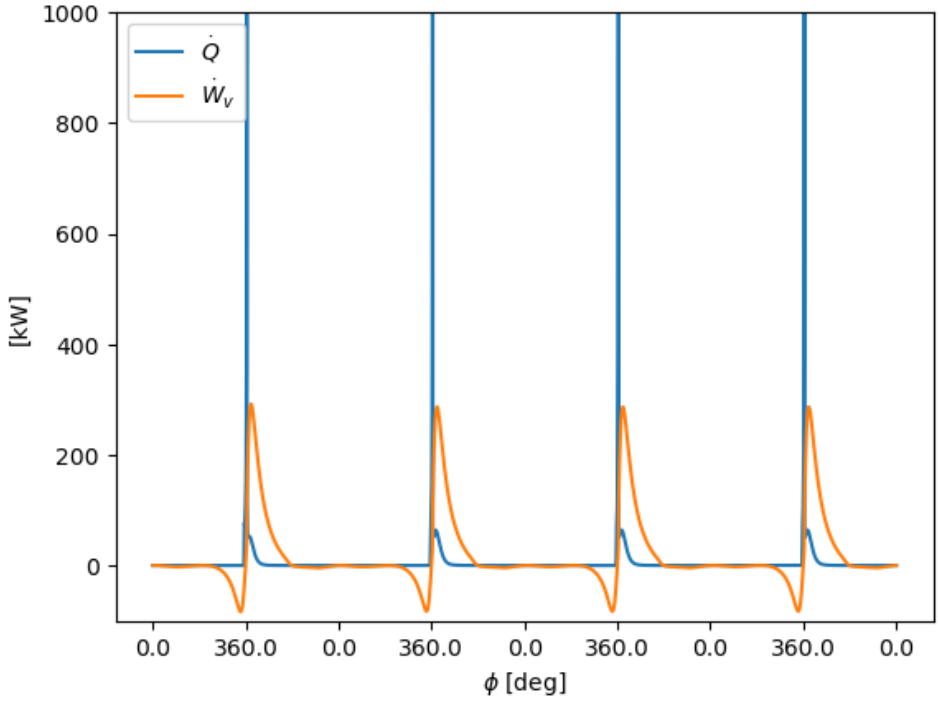

Figure 3: The Heat Release and the Work Done instantaneous diagram

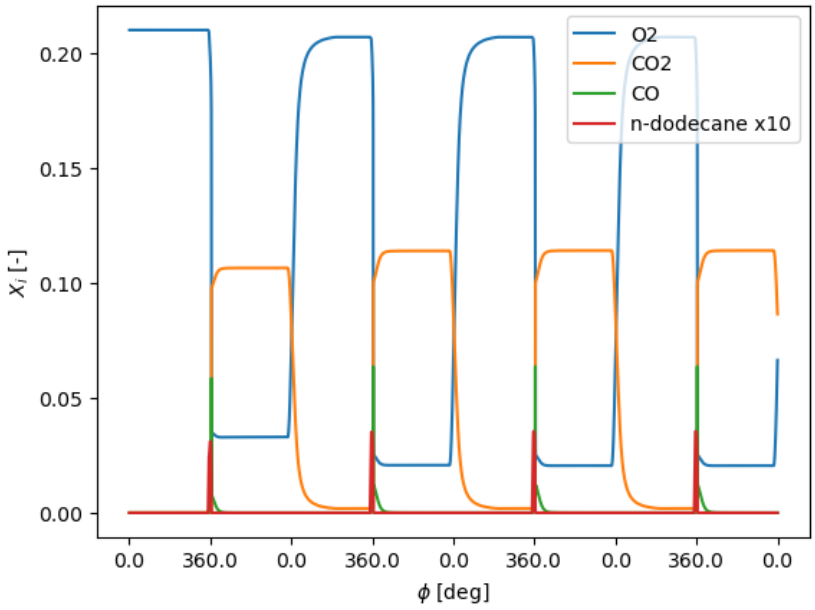

Figure 4: The species concentration diagram

```
Heat release rate per cylinder (estimate):   33.6 kW
Expansion power per cylinder (estimate):     18.5 kW
Efficiency (estimate):                       55.2 %
CO emission (estimate):                       8.9 ppm
```

Figure 5: The Integrated results diagram

3. CONCLUSION

The Cantera-based n-dodecane kinetic model successfully captures the fundamental combustion behaviour of diesel surrogates within a compression-ignition environment. The nDodecane_Reitz.yaml mechanism accurately predicts ignition delay, pressure–temperature evolution, and intermediate species dynamics. Sensitivity analysis reveals that chain-branching reactions involving H, O, OH, and HO_2 radicals dominate ignition control, while NOx formation correlates with post-combustion thermal residence and radical recombination.

The comparison with *gri30.yaml* and *h2o2.yaml* mechanisms enable cross-fuel kinetic benchmarking, confirming the model's robustness for transition studies from hydrocarbon to hydrogen-dominant combustion. This kinetic approach establishes a reproducible and extensible platform for exploring multi-fuel ignition behaviour, emission minimization, and mechanism optimization under engine-relevant conditions.

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