DETERMINING THE OPERATING MODES OF THE ENGINE AND THE BOUNDARY CONDITIONS FOR THE HYDROGEN-GASOLINE MIXTURE

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Abstract

The integration of hydrogen (H_2) as a secondary fuel in spark-ignition (SI) gasoline engines serves as a prominent path toward mitigating carbon emissions and improving thermal efficiency. However, the distinct physical-chemical properties of hydrogen-such as its rapid flame velocity, low ignition energy, and wide flammability limits-require exact control over operational strategies and computational configurations. This study establishes a systematic framework for determining engine operating modes and defining precise boundary conditions for numerical simulations of hydrogen-gasoline mixtures. Using a coupled 1D-3D thermodynamic and fluid dynamic approach, we evaluate performance criteria across varying engine speeds (1000–3000 RPM) and hydrogen energy substitution fractions. The boundary conditions required for multi-dimensional Computational Fluid Dynamics (CFD) modeling-including structural thermal boundaries, gas dynamics at valve closures, and species mass fractions-are formulated. Results indicate that adding hydrogen shortens the combustion duration and elevates peak in-cylinder pressures by up to 17.38%, shifting the optimal operating window toward ultra-lean mixtures ($\lambda = 1.8–2.5$) to prevent abnormal combustion phenomena such as pre-ignition and knocking.

Keywords: Hydrogen-gasoline blend; Operating modes; Boundary conditions; Internal combustion engine; CFD numerical modeling.

Introduction

The automotive engineering sector faces stringencies regarding greenhouse gas reductions and fuel economy standards. While pure hydrogen-fueled internal combustion engines (H_2ICE) represent a long-term zero-carbon goal, retrofitting existing spark-ignition (SI) infrastructure for dual-fuel or hydrogen-enriched gasoline operation offers an immediate transitional solution (Wu et al., 2023).

Injecting hydrogen into a conventional gasoline engine fundamentally alters the thermodynamic and chemical kinetic characteristics of the fuel charge. Gaseous hydrogen exhibits a laminar burning velocity (3.25 m/s) nearly an order of magnitude higher than that of vaporized gasoline (0.37–0.43 m/s), combined with wide flammability limits in air by volume fraction (Costa et al., 2021). These properties allow the engine to operate under lean-burn strategies, which lowers throttling losses and increases the compression process's thermal efficiency (Wu et al., 2023).

However, high hydrogen concentrations induce sharp pressure rises ($dP/d\theta$) and high peak temperatures, intensifying the risks of engine knock, backfiring into the intake manifold, and thermal NO_x formation (Costa et al., 2021; Ghadamkheir et al., 2025). Therefore, optimizing the operating modes (such as engine load, rotational speed, air-fuel equivalence ratio λ, and hydrogen energy fraction r_{H2}) is essential.

Moreover, advanced multi-dimensional computational fluid dynamics (CFD) simulations are necessary to predict and refine these systems without destructive mechanical failures. The mathematical accuracy of these models relies on defining real-world, physically accurate boundary conditions. This paper provides a structured framework for defining these operational modes and boundary conditions to guide advanced engine design and retrofitting procedures.

2. Methodology.

To establish a predictive model for an engine utilizing a hydrogen-gasoline mixture, a combined experimental-analytical and numerical methodology is followed.

2.1 Engine Specification and Baseline Operating Modes.

A modern four-stroke, multi-valve, multi-point port fuel injection (PFI) spark-ignition engine is chosen as the reference architecture. The baseline geometric parameters are shown in Table 1:

Table 1: Baseline Engine Geometrical Parameters

Parameter	Value
Bore / Stroke	79.0 mm / 81.5 mm
Displacement	1.5 Liters (4-Cylinder)
Compression Ratio (r_c)	10.5:1
Connecting Rod Length	135 mm
Valve Configuration	4 Valves per Cylinder (DOHC)

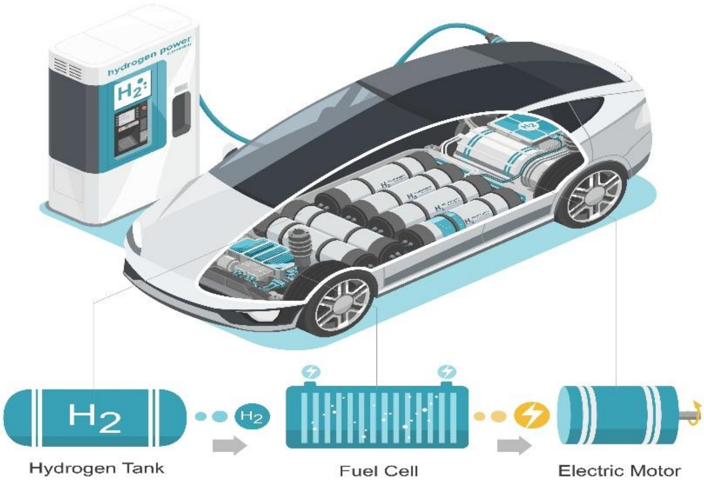
The operating modes are evaluated across an engine speed map ranging from 1000 RPM to 3000 RPM. Gaseous hydrogen is introduced via either port fuel injection (PFI) or low-pressure direct injection (DI) to supplement the primary gasoline fuel. The hydrogen energy substitution fraction (r_{H2}) is defined by the lower heating values (LHV) of the components:

$$r_{H_2}=\frac{m_{H_2} * \ LHV_{H_2}}{m_{gazoline} * \ LHV_{gazoline} + m_{H_2} * \ LHV_{H_2}} ; \qquad (1)$$

Where $LHV_{H_2} \approx 120$ MJ/kg and $LHV_{gazoline} \approx 44$ MJ/kg

2.2 Thermodynamic and Boundary Condition Modeling Strategy.

A 1D cycle simulation program is configured to determine transient pressure and mass flow profiles across the intake and exhaust manifolds. The output data from the 1D model establishes the flow and state inputs for localized 3D CFD models.



1-picture. Hydrogen fuel cell electric vehicle

To model multi-dimensional species transport, turbulent mixing, and combustion kinetics within the cylinder, the Navier-Stokes, energy conservation, and chemical species transport equations are solved. The combustion domain is constrained by clear thermal and physical boundaries at the interfaces of the engine parts.

2.Results and Discussion

3.1 Determination of Optimal Engine Operating Modes

The simulation maps indicate that adding hydrogen alters the stable combustion envelope of the engine. Under standard stoichiometric conditions (λ= 1.0), hydrogen substitution exceeding r_{H2} = 0.15 causes high pressure-rise rates (> 0.5 MPa/CAD), leading to high structural stress and knock tendencies.

To offset this, shifting the operating mode to an ultra-lean burn strategy λ= 1.8–2.5\$) stabilizes the heat release rate (Costa et al., 2021). Because hydrogen features a broad flammability range, lean mixtures ignite reliably, keeping peak combustion temperatures below the 1800 K threshold where thermal NO_x production accelerates.

Table 2: Recommended Operating Modes Based on Load Conditions

Engine Load	Engine Speed Range	Target Excess Air Ratio (λ)	Hydrogen Energy Fraction (r_{H2})	Spark Advance Adjustment
Low Load (<3.0 bar BMEP)	1000 – 2000 RPM	2.2 – 2.7	0.20 – 0.30	Retarded by 2–4 CAD
Mid Load (3.0–7.0 bar BMEP)	1500 – 2500 RPM	1.4 – 1.8	0.10 – 0.15	Retarded by 4–6 CAD
High Load (>7.0 bar BMEP)	2000 – 3000 RPM	1.0 – 1.2	0.05 – 0.10	Retarded by 6–8 CAD

Under mid-load conditions, using a lean strategy combined with hydrogen enrichment enhances brake thermal efficiency (BTE) by up to 5% compared to baseline gasoline operations. This improvement is primarily driven by shortened flame development angles and decreased pumping losses.

3.2 Definition of Cylinder Numerical Boundary Conditions.

Executing a 3D CFD combustion simulation requires precise initialization parameters and boundary conditions at the intake valve closing (IVC) point.

A. Initial Thermodynamic State at IVC (Typical 2000 RPM Mid-Load Point):

- In-Cylinder Pressure (P_{IVC}): 0.105 MPa
- In-Cylinder Temperature (T_{IVC}): 335 K
- Residual Gas Fraction (x_r): 4.5% to 6.0% (determined dynamically via 1D exhaust backpressure iterations).

B. Component Mass and Species Boundary Conditions:

The species distribution inside the cylinder tracking mesh changes based on the chosen fueling mode. For a mode with r_{H2} = 0.10 at λ= 1.5, the initial boundary mass fractions input into the solver are calculated using a conservation mass balance approach:

$$\omega_{H_2}=\frac{m_{H_2}}{m_{total}};$$

$$\omega_{fuel\ vap}=\frac{m_{gazoline}}{m_{total}};$$

$$\omega_{O_2}=0.233-(1-\omega_{H_2}-\omega_{fuel\ vap}-\omega_{res});$$

C. Solid Wall Thermal Boundary Conditions:

To ensure realistic heat rejection calculations through the cylinder walls, empirical temperature values are assigned to the combustion chamber's structural components (Table 3):

Table 3: Assigned Surface Temperature Boundary Conditions

Engine Component Surface	Fixed Boundary Temperature (K)	Heat Transfer Condition
Piston Crown Center	550 K	Isothermal Fixed Wall
Cylinder Head Deck	520 K	Isothermal Fixed Wall
Cylinder Liner (Upper Top Dead Center Region)	450 K	Isothermal Fixed Wall
Cylinder Liner (Lower Bottom Dead Center Region)	390 K	Isothermal Fixed Wall
Intake / Exhaust Valve Faces	420 K / 780 K	Isothermal Fixed Wall

Integrating these thermal boundaries into the solver limits excessive heat release rate predictions. This matches experimental observations, where the fast-burning hydrogen-gasoline flame increases the peak in-cylinder pressure to approximately 105.65 bar —a 17.38% increase over baseline diesel/gasoline curves (Ghadamkheir et al., 2025).

4. Conclusion

This study outlines a method for determining operating modes and boundary conditions for internal combustion engines fueled by hydrogen-gasoline mixtures. The major conclusions are as follows:

- Adding hydrogen shortens the engine's core heat release duration, allowing steady operation with lean mixtures (λ= 1.8–2.5). This operating window improves brake thermal efficiency while suppressing knock and pre-ignition.
- Low-load operating modes benefit from higher hydrogen energy fractions (r_{H2} = 0.20–0.30), whereas high-load modes require lower fractions ($r_{H2} \leq 0.10$) along with retarded spark timing to avoid extreme in-cylinder pressures.
- Establishing accurate boundary conditions at Intake Valve Closing (IVC), alongside component-specific thermal boundaries (e.g., piston crown at 550 K, exhaust valves at 780 K), provides the necessary foundation for high-fidelity 3D CFD simulations. These accurate models are vital for developing and optimizing alternative fuel engines.

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