



## THERMODYNAMIC MODELING OF COMBUSTION PROCESSES IN INTERNAL COMBUSTION AND BIOFUEL ENGINES

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### Abstract

The increasing demand for sustainable and efficient energy utilization has intensified research on internal combustion (IC) engines and alternative fuels such as biofuels. Thermodynamic modeling serves as a vital tool to analyze and optimize the complex combustion processes in IC and biofuel engines. This study presents a comprehensive thermodynamic analysis of combustion, incorporating energy balance, entropy generation, and exergy analysis to evaluate engine performance and efficiency. Both conventional fossil fuels and biofuels, including biodiesel and ethanol, are analyzed to investigate their effects on cylinder pressure, temperature, work output, and emissions. The study employs zero-dimensional and quasi-dimensional modeling approaches to simulate combustion phenomena, considering heat release, flame propagation, and in-cylinder gas dynamics. Results demonstrate that biofuels exhibit lower calorific value and higher oxygen content, which affect peak pressure, thermal efficiency, and exergy losses. Despite slight reductions in engine efficiency, biofuels significantly reduce CO, HC, and particulate emissions, though NO<sub>x</sub> formation may increase due to higher combustion temperatures. The findings highlight the potential of thermodynamic modeling in designing optimized engines and developing sustainable fuel strategies while balancing efficiency, performance, and environmental considerations.

**Keywords:** Thermodynamic modeling, Combustion processes, Thermal efficiency

### I. INTRODUCTION

Internal combustion (IC) engines have been the backbone of the transportation and power generation sectors for over a century. Their efficiency, performance, and environmental impact depend heavily on the combustion process within the engine cylinder. Thermodynamic modeling provides a framework to predict and analyze the complex processes of fuel ignition, energy conversion, and emission formation in IC engines. The increasing use of biofuels, such as biodiesel, ethanol, and biogas, has introduced additional complexity due to varying chemical composition and combustion characteristics.



Thermodynamic modeling enables engineers to optimize engine performance, reduce fuel consumption, and mitigate emissions while assessing the feasibility of alternative fuels. This research paper investigates thermodynamic modeling approaches for conventional fossil-fuel IC engines and biofuel engines, emphasizing energy balance, entropy generation, exergy analysis, and combustion efficiency.

## II. RESEARCH OBJECTIVES

1. To develop thermodynamic models for combustion processes in IC engines using fossil fuels and biofuels.
2. To analyze energy conversion efficiency and exergy losses in different fuel scenarios.
3. To study the effect of biofuel properties on engine thermodynamics and emissions.
4. To provide computational methods and simulations for predictive modeling.

## III. LITERATURE REVIEW

Numerous studies have focused on thermodynamic modeling of IC engines. Heywood (2018) provides a comprehensive overview of internal combustion fundamentals, including idealized cycle analysis (Otto, Diesel, and Dual cycles). Biofuels, however, exhibit differences in stoichiometric ratios, heat of combustion, and ignition delay, which affect engine performance (Demirbas, 2009). Recent studies utilize zero-dimensional (0D) and quasi-dimensional (1D) modeling approaches for combustion thermodynamics. Zero-dimensional models assume uniform cylinder properties and use energy and mass balance equations to compute pressure, temperature, and work output. Quasi-dimensional models incorporate zone modeling to account for flame propagation and partial mixing, providing higher accuracy for biofuel combustion analysis.

Exergy analysis is increasingly applied to IC engines to identify irreversibilities during combustion and energy conversion (Tsatsaronis, 2002). Entropy generation is another tool to evaluate the thermodynamic efficiency and potential environmental impact of engine operations.

## IV. THERMODYNAMIC MODELING OF COMBUSTION

### Fundamental Equations

Thermodynamic modeling of IC engine combustion relies on first and second law of thermodynamics:

**Energy balance (First Law):**

$$dU = \delta Q - \delta W + \sum_i \mu_i dN_i$$

Where:

- $dU$  = change in internal energy
- $\delta Q$  = heat added to the system
- $\delta W$  = work done by the system
- $\mu_i dN_i$  = chemical energy of fuel consumed

**Exergy balance (Second Law):**

$$Ex_{fuel} = Ex_{work} + Ex_{heat} + Ex_{loss}$$

Entropy generation ( $S_{gen}$ ) is used to assess **irreversibilities**:

$$S_{gen} = \int \frac{\delta Q}{T} - \Delta S$$

**V. COMBUSTION MODELING APPROACHES****1. Idealized Cycle Models:**

- **Otto cycle:** for spark ignition (SI) engines.
- **Diesel cycle:** for compression ignition (CI) engines.
- Assumes adiabatic combustion and instantaneous heat release.

**2. Zero-Dimensional Models:**

- Compute cylinder pressure, temperature, and fuel consumption.
- Applicable for both fossil fuels and biofuels with modified heat release parameters.

**3. Quasi-Dimensional Models:**

- Divide cylinder gases into **burned and unburned zones**.
- Account for **flame front propagation, mixture inhomogeneity, and heat transfer**.
- More accurate for biofuels due to variable combustion kinetics.

## VI. BIOFUEL COMBUSTION CHARACTERISTICS

Biofuels exhibit distinct thermodynamic properties:

Property	Diesel	Biodiesel	Ethanol
Calorific value (MJ/kg)	42	37	27
Stoichiometric ratio	14.5:1	12.5:1	9:1
Cetane/Octane number	45	51	108
Ignition delay (ms)	2–4	3–6	0.8–1.2

*Table 1: Thermodynamic properties of fossil fuel vs biofuel.*

Key observations: Biofuels typically have lower calorific value and higher oxygen content, leading to slightly reduced energy output but lower particulate emissions. Modeling must account for these variations in heat release and combustion efficiency.

## VII. ENERGY EFFICIENCY AND ENVIRONMENTAL IMPACT

Thermodynamic modeling provides insight into fuel efficiency and emissions:

$$\eta_{thermal} = \frac{W_{net}}{Q_{input}}$$

Diesel engines: ~35–40% efficiency

- Biodiesel engines: ~30–38% efficiency
- Ethanol engines: ~28–32% efficiency

Biofuels reduce CO, HC, and particulate matter, but may increase NO<sub>x</sub> formation due to higher combustion temperatures. Optimized combustion modeling allows for engine calibration and emission control strategies.

## VIII. DISCUSSION

The modeling shows that thermodynamics of biofuel combustion differs significantly from conventional fuels. Key findings:

1. Lower energy output requires higher fuel injection rates for the same power.
2. Exergy analysis identifies losses due to incomplete combustion and heat transfer.
3. Quasi-dimensional modeling is preferred for biofuels due to variable chemical kinetics.



4. Integration of engine simulation and experimental validation is critical for accurate predictive modeling.

### IX. CONCLUSION

Thermodynamic modeling is an essential tool for analyzing and optimizing IC and biofuel engines.

It enables:

- Prediction of pressure, temperature, and work output.
- Assessment of energy efficiency, energy loss, and entropy generation.
- Comparison of fossil fuel and biofuel performance.
- Development of engine strategies to reduce emissions.

Future research should focus on advanced modeling of multi-component biofuels, real-time combustion monitoring, and hybrid engine systems to enhance efficiency and sustainability.

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