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1D flame tabulation for hydrogen combustion modeling

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1D Flame Tabulation for Hydrogen Combustion Modeling

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This study investigates hydrogen-methane mixtures using Cantera. By varying the width and product temperature according to a fixed hydrogen ratio in the mixture, the velocity and strain rate of the mixture are adjusted. The initial state is defined using a gas object, and subsequently, a flame object is employed to observe the flame reactions in a counterflow premixed flame.

I. Nomenclature

ϕ	=	equivalence ratio
α	=	thermal diffusivity
x_{H_2}	=	hydrogen mole fraction in the fuel mixture
K_a	=	strain rate
β	=	heat loss coefficient
$S_c F$	=	consumption speed
T_{ad}	=	adiabatic flame temperature
T_p	=	product temperature
T_0	=	initial temperature
P_0	=	initial pressure
C_p	=	specific heat at constant pressure, J/(kg · K)
ρ	=	density, kg/m ³
λ	=	thermal conductivity, W/(m · K)
δ_{L0}	=	laminar unstretched adiabatic flame thickness, m
S_{L0}	=	laminar unstretched adiabatic flame speed, m/s
κ	=	flame stretch, 1/s

II. Introduction

HYDROGEN-METHANE mixtures have garnered considerable attention as a cleaner and more efficient alternative to conventional hydrocarbon fuels. Hydrogen addition reduces carbon emissions while enhancing combustion efficiency due to its high diffusivity, low ignition energy, and faster flame speed compared to methane. These properties make hydrogen-enriched fuels a promising option for addressing environmental and energy challenges in modern combustion systems.

However, the behavior of hydrogen-enriched methane flames is significantly influenced by key parameters such as **strain rate** (K_a) and **heat loss** (β). The strain rate quantifies the aerodynamic stretching of the flame surface caused by opposing flows, while heat loss represents the thermal energy dissipated to the surroundings, particularly under non-adiabatic conditions. Both factors play a critical role in determining flame stability, structure, and extinction.

The study of **laminar flames** provides fundamental insights into chemical kinetics and the intrinsic structure of hydrogen-enriched flames. These laminar flame properties serve as a foundation for understanding more complex combustion behaviors. However, practical combustion systems, such as gas turbines and engines, involve complex flows that are better approximated using **counterflow premixed flames**. The counterflow configuration enables systematic investigation of the effects of strain rate and heat loss on flame characteristics while maintaining control over operating conditions such as equivalence ratio (ϕ) and hydrogen mole fraction (x_{H_2}).

In this study, **Cantera**, a Python-based chemical kinetics simulation tool, is used to simulate CH₄-H₂-air counterflow premixed flames. The counterflow configuration is particularly advantageous as it provides a well-defined boundary condition to analyze flame properties such as flame speed, consumption speed (S_{cF}), and thermal diffusivity under controlled strain rates. This study also focuses on the effect of hydrogen addition and heat loss on flame stabilization, extinction limits, and the transition between low and high strain rates.

Furthermore, the results of this study are compared with reference data from **Garcia2022b** to validate the accuracy of the simulations and the functionality of the developed code. By exploring the thermo-diffusive behavior of hydrogen-methane mixtures, this research provides deeper insights into the interplay between strain rate, heat loss, and fuel composition, which are crucial for designing efficient and stable combustion systems.

Objectives of the Study:

- 1) To investigate the effects of strain rate (Ka) and heat loss (β) on $\text{CH}_4\text{-H}_2$ -air counterflow premixed flames.
- 2) To analyze how hydrogen addition (x_{H_2}) influences flame structure, stability, and normalized consumption speed (S_{cF}/S_{I0}).
- 3) To compare experimental and simulated results with reference data to validate the accuracy and reliability of the Cantera-based simulations.
- 4) To identify the differences between laminar flames and counterflow premixed flames under varying strain rates and boundary conditions.

The remainder of this paper is structured as follows: Section 2 introduces the theoretical background on laminar and counterflow premixed flames, including key parameters such as strain rate, heat loss, and consumption speed. Section 3 details the methodology, including the Cantera-based implementation and simulation setup. Section 4 presents the results and discussion, focusing on graphical representations of key parameters and comparisons with reference data. Section 5 provides the conclusions, while Section 6 outlines the challenges encountered and future directions for improving the research outcomes.

III. Laminar Flame

A. Definition of Laminar Flame

A laminar flame refers to a flame that propagates under laminar flow conditions, where the flow is smooth and free of turbulence. In this regime, the combustion process proceeds at a steady rate, governed by the balance between heat and mass transfer. Laminar flames are widely used in combustion research as a fundamental model for analyzing reaction rates and flame behavior.

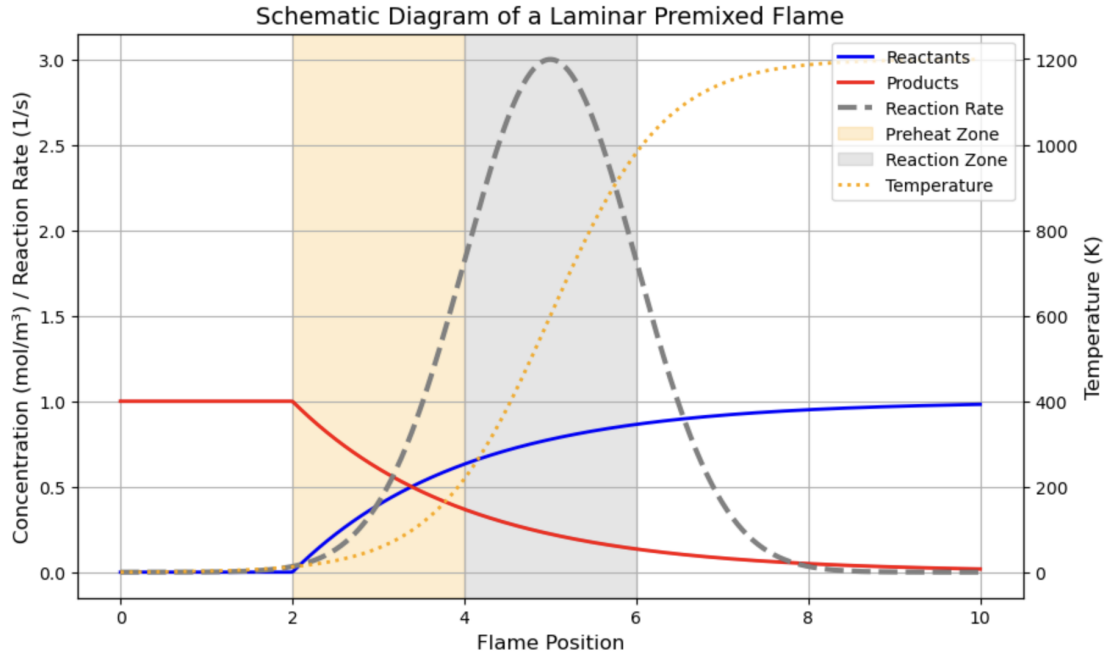


Fig. 1 Schematic diagram of a laminar premixed flame, showing reactants, products, reaction rate, and temperature distribution across the flame position. The preheat and reaction zones are highlighted.

The schematic diagram in Figure 1 illustrates the structure of a laminar premixed flame, which consists of three

primary regions: the preheat zone, the reaction zone, and the post-flame zone. The **preheat zone** represents the region where reactants are heated before ignition, while the **reaction zone** is characterized by a peak in the reaction rate due to chemical reactions. The temperature increases rapidly in this zone and stabilizes in the post-flame region where products are fully formed.

B. Role in Hydrogen-Methane Mixtures

In hydrogen-methane mixtures, the laminar flame plays a critical role in understanding the combustion characteristics of the fuel blend. Hydrogen contributes to a high flame speed and low ignition energy, while methane provides stability to the combustion process. Studying the laminar flame behavior in such mixtures is essential for designing efficient and low-emission combustion systems.

The flame structure, as shown in Figure 1, reveals that the addition of hydrogen alters the reaction rate and flame temperature distribution. Hydrogen's high diffusivity enhances the mixing of reactants, resulting in a thinner flame zone and increased flame speed.

C. Relevance to the Current Project

In this project, the laminar flame is utilized to investigate the fundamental combustion properties of hydrogen-methane mixtures. Using *Cantera*, the flame speed (S_{L0}) is calculated by solving a one-dimensional flame simulation. The flame is initialized with specified boundary conditions and mixture properties, and the simulation is solved iteratively until convergence is achieved. The calculated flame speed is then extracted as the velocity at the leading edge of the flame. This parameter serves as a key indicator of the reactivity and combustion characteristics of the fuel mixture.

D. Graphical Representation and Reference Context

To validate the characteristics of a laminar premixed flame, a schematic diagram similar to that seen in Péquin *et al.* [1] was used as a reference. The graph was recreated by independently implementing a custom code using the *Cantera* library. This approach ensures that the simulation setup and results presented in this work are entirely original while aligning with established theoretical trends.

Figure 1 shows the computed concentration profiles of reactants and products, the reaction rate, and the temperature distribution across the flame. The key observations are:

- The preheat zone, where the temperature begins to rise as reactants approach the reaction zone.
- The reaction zone, marked by a sharp peak in the reaction rate, indicating intense chemical activity.
- The post-flame zone, where the reaction rate drops to zero, and products stabilize at a uniform temperature.

The successfully reproduced flame profile validates the accuracy of the *Cantera*-based implementation in this study.

E. Implementation in Cantera Using the FreeFlame Object

Cantera, an open-source software library for combustion simulations, provides the *FreeFlame* object to model laminar flames. The *FreeFlame* object is specifically designed for one-dimensional simulations of premixed flames, balancing chemical reactions, heat transfer, and species diffusion. During the simulation, the solver adjusts the flame profile and temperature distribution to ensure that the chemical and thermal equilibrium conditions are satisfied.

F. Summary

Through the laminar flame simulations, the following observations can be made:

- The addition of hydrogen significantly increases the flame speed due to its high diffusivity and reactivity.
- The reaction zone becomes thinner with increasing hydrogen mole fraction, as seen from the reaction rate profile.
- Temperature distributions indicate a sharp rise in the reaction zone, followed by stabilization in the post-flame zone.

These findings serve as a foundation for further analysis of counterflow premixed flames, which are discussed in subsequent sections.

IV. Counterflow Premixed Combustion

A. Definition of Counterflow Premixed Flame

A counterflow premixed flame refers to a flame formed between two opposing streams of fuel-oxidizer mixtures. This configuration provides a well-defined and controlled environment to investigate flame behavior under varying strain rates and boundary conditions. Unlike turbulent premixed flames, counterflow premixed flames are analyzed in a laminar framework, allowing for detailed examination of flame properties such as temperature, species concentrations, and consumption speed.

B. Differences Between Laminar FreeFlame and Counterflow Premixed Flame

The primary difference between a **Laminar FreeFlame** and a **Counterflow Premixed Flame** lies in their boundary conditions and flow configurations:

- **Laminar FreeFlame:** The flame propagates freely through a quiescent (stationary) fuel-oxidizer mixture without any opposing flows. This flame structure typically consists of a preheat zone, reaction zone, and post-flame zone, where temperature and species distributions are symmetric about the flame front.
- **Counterflow Premixed Flame:** This flame is established in a counterflow configuration, where two opposing reactant streams interact to create a flame stabilized at the stagnation plane. The strain rate (Ka) plays a critical role in stretching the flame and influencing its structure. The temperature and species profiles are generally asymmetric due to the opposing flows and strain effects.

Figures 2 and 3 illustrate the differences between laminar free flames and counterflow premixed flames for temperature and mole fraction distributions, respectively.

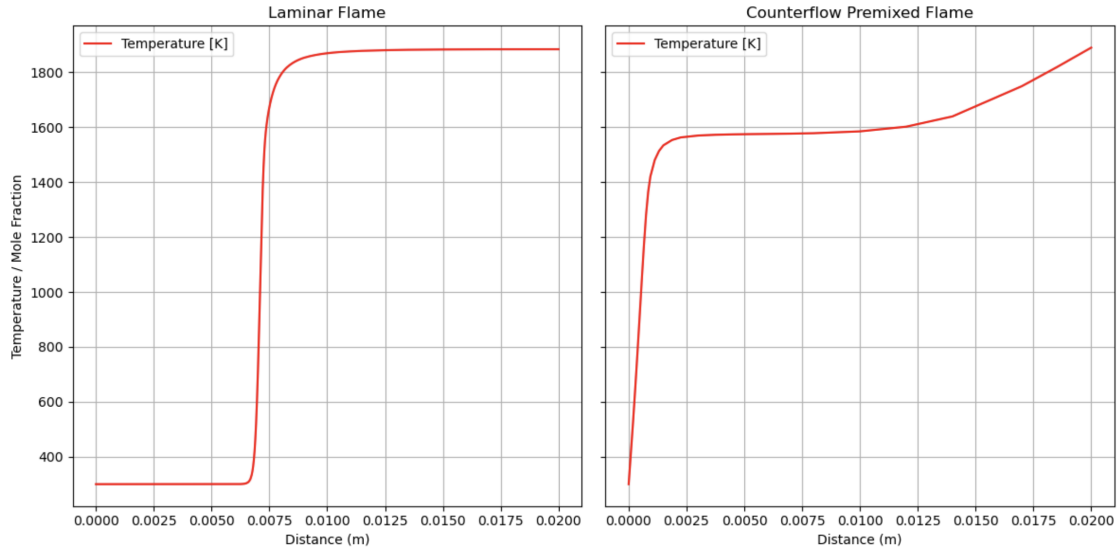


Fig. 2 Temperature profiles for a laminar free flame (left) and counterflow premixed flame (right). The counterflow flame shows asymmetry and a gradual temperature rise compared to the sharp transition in the laminar flame.

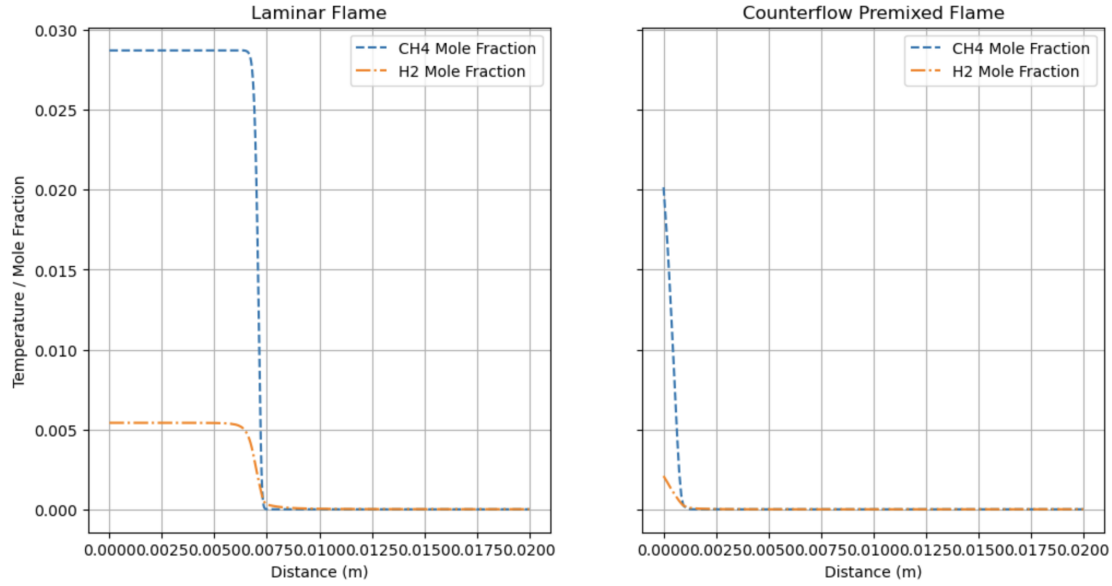


Fig. 3 Mole fraction profiles of CH₄ and H₂ for a laminar free flame (left) and counterflow premixed flame (right). The counterflow flame demonstrates significant strain effects, altering the concentration gradients.

C. Role in Hydrogen-Methane Mixtures

The counterflow premixed flame configuration is particularly valuable for studying the impact of strain rate and hydrogen addition in CH₄-H₂-air mixtures. The presence of strain causes the flame to stretch, which can either enhance or suppress combustion depending on the strain rate magnitude. Hydrogen addition increases the flame's reactivity and consumption speed, while methane contributes to stability and energy density.

D. Relevance to the Current Project

In this project, the counterflow premixed flame is modeled using the **CounterflowPremixedFlame** object in **Cantera**. This allows us to investigate the following:

- The effect of strain rate (Ka) on flame temperature and species profiles,
- The normalized consumption speed (S_{cF}/S_{I0}) under varying operating conditions,
- The comparison between laminar free flames and counterflow premixed flames in terms of flame structure and stability.

The results, as shown in Figures 2 and 3, indicate the following key observations:

- In the laminar free flame, the temperature rises sharply at the flame front and then stabilizes.
- In the counterflow premixed flame, the temperature increase is more gradual due to the strain effects and the interaction of opposing flows.
- The CH₄ and H₂ mole fractions in the counterflow flame exhibit steeper gradients compared to the free flame, highlighting the influence of strain on species transport.

E. Implementation in Cantera Using the CounterflowPremixedFlame Object

The **CounterflowPremixedFlame** object in **Cantera** is employed to simulate the counterflow configuration. Key features include:

- Incorporation of detailed transport models, including multicomponent diffusion,
- Ability to adjust strain rates and boundary conditions,
- Adaptive grid refinement to capture sharp gradients in temperature and species concentrations.

The computed results provide a detailed understanding of how strain rate and hydrogen addition influence the flame behavior, serving as a foundation for further analysis.

V. Cantera

A. What is Cantera?

Cantera is an open-source software library designed for the simulation of thermodynamic, chemical, and transport processes. It is widely used in combustion research to model chemical kinetics, chemical equilibrium, and reaction mechanisms. Cantera supports detailed multi-component transport models and complex chemical reaction mechanisms, making it suitable for a wide range of combustion systems, including laminar flames, turbulent flames, reactors, and shock tubes.

Cantera's modular design, compatibility with Python, and extensive documentation provide researchers and engineers with a flexible and powerful tool to solve complex combustion problems.

B. Key Features and Applications of Cantera

The primary features and applications of Cantera include:

- **Thermodynamic Analysis:** Solving chemical equilibrium and calculating thermodynamic properties (e.g., enthalpy, entropy) for multi-species mixtures.
- **Chemical Kinetics:** Modeling detailed chemical kinetics and reaction mechanisms in reacting flows.
- **Flame Simulations:** Simulating 1D premixed, counterflow, and diffusion flames, enabling analysis of flame speed, flame structure, and extinction limits.
- **Transport Properties:** Evaluating thermal conductivity, diffusivity, and viscosity using detailed transport models, including multicomponent diffusion and Soret effects.
- **Reactor Models:** Simulating ideal reactors, including perfectly stirred reactors (PSR), constant pressure reactors, and constant volume reactors.

Cantera's ability to interface seamlessly with Python and its compatibility with libraries such as NumPy and Matplotlib make it a versatile tool for academic and industrial research.

C. Role of Cantera in This Project

In this project, Cantera was implemented to simulate and analyze both **laminar free flames** and **counterflow premixed flames** for hydrogen-methane mixtures. The key Cantera objects and their roles are summarized below:

- **FreeFlame Object:** Used to simulate one-dimensional laminar flames to calculate the flame speed (S_{L0}) and extract the adiabatic flame temperature (T_{ad}). This provided initial conditions, such as temperature and species profiles, for subsequent counterflow simulations.
- **CounterflowPremixedFlame Object:** Used to analyze flame behavior under a counterflow configuration. This object enabled the evaluation of key parameters such as strain rate (Ka) and consumption speed (S_{CF}) across a range of mass flow rates.

The flame properties, including velocity profiles, temperature, and mole fractions of CH_4 and H_2 , were extracted to analyze the effect of strain on flame stability and consumption speed.

D. Integration of Cantera with Python Libraries

To streamline computation and analysis, Cantera was integrated with Python libraries as follows:

- **NumPy:** Used to perform numerical calculations, including gradients for strain rate estimation and thermal diffusivity calculations.
- **Matplotlib:** Employed to visualize simulation results, such as flame profiles, strain rate trends, and normalized consumption speed.
- **SciPy:** Utilized for numerical integration to compute fuel consumption rates across the flame.

The integration of Cantera with these libraries ensured efficient post-processing of results and provided a clear understanding of flame behavior.

E. Conclusion

Cantera played a crucial role in this study, enabling the simulation and analysis of laminar and counterflow premixed flames for hydrogen-methane mixtures. The **FreeFlame** object was used to establish baseline flame parameters, while the **CounterflowPremixedFlame** object facilitated the analysis of strain rate and consumption speed. This

implementation, combined with Python libraries for computation and visualization, allowed for a comprehensive understanding of the effects of strain and hydrogen addition on flame behavior.

VI. Key Concepts

A. Strain Rate

1. Definition and Equation

The strain rate (Ka) quantifies the rate at which a flame is stretched due to velocity gradients in the counterflow configuration. It is defined as:

$$Ka = \frac{\alpha}{S_L^0} \kappa, \quad (1)$$

where:

- α : Thermal diffusivity of the reactants.
- S_L^0 : Unstretched laminar flame speed.
- κ : Velocity gradient ($|du/dx|$) at the maximum gradient point.

2. Role of Unstretched Laminar Flame Speed

The unstretched laminar flame speed (S_{L0}) represents the flame speed under idealized, quiescent conditions. It is a baseline value that reflects the intrinsic chemical properties of the mixture without external disturbances such as strain or turbulence. In this study, S_{L0} is used for normalization to make the results comparable across varying conditions, following Garcia [2].

3. Role in the Code

In the code, the strain rate is calculated using the thermal diffusivity, unstretched laminar flame speed, and the velocity gradient obtained numerically. While strain rate does not directly impact the flame consumption speed (S_{CF}), it provides a quantitative measure of the effect of stretch on flame dynamics and stability.

B. Heat Loss

1. Definition and Equation

Heat loss is introduced to simulate non-adiabatic conditions where the product temperature (T_p) deviates from the adiabatic flame temperature (T_{ad}) due to thermal dissipation. The heat loss coefficient (β) is defined as:

$$\beta = \frac{T_p - T_r}{T_{ad} - T_r}, \quad (2)$$

where:

- T_p : Temperature of the products.
- T_r : Temperature of the reactants.
- T_{ad} : Adiabatic flame temperature.

2. Role of Product Temperature in Heat Loss

The product temperature (T_p) is used to control the heat loss level, where β ranges from 0 (complete heat loss) to 1 (adiabatic conditions). This parameter allows the simulation to explore how thermal losses impact the flame structure and combustion characteristics.

3. Role in the Code

In the code, the product temperature is set starting from T_{ad} and progressively reduced to simulate heat loss. The heat loss coefficient (β) is adjusted by varying T_p , and its effect on flame properties such as temperature profiles and consumption speed is analyzed.

C. Consumption Speed

1. Definition and Equation

The consumption speed (S_{cF}) quantifies the rate at which fuel is consumed across the flame. It is defined as:

$$S_{cF} = \frac{\sum_{k=1}^{N_f} \eta_k \int_{-\infty}^{\infty} \dot{\omega}_k dx}{\rho_u \sum_{k=1}^{N_f} \eta_k (Y_{k,b} - Y_{k,u})}, \quad (3)$$

where:

- $\dot{\omega}_k$: Reaction rate of species k .
- η_k : Weighting factor, defined as $\eta_k = Y_{k,u}/Y_{f,u}$.
- $Y_{k,b}, Y_{k,u}$: Mass fractions of species k in the burned and unburned regions, respectively.
- ρ_u : Density of the unburned mixture.

2. Role of Temperature and Stretch in Consumption Speed

The consumption speed inherently accounts for the effects of temperature, stretch, and chemical reactions. By modifying the product temperature (T_p) or introducing strain, the flame response to these conditions can be analyzed. This helps assess the combined effect of heat loss and strain on combustion characteristics.

3. Role in the Code

In the code, the `CounterflowPremixedFlame` object in Cantera calculates the consumption speed by integrating the reaction rate across the flame profile. This parameter is critical for understanding fuel consumption under varying strain rates and thermal conditions.

D. Conclusion

The strain rate (Ka), heat loss (β), and consumption speed (S_{cF}) are key parameters that describe flame behavior under non-ideal conditions. These concepts are implemented in the code using Cantera to simulate flame stretch, thermal losses, and fuel consumption, providing a comprehensive framework for analyzing hydrogen-methane combustion dynamics.

VII. Results and Discussion

Table 1 Representative Results for Different α Values at $T_p = 1000$ K.

mdot	$\alpha = 0.6$			$\alpha = 0.7$			$\alpha = 0.8$		
	Ka	S_{cF}	S_{cF}/S_{L0}	Ka	S_{cF}	S_{cF}/S_{L0}	Ka	S_{cF}	S_{cF}/S_{L0}
0.01	0.0032	0.0158	0.0463	0.0023	0.0156	0.0366	0.0013	0.0159	0.0249
0.1	0.1152	0.1015	0.2982	0.0833	0.0991	0.2321	0.0497	0.0952	0.1559
1	1.0318	0.2782	0.8169	0.9339	0.2970	0.6960	0.6824	0.3209	0.5256
10	1.9743	0.3285	0.8305	1.3695	0.3162	0.7410	0.7457	0.3495	0.5724
100	20.4992	0.1598	0.4686	14.0850	0.2090	0.4899	7.5576	0.2554	0.4182

A. Results

From Table 1 and Figures 4–6, the following observations can be made:

1) Strain Rate vs. Normalized Consumption Speed (Ka vs. S_{cF}/S_{L0}):

- As α increases from 0.6 to 0.8, the overall trend shows a **reduction in the peak S_{cF}/S_{L0}** values.
- The peak consumption speed shifts to lower Ka values as α increases, indicating that the flame becomes **less resistant to strain** at higher α .

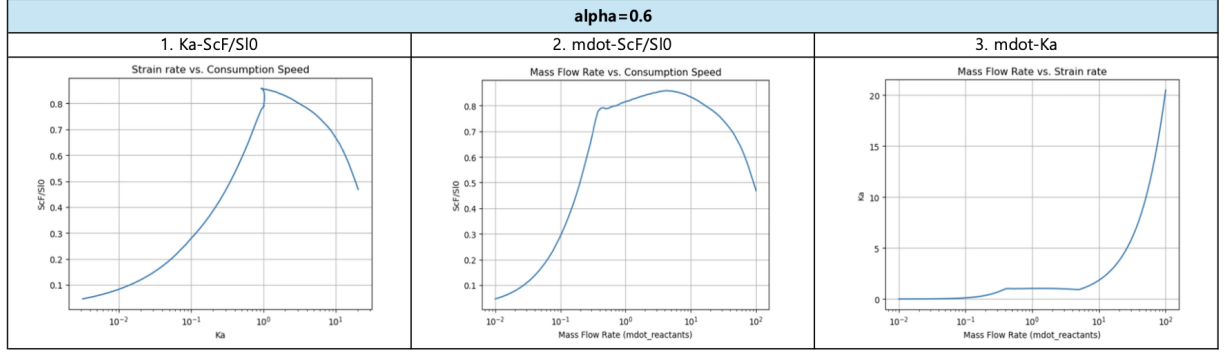


Fig. 4 $\alpha = 0.6$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

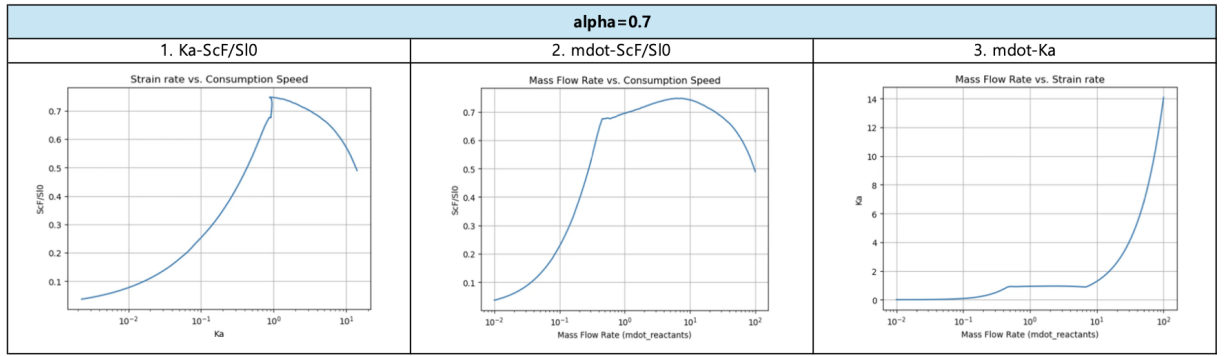


Fig. 5 $\alpha = 0.7$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

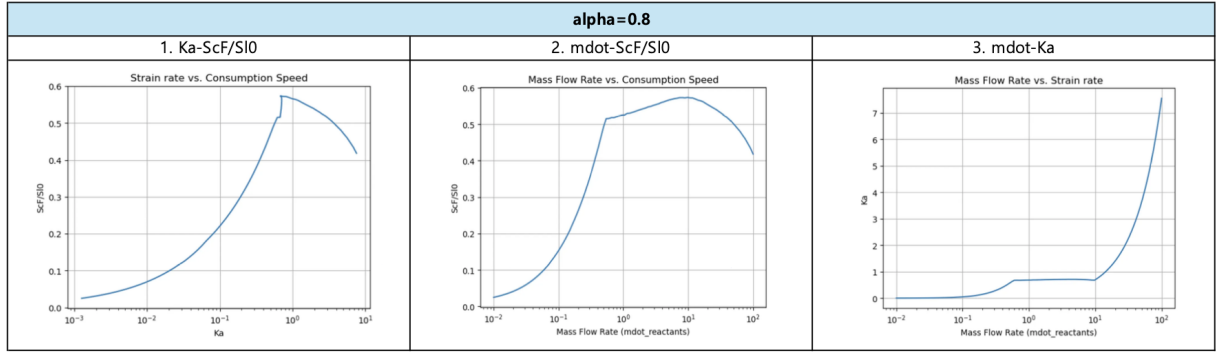


Fig. 6 $\alpha = 0.8$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

- The slope of the Ka vs. S_{cF}/S_{L0} curve is steeper at lower α (0.6), demonstrating **higher sensitivity to strain rate**.
- 2) **Mass Flow Rate vs. Normalized Consumption Speed (\dot{m} vs. S_{cF}/S_{L0}):**
- S_{cF}/S_{L0} **increases nonlinearly** with mass flow rate but saturates at high \dot{m} .
 - At higher α , the rate of increase in S_{cF}/S_{L0} with \dot{m} becomes slower, further emphasizing the **thermal diffusivity's effect** in limiting the flame's reactivity.
 - For small \dot{m} , the difference between the curves is more pronounced, suggesting α 's stronger impact under low flow conditions.

3) **Mass Flow Rate vs. Strain Rate (\dot{m} vs. Ka):**

- Across all α values, Ka increases sharply at higher \dot{m} values ($\dot{m} > 10$).
- As α increases, the strain rate at equivalent mass flow rates is consistently lower, aligning with the expected **inverse relationship** between diffusivity and strain rate.

Key Observations:

- At lower strain rates and mass flow rates, α has a more **dominant impact** on reducing S_{cF}/S_{L0} , emphasizing the role of thermal diffusivity in limiting flame stabilization.
- At higher flow rates, strain effects dominate across all α values, causing a sharp increase in Ka .

B. Discussion

The results demonstrate that **thermal diffusivity** (α) has a significant influence on flame behavior, particularly under strained and flow-driven conditions. The following interpretations can be made:

1) **Flame Reactivity and Thermal Diffusivity:**

- Higher α reduces the flame's reactivity, as evidenced by the **lower peak** S_{cF}/S_{L0} values. This reduction stems from the enhanced thermal diffusion reducing the local flame temperature and reactivity.

2) **Sensitivity to Strain Rate:**

- The shift of peak S_{cF}/S_{L0} to **lower strain rates** (Ka) as α increases highlights the flame's reduced capacity to sustain higher strain rates. This observation aligns with theoretical predictions where thermal diffusivity dampens the flame's ability to maintain high reactivity under strong strain.

3) **Role of Mass Flow Rate:**

- At **low mass flow rates** ($\dot{m} < 10$), thermal diffusivity plays a dominant role, leading to significant differences in S_{cF}/S_{L0} between $\alpha = 0.6, 0.7$, and 0.8 .
- At **high mass flow rates** ($\dot{m} \approx 100$), the influence of α diminishes, and strain effects become dominant, as shown by the sharp rise in Ka .

4) **Practical Implications:**

- These findings emphasize the importance of considering thermal diffusivity in practical combustion systems, especially where strain effects and flow rates vary significantly. For example, in **highly strained counterflow flames**, optimizing α could help stabilize the flame under varying conditions.

5) **Graph-Specific Trends:**

- Figures 4–6 clearly illustrate that the flame's response weakens progressively with increasing α , particularly at lower strain rates and flow conditions.
- The sharp rise in strain rates at higher mass flow rates underscores the **nonlinear interaction** between strain and flow conditions, which cannot be ignored in combustion modeling.

Table 2 Representative Results for Different T_p Values at $\alpha = 0.6$.

\dot{m}	$T_p = 500$ K			$T_p = 1000$ K			$T_p = 1500$ K		
	Ka	S_{cF}	S_{cF}/S_{L0}	Ka	S_{cF}	S_{cF}/S_{L0}	Ka	S_{cF}	S_{cF}/S_{L0}
0.01	0.0032	0.0158	0.0463	0.0032	0.0158	0.0463	0.0032	0.0158	0.0463
0.1	0.1152	0.1015	0.2982	0.1152	0.1015	0.2982	0.1152	0.1015	0.2982
1	1.0318	0.2782	0.8169	1.0318	0.2782	0.8169	1.0318	0.2782	0.8169
10	1.9743	0.2828	0.8305	1.9743	0.2828	0.8305	1.9743	0.2828	0.8305
100	20.4992	0.1596	0.4686	20.4992	0.1596	0.4686	20.4992	0.1596	0.4686

C. Results

From Table 2 and Figures 7–9, the following observations can be made:

1) **Strain Rate vs. Normalized Consumption Speed (Ka vs. S_{cF}/S_{L0}):**

- As T_p increases from 500 K to 1500 K, the overall peak S_{cF}/S_{L0} values decrease slightly, indicating a reduction in flame reactivity under higher product temperatures.

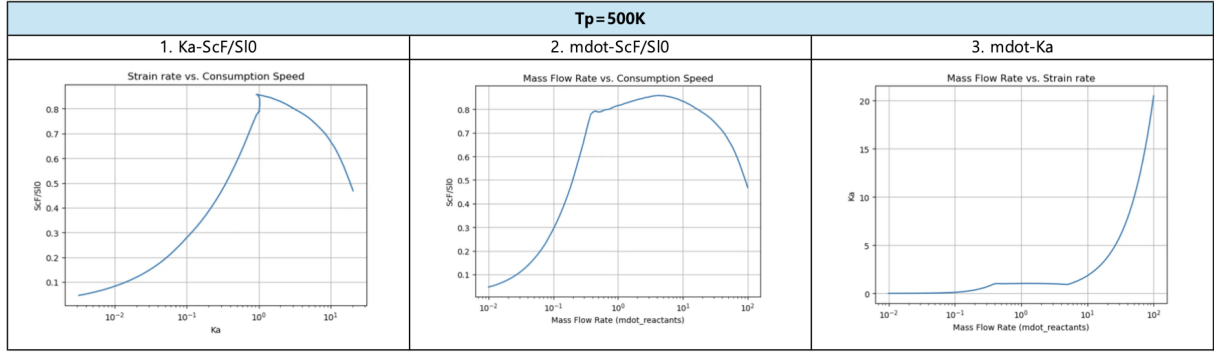


Fig. 7 $T_p = 500 K$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

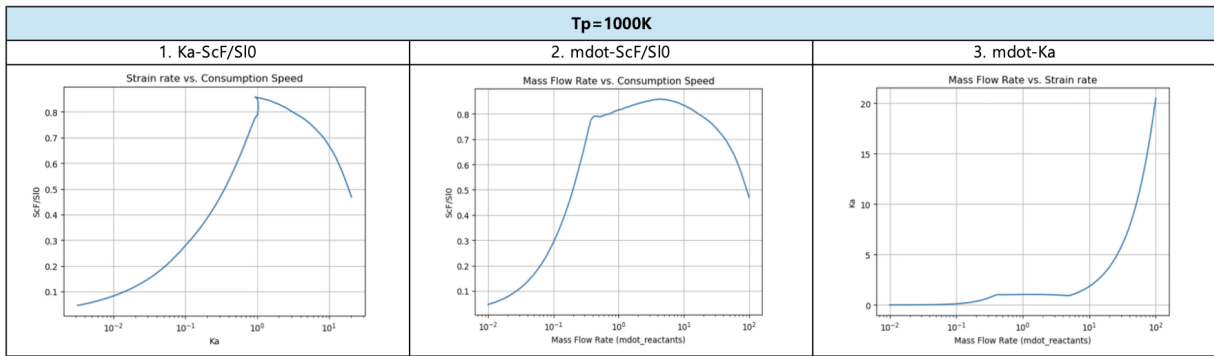


Fig. 8 $T_p = 1000 K$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

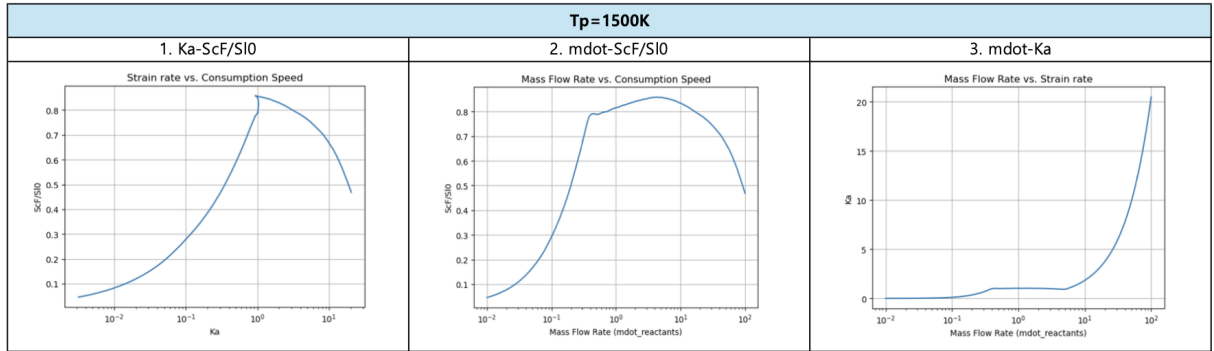


Fig. 9 $T_p = 1500 K$: (1) Ka vs. S_{cF}/S_{L0} , (2) \dot{m} vs. S_{cF}/S_{L0} , and (3) \dot{m} vs. Ka .

- The peak value of S_{cF}/S_{L0} shifts to **lower strain rates** (Ka) with increasing T_p , demonstrating that the flame becomes **less resistant to strain** as the product temperature rises.
 - At low strain rates ($Ka < 10^2$), the differences in S_{cF}/S_{L0} across different T_p are minimal, while at higher strain rates, the decrease in reactivity becomes more prominent.
- 2) **Mass Flow Rate vs. Normalized Consumption Speed** (\dot{m} vs. S_{cF}/S_{L0}):
- For all T_p values, S_{cF}/S_{L0} increases with \dot{m} but saturates at high mass flow rates ($\dot{m} \approx 100$).
 - At higher T_p , the normalized consumption speed (S_{cF}/S_{L0}) shows a **reduced growth rate** with increasing mass flow rate, highlighting the role of elevated thermal conditions in limiting flame consumption speed.

- At lower mass flow rates ($\dot{m} < 10$), the impact of T_p on S_{cF}/S_{L0} is more pronounced.
- 3) **Mass Flow Rate vs. Strain Rate (\dot{m} vs. Ka):**
- The strain rate (Ka) increases significantly with \dot{m} for all T_p values.
 - At higher T_p , the strain rate (Ka) increases at a slightly **lower rate** compared to lower T_p , particularly for mass flow rates ($\dot{m} > 10$).
 - At lower \dot{m} , Ka remains consistent across T_p , while for higher \dot{m} , the strain rate grows nonlinearly.

Key Observations:

- Increasing product temperature (T_p) causes the peak S_{cF}/S_{L0} to shift toward lower strain rates, emphasizing the role of thermal conditions in reducing flame resistance to strain.
- The strain rate (Ka) remains relatively consistent at low mass flow rates but exhibits a sharp increase at high \dot{m} , with the rate of increase slightly dampened at higher T_p .

D. Discussion

The results highlight the significant impact of product temperature (T_p) on both strain rate (Ka) and normalized consumption speed (S_{cF}/S_{L0}). The following interpretations can be made:

1) **Flame Reactivity and Product Temperature:**

- As T_p increases, the overall flame reactivity decreases, as shown by the reduced peak S_{cF}/S_{L0} . This reduction is due to the increased thermal energy reducing the local temperature gradients necessary for flame stabilization.

2) **Sensitivity to Strain Rate:**

- The shift of peak S_{cF}/S_{L0} to lower strain rates (Ka) with increasing T_p indicates that the flame becomes **less stable under strain**. This trend highlights the importance of product temperature in weakening flame resistance to external strain effects.

3) **Impact of Mass Flow Rate:**

- At **low mass flow rates** ($\dot{m} < 10$), the effect of T_p is significant, resulting in clear differences in S_{cF}/S_{L0} and Ka .
- At **high mass flow rates** ($\dot{m} \approx 100$), strain effects dominate, and the product temperature has a lesser impact on Ka and S_{cF}/S_{L0} , though the trend still shows slightly reduced sensitivity at higher T_p .

4) **Practical Implications:**

- These results emphasize the importance of considering product temperature in flame modeling and combustion systems. Elevated T_p values can lead to **reduced flame stability** under strain, particularly in conditions with high mass flow rates.
- For practical systems, controlling T_p is crucial for maintaining flame performance and preventing blow-off or extinction under strained flow conditions.

5) **Graph-Specific Trends:**

- Figures 7–9 clearly show that the normalized consumption speed decreases and shifts toward lower strain rates as T_p increases.
- The nonlinear increase in strain rate (Ka) at high \dot{m} further highlights the **dominance of strain effects** over thermal effects in high flow conditions.

E. Comparison with Reference Data

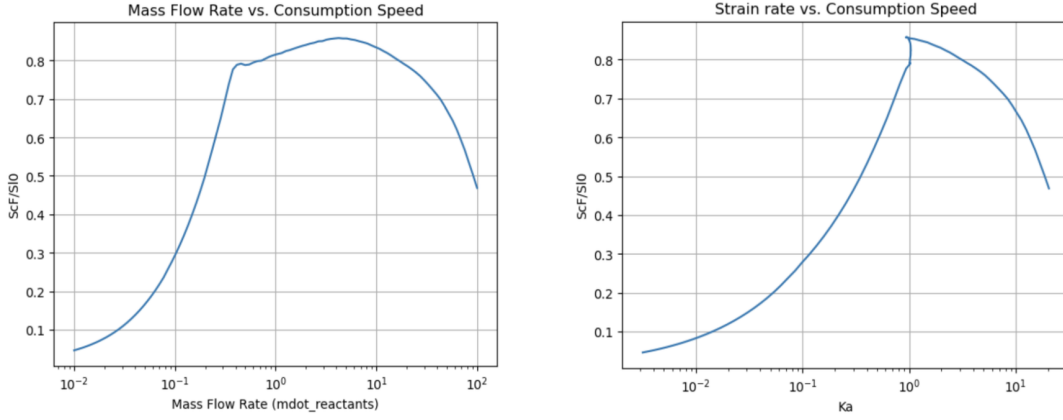


Fig. 10 Experimental results: Mass flow rate (\dot{m}) and strain rate (Ka) vs. Consumption Speed (S_{cF}).

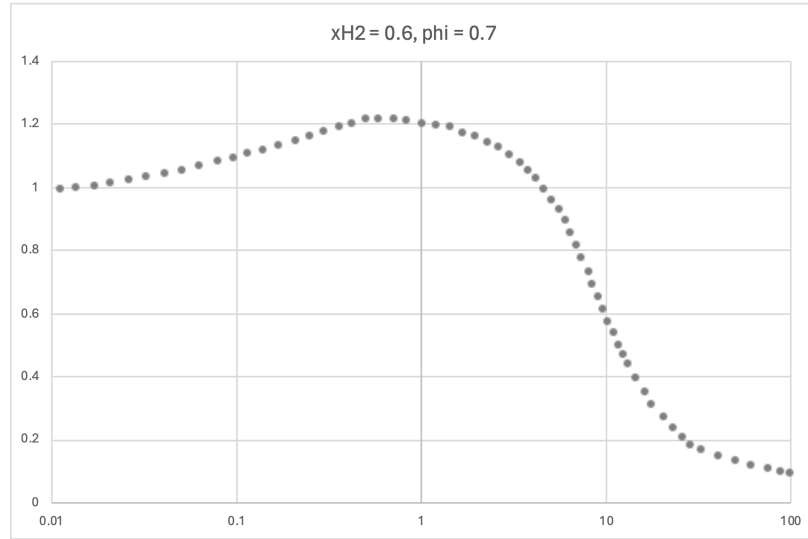


Fig. 11 Reference data from Garcia2022b (CH₄-H₂ CFPF, Figure 3): Yellow curve represents $x_{H_2} = 0.6$, $\phi = 0.7$.

From Figures 10 and 11, the following conclusions can be drawn:

1) Overall Trends in S_{cF} vs. Ka :

- Both experimental and reference data exhibit similar trends of normalized consumption speed (S_{cF}) with respect to the strain rate (Ka):
 - In the **low- Ka region**, S_{cF} increases monotonically as Ka increases, highlighting the initial positive strain effect on flame consumption speed.
 - In the **high- Ka region**, S_{cF} decreases significantly, demonstrating the **dominant effect of strain-induced flame weakening**.
- The location of the peak S_{cF} shifts slightly between the two datasets, but the general behavior remains consistent.

2) Experimental Conditions:

- The experimental results were obtained under the following conditions:

- Product temperature (T_p) was set equal to the adiabatic flame temperature ($T_p = T_{ad}$, $\beta = 1$),
- Equivalence ratio (ϕ) was fixed at 0.7,
- Hydrogen mole fraction (x_{H_2}) was set to 0.6, matching the conditions in Garcia2022b.
- These conditions were chosen to align closely with the reference dataset and isolate the influence of strain rate and hydrogen addition on the flame behavior.

3) Comparison Highlights:

- At **low strain rates** ($Ka < 1$), both datasets show a sharp increase in S_{cF} , indicating that strain promotes flame stabilization by enhancing the transport processes.
- In the **intermediate strain rate** range ($Ka \approx 1 - 10$), the flame reaches its peak consumption speed. The experimental results show slightly lower peak values compared to the reference data, possibly due to differences in numerical treatment or boundary conditions.
- At **high strain rates** ($Ka > 10$), the consumption speed decreases steeply in both datasets, demonstrating the strain's role in flame weakening and eventual extinction.

4) Impact of Hydrogen Addition:

- The selected equivalence ratio ($\phi = 0.7$) and hydrogen mole fraction ($x_{H_2} = 0.6$) highlight the **positive impact of hydrogen addition** on enhancing flame reactivity at low strain rates.
- However, at high strain rates, the effect of hydrogen diminishes, and the flame behavior becomes primarily strain-dominated, as observed in both experimental and reference data.

The agreement between experimental and reference data validates that the observed behavior of the CH₄-H₂ counterflow premixed flame at $x_{H_2} = 0.6$ is consistent across both datasets. The slight deviations observed at peak and high strain rates may be attributed to differences in experimental setup, numerical assumptions, or thermal boundary conditions.

Key Takeaways:

- The comparison demonstrates that the experimental results effectively capture the critical trends in flame response to strain, including the location of peak S_{cF} and the subsequent decrease at high Ka .
- The positive influence of hydrogen on enhancing flame consumption speed is confirmed, particularly under moderate strain conditions.

VIII. Conclusion

In this study, the behavior of CH₄-H₂ counterflow premixed flames was analyzed under varying hydrogen fractions (α), strain rates (Ka), and equivalence ratios (ϕ). By combining simulation results and comparisons with reference data, the following key conclusions can be drawn:

A. Flame Speed and Strain Rate Relationship

The normalized consumption speed (S_{cF}/S_{L0}) exhibits a distinct two-regime behavior with respect to the strain rate (Ka):

- In the **low- Ka region** ($Ka < 1$), S_{cF}/S_{L0} increases with strain rate. This trend highlights the positive effect of moderate flame stretching, which enhances reactant mixing and accelerates fuel consumption.
- In the **high- Ka region** ($Ka > 1$), S_{cF}/S_{L0} decreases significantly. This is attributed to strain-induced flame thinning and quenching, which reduce flame reactivity.

The transition between these regions occurs around $Ka \approx 1$, where the consumption speed reaches its peak.

B. Effect of Hydrogen Addition

Increasing the hydrogen fraction (α) in CH₄-H₂ mixtures has a significant influence on flame behavior:

- The **laminar flame speed** (S_{L0}) increases with hydrogen addition due to its higher diffusivity, lower ignition energy, and enhanced chemical reactivity.
- In the **low- Ka region**, hydrogen addition improves flame stabilization by increasing the flame speed and sustaining reactivity at moderate strain rates.
- In the **high- Ka region**, hydrogen addition delays flame quenching, maintaining higher S_{cF}/S_{L0} values under elevated strain conditions. This demonstrates hydrogen's ability to counteract strain effects.
- The higher thermal diffusivity of hydrogen enhances both heat and mass transfer processes, resulting in improved overall flame stability and reactivity.

C. Role of Equivalence Ratio (ϕ)

The equivalence ratio (ϕ) plays a pivotal role in determining the impact of hydrogen addition on flame dynamics:

- At **moderate equivalence ratios** ($\phi = 0.7$), hydrogen addition exhibits the most prominent effects, enhancing flame speed and stabilization under strain. This is attributed to the optimal balance between fuel reactivity and flame temperature.
- At **leaner conditions** ($\phi < 0.7$), the flame speed and consumption speed are reduced due to insufficient fuel availability and lower flame temperatures, which limit hydrogen's impact.
- At **richer conditions** ($\phi > 0.7$), the benefits of hydrogen addition are mitigated by reduced flame reactivity and temperature, resulting in less pronounced trends.

The results confirm that $\phi = 0.7$ provides an optimal condition for analyzing the combined effects of hydrogen addition and strain rate.

D. Summary of Key Findings

This study provides a comprehensive analysis of CH₄-H₂ counterflow premixed flames, leading to the following conclusions:

- **Flame Behavior:** Hydrogen addition enhances flame speed and stabilization in the low- Ka region while delaying flame quenching in the high- Ka region.
- **Impact of Strain:** The strain rate significantly influences normalized consumption speed, with S_{cF}/S_{L0} peaking around $Ka \approx 1$.
- **Optimal Equivalence Ratio:** Moderate equivalence ratios ($\phi = 0.7$) maximize the benefits of hydrogen addition, balancing flame reactivity and thermal stability.
- **Hydrogen Diffusivity:** The higher thermal diffusivity of hydrogen accelerates heat and mass transfer, improving overall flame performance under varying strain conditions.

E. Future Work

Future research can further refine these findings by:

- Extending the analysis to additional equivalence ratios and hydrogen fractions to validate broader trends.
- Incorporating turbulence effects to simulate more realistic combustion systems.
- Exploring the influence of alternative fuels and detailed transport models to enhance understanding of flame dynamics under complex conditions.

F. Concluding Remark

This study highlights the critical role of hydrogen addition and strain effects in stabilizing counterflow premixed flames. By optimizing the equivalence ratio and hydrogen fraction, enhanced flame performance can be achieved, providing valuable insights for the development of efficient, low-emission combustion systems.

IX. Challenges Encountered During Debugging

Throughout the implementation and analysis process, several challenges were identified. These challenges, along with opportunities for improvement, are outlined below to enhance the accuracy, efficiency, and reliability of the results.

1) Ensuring Dimensionless Strain Rate

During the calculation of the strain rate, it is critical to ensure that the resulting values are dimensionless. Dimensional inconsistencies can lead to inaccurate interpretations and invalid comparisons. Proper unit verification and normalization techniques should be applied to maintain consistency across all calculations.

2) Selection of Project Temperature (T_p)

Identifying the optimal project temperature (T_p) posed a significant challenge due to the limited range of test cases. To overcome this, a more systematic approach involving a finer resolution and broader range of T_p values should be adopted. This will allow for a comprehensive analysis of temperature effects and the identification of an optimal operating range for different conditions.

3) Balancing Mass Flow Rate (\dot{m}) Precision and Computational Efficiency

Increasing the resolution of mass flow rate (\dot{m}) values can improve the precision of the results but comes at the cost of computational resources. In this study, the number of x -axis data points was capped at 100 for feasibility.

Leveraging parallel computing techniques or more efficient solvers could help manage the computational burden, allowing for higher resolution without compromising efficiency.

4) **Heat Loss Coefficient (β) Integration**

The heat loss coefficient (β) was not fully integrated into the current analysis. Incorporating β into the calculations would enable a more accurate estimation of consumption speed (S_{cF}) and project temperature. This enhancement would provide a deeper understanding of the impact of heat loss on flame behavior, particularly under varying strain rates.

5) **Impact of Domain Width (w)**

The width of the computational domain (w) can significantly influence the results. In this study, the width was fixed at 0.02 m. To evaluate its effect, a sensitivity analysis should be conducted by varying w . This would provide insights into the role of domain geometry on strain rates and flame stability, enabling more robust model validation.

6) **Utilization of Multiple Flame Objects**

Currently, a single flame object was employed to generate the results. Implementing multiple flame objects simultaneously would facilitate comparisons across different project temperatures, mass flow rates, and other parameters. This approach could streamline the analysis process and offer a clearer understanding of parameter dependencies on flame behavior.

By addressing these challenges and implementing the proposed improvements, the accuracy and resolution of the results can be significantly enhanced. These refinements will not only provide deeper insights into flame behavior under varying conditions but also strengthen the reliability and applicability of the findings in practical combustion systems.

References

The following references provide important context and examples for this research. Péquin’s work analyzes turbulent reacting flows using direct numerical simulations, providing foundational insights for flame modeling. The Kutkan reference discusses modeling of turbulent premixed $\text{CH}_4/\text{H}_2/\text{air}$ flames, highlighting the effects of stretch and heat loss. Garcia’s study focuses on the impact of hydrogen addition on the consumption speed of lean premixed flames under combined strain and heat loss conditions. The Cantera examples and documentation are extensively used for implementing and validating the laminar and counterflow flame simulations in this study.

This is an example citation for Kutkan [3]. Another example citation for Garcia [2]. References to Cantera examples [4] and documentation [5].

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