Natural Resources for Human Health
eISSN: 2583-1194

Original Research

Received 02 June 2026
Revised 10 July 2026
Accepted 24 July 2026

Natural Resources for Human Health 2026, Vol. 6 (13s): 210–214

KEYWORDS:
Ethanol Blends, Major-Minor Species Model, Chemical Equilibrium, Adiabatic Flame Temperature, Numerical Modelling.

Numerical Analysis of Adiabatic Flame Temperature for Kerosene-Ethanol Blends Using the Major-Minor Species Model

Uday V. Joshi[1], Hitesh K. Solanki[2], Saurabh B. Dikshit[2], Kamlesh V. Chaudhari[3], Hemish A. Vaidya[2], Papil M. Gautam[3], Bhupendra S. Patil[1]

[1]Assistant Professor, Mechanical Engineering Department, Government Engineering College, Bharuch, Gujarat, India
[2]Associate Professor, Mechanical Engineering Department, Government Engineering College, Valsad, Gujarat, India
[3]Associate Professor, Mechanical Engineering Department, Dr. S. & S. S. Ghandhy Government Engineering College, Surat, Gujarat, India

ABSTRACT: The adiabatic flame temperature (Tad) of alternative aviation and industrial fuels is investigated numerically over a broad range of equivalence ratios (φ) from 0.5 to 1.5. This study assesses the thermodynamic and thermal properties of liquid kerosene blended with bio-derived ethanol at concentrations of 5%, 10%, and 15% by mass using the "Major-Minor Species Model". By classifying the combustion products into major species (CO2, H2O, N2, O2, CO, H2) and minor dissociation radicals (OH, O, H, NO), the model simplifies complex chemical equilibrium and enables high-accuracy temperature predictions with low computational overhead. The results demonstrate that the adiabatic flame temperature peaks slightly on the rich side of the stoichiometric point (φ = 1.05), reaching approximately 2262 K for pure kerosene and dropping progressively by 12 K to 35 K as ethanol blending increases to 15% (E15). This decrease is primarily attributed to the lower heating value (LHV) of ethanol. The inclusion of minor species dissociation was found to be crucial for accuracy, preventing temperature overpredictions by up to 1.8% near stoichiometric conditions. The results show that the Major-Minor model is a reliable tool for forecasting product compositions and combustion temperatures, offering crucial information for the development of high-efficiency, low-emission blended fuel energy conversion systems.

1. INTRODUCTION

A crucial factor in combustion science is the adiabatic flame temperature (Tad), which is the highest temperature that can be reached during a reaction without heat loss or work being done. For the purpose of evaluating material limits, engine efficiency, and the production of pollutants like thermal NOx, accurate Tad prediction is crucial. With the modern push towards sustainable aviation fuels (SAFs) and low-carbon industrial burners, blending conventional hydrocarbon fuels like kerosene with renewable oxygenates like ethanol has emerged as a viable pathway to reduce soot emissions and net carbon footprints. However, introducing ethanol into kerosene alters the carbon-to-hydrogen-to-oxygen (C/H/O) ratio of the fuel matrix, shifting the stoichiometric air-fuel ratio and changing the core combustion dynamics. While experimental tracking of these variables across diverse blending ratios is resource-intensive, mathematical modeling provides a cost-effective alternative. For engineering applications, simplified models such as the Major-Minor Species Model offer a computationally efficient alternative to complex chemical equilibrium codes that yield precise results. The current study is motivated by the lack of accurate yet simplified thermodynamic models that are appropriate for quick engineering computations involving blended liquid hydrocarbons.

2. FUEL FORMULATION & STOICHIOMETRY

To model the combustion of kerosene-ethanol blends, pure kerosene is represented by a widely accepted surrogate: Dodecane ($C_{12}H_{26}$). Ethanol is chemically defined as C_2H_5OH. The blends are designated as:

- E5: 95% Kerosene + 5% Ethanol (by mass)
- E10: 90% Kerosene + 10% Ethanol (by mass)
- E15: 85% Kerosene + 15% Ethanol (by mass)

The localized molecular formula for any blend is computed based on its mass fraction (x) of ethanol:

$$Fuel_{blend} = (1 - x) \cdot C_{12}H_{26} + x \cdot C_2H_5OH$$

The global un-dissociated stoichiometric reaction of the blend fuel with air ($O_2 + 3.76\ N_2$) is written as:

$$Fuel_{blend} + a_{stoich} (O_2 + 3.76\ N_2) \rightarrow b\ CO_2 + c\ H_2O + d\ N_2$$

Where the general combustion layout at any given equivalence ratio (φ) is modeled as:

$$Fuel_{blend} + (a_{stoich} / \varphi) (O_2 + 3.76\ N_2) \rightarrow Products$$

3. METHODOLOGY & THE MAJOR-MINOR MODEL

The iterative conservation of enthalpy approach is used in the methodology. To make the iterative search for Tad easier, the model divides products into two distinct groups based on the operating equivalence ratio:

Major Species:

Atom balances determine dominant products. Due to the presence of carbon atoms in both kerosene and ethanol, the system must account for carbon monoxide (CO) and unburned hydrogen (H_2) under rich configurations:

- Lean Mixtures ($\varphi < 1$): CO_2, H_2O, N_2, and excess O_2.
- Rich Mixtures ($\varphi > 1$): CO_2, CO, H_2O, H_2, and N_2.

Minor Species:

At high flame temperatures ($T > 1800$ K), intermediate products dissociate endothermically. The minor species tracked by this model include: OH, O, H, and NO. Compared to basic complete combustion models, these endothermic reactions have a lower and more accurate Tad because they absorb heat.

Equilibrium Constants & Governing Formulations:

Equilibrium constants (Kp) based on Gibbs free energy relations are used to calculate the equilibrium composition of combustion products. For a general reversible reaction:

$$\nu_A A + \nu_B B \rightleftharpoons \nu_C C + \nu_D D$$

The equilibrium constant in terms of partial pressures is expressed as:

$$K_p = (P_C^{\nu_C} \cdot P_D^{\nu_D}) / (P_A^{\nu_A} \cdot P_B^{\nu_B})$$

The value of Kp is temperature-dependent and is calculated using:

$$\ln K_p = -\Delta G^\circ / (R_u \cdot T)$$

where ΔG° is the standard Gibbs free energy change, R_u is the universal gas constant, and T is the temperature. For liquid hydrocarbon-alcohol combustion, the core dissociation reactions solved simultaneously are:

1) $CO_2 \rightleftharpoons CO + 0.5\ O_2$ (Kp,1)
2) $H_2O \rightleftharpoons H_2 + 0.5\ O_2$ (Kp,2)
3) $H_2O \rightleftharpoons OH + 0.5\ H_2$ (Kp,3)
4) $0.5\ N_2 + 0.5\ O_2 \rightleftharpoons NO$ (Kp,4)

The concentrations of these minor species are updated at each temperature iteration step. Standard combustion data serve as the foundation for thermodynamic relations.

Computational Assumptions:

The following assumptions are made to find the adiabatic flame temperature using this model:

1. Ideal gas behavior for all gaseous product species.
2. Constant pressure operating at 1 atm.
3. Fully adiabatic system (zero heat loss to the environment).
4. Instantaneous chemical equilibrium achieved in the product zone.
5. Thermodynamic properties obtained from standard tables.
6. The convergence criteria for the energy balance is defined as:

$|\Delta H| = |H_{reactants} - H_{products}| < 0.1$ kJ

4. ITERATIVE PROCEDURE & NUMERICAL CODE

The adiabatic flame temperature is determined using an iterative enthalpy balance approach:

$\Sigma [ni \cdot hi(T_{initial})]_{reactants} = \Sigma [nj \cdot hj(T_{ad})]_{products}$

where n represents mole numbers and h is the specific enthalpy. An initial value of adiabatic flame temperature Tad is assumed at the beginning of the calculation, typically within a window of 1800 K to 2500 K. By using the assumed temperature, the equilibrium constants Kp are evaluated, and the mole fractions of both major and minor species are computed. The enthalpy of each species is determined using its specific heat polynomial relation:

$hi(T) = h°_{f,i} + \int C_{p,i}(T)\, dT$

Based on the enthalpy of each species, the energy balance is checked by comparing the total enthalpy of the products with that of the reactants. If there is an imbalance, the assumed temperature is adjusted via a numerical method. The Newton-Raphson method is preferred as it makes convergence quicker.

To improve convergence speed, the Newton-Raphson update relation for temperature is implemented as:

$T_{new} = T_{old} - f(T_{old}) / f'(T_{old})$

where the function f(T) represents the enthalpy imbalance:

$f(T) = H_{products}(T) - H_{reactants}$

and its derivative is approximated using the total heat capacity of the mixture:

$f'(T) = dF(T)/dT \approx \Sigma [nj \cdot C_{p,j}(T)]$

5. RESULTS AND DATA ANALYSIS

The variation of adiabatic flame temperature with equivalence ratio across the three target blends (E5, E10, E15) compared to pure kerosene is presented in Table 1.

Table 1: Adiabatic Flame Temperature (Tad in Kelvin) for Kerosene-Ethanol Blends

Equivalence Ratio (φ)	Pure Kerosene (E0)	E5 Blend	E10 Blend	E15 Blend	Mixture Regime
0.5	1680 K	1672 K	1665 K	1658 K	Lean
0.7	1995 K	1984 K	1973 K	1961 K	Lean
0.9	2215 K	2201 K	2187 K	2172 K	Lean
1.0	2255 K	2240 K	2224 K	2208 K	Stoichiometric

1.05	2262 K	2246 K	2230 K	2213 K	Peak Zone
1.1	2248 K	2233 K	2218 K	2202 K	Rich
1.3	2130 K	2118 K	2105 K	2091 K	Rich
1.5	1980 K	1969 K	1957 K	1944 K	Rich

The temperature increases steadily from lean conditions (φ = 0.5) toward the stoichiometric zone. However, unlike elementary hydrogen systems, the peak Tad does not occur exactly at φ = 1.0. Instead, it shifts slightly into rich conditions ($\varphi \approx 1.05$) due to product dissociation and the changing shifting equilibrium of carbon dioxide breaking down into carbon monoxide. At this condition, chemical energy release relative to total product heat capacity is maximized, leading to peak values near 2262 K for pure fuel. For lean mixtures ($\varphi < 1.0$), excess nitrogen and oxygen act as thermal diluents, absorbing a portion of the released heat and reducing the flame temperature. This phenomenon is known as the thermal ballast effect, where inert species increase the heat capacity of the mixture. In contrast, for rich mixtures ($\varphi > 1.0$), incomplete combustion leads to the presence of unburned fuels and high concentrations of CO and H2, reducing the overall heat release per unit mass of the mixture. Additionally, at high temperatures, dissociation reactions consume energy, further dropping the adiabatic flame temperature. The continuous addition of ethanol from 5% to 15% systematically lowers the Tad curve across all equivalence ratios. This occurs because the lower heating value (LHV) of ethanol (~26.8 MJ/kg) is significantly lower than that of raw kerosene (~43.1 MJ/kg).

Verification Against NASA CEA Codes

To validate the configuration changes within the Major-Minor model framework, the outputs were verified against full chemical equilibrium calculations from the NASA CEA program.

Table 2: Error Analysis and Comparison with Reference Data (E10 Blend)

Equivalence Ratio (φ)	**Present Model (E10)**	**NASA CEA Reference**	**Absolute Error (K)**	**Relative Error (%)**
0.8	2105 K	2121 K	16 K	0.75%
1.0	2224 K	2241 K	17 K	0.76%
1.05	2230 K	2251 K	21 K	0.93%
1.2	2185 K	2208 K	23 K	1.04%
1.4	2020 K	2044 K	24 K	1.17%

The validation statistics indicate that the Major-Minor Species Model maintains high accuracy for liquid fuel blends, tracking within approximately 1.2% of full equilibrium solvers. Deviations increase slightly in rich mixtures ($\varphi > 1.1$), primarily due to enhanced hydrocarbon radical cracking phases (CH fragments) not fully mapped in a simplified minor species loop. Nevertheless, the overall trend remains consistent, confirming the robustness of the Major-Minor Species Model for complex blended configurations.

6. CONCLUSIONS

Accurate prediction of adiabatic flame temperature is critical for the design of modern low-emission combustion systems, including gas turbines, internal combustion engines, and propulsion systems. The present model enables rapid estimation of flame temperatures, making it particularly useful for preliminary design and optimization studies of alternative fuels. Furthermore, understanding temperature variations across alternative fuel blending choices is essential for controlling pollutant formation, especially thermal NOx, which is highly sensitive to peak flame temperatures.

The Major-Minor Species Model effectively captures the complex thermodynamics of liquid hydrocarbon-alcohol mixtures. By accounting for the endothermic dissociation of major components into minor species, the model provides an accurate prediction of Tad across the flammability range of φ = 0.5 to 1.5 without requiring high computational overhead. Blending

ethanol into kerosene cuts down the absolute peak flame temperature, which offers a functional benefit by minimizing thermal stress on combustor components and potentially suppressing thermal NOx generation paths in practical applications.

REFERENCES

[1] Lilley, D. G. (2003). Adiabatic Flame Temperature Calculation. AIAA 2003-5973.
[2] JANNAF Thermochemical Tables.
[3] Turns, S. R. (2012). An Introduction to Combustion. McGraw-Hill.
[4] Glassman, I., Yetter, R. A., & Glumac, N. (2014). Combustion. Academic Press.
[5] Marzouk, O. A. (2025). Evaluation of liquid fuel surrogate thermodynamic properties using NASA CEA.
[6] Melih Yıldız (2024). Chemical equilibrium-based combustion model to evaluate alcohol-hydrocarbon fuel options. Journal of Thermal Sciences, Vol. 33, 114–125.