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RESEARCH ARTICLE

Numerical investigation of syngas combustion considering effect of inlet air temperatures along with hydrogen to carbon monoxide ratio

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Abstract

A two-dimensional detailed numerical combustion analysis is performed to explore syngas combustion inside a non-premixed combustion chamber. A detailed transport model coupled with a chemical kinetic mechanism is used to study combustion behavior. The combustion chamber supplied with syngas comprising Hydrogen (H_2), Carbon Monoxide (CO), and Nitrogen (N_2) as constituents such that H_2 and CO molar ratios are changed while N_2 constant. The numerical study uses co-flow air delivery to control the inlet air temperature to analyze its impact on reaction rate performance. The study analyzes both the ignition zone structure and the effects of changing H_2/CO molar ratios on adiabatic flame temperature. Perfecting syngas H_2/CO ratios together with inlet air temperature leads to best reaction rate balances between H_2 and CO molar ratios. The simulated results reveal information about temperature distribution along with reaction rates and flame topologies that help perfect combustion performance.

Keywords: Syngas, H_2/CO ratio, inlet air temperature, non-premixed combustion

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1. Introduction

Syngas stands as an industrially important resourceful fuel which gains increasing significance for boiler and steam generation purposes [1]. The main components of Syngas include hydrogen (H_2) and carbon monoxide (CO) while methane, nitrogen and minor other gases are present in small amounts. The gasification process transforms different raw materials including coal and biomass and waste into Syngas which enables integration into energy systems at different sustainability levels for alternative fuel usage [2]. The H_2-to-CO ratio decides syngas combustion efficiency because it influences the composition of syngas [3]. Controlling the H_2-to-CO ratio enables the optimization of performance characteristics which includes ignition properties together with flame stability and thermal efficiency and emission output.

The combustion reactivity of syngas enhances with higher hydrogen content because this produces shorter ignition delays and faster burn rates that drive thermal efficiency upward [4]. More energy from hydrogen-rich syngas releases quickly in short periods of time which generates intense heat release rates and higher peak pressures during combustion. Contrary to this effect disproportionate CO causes combustion delays through decreased oxidation rates and possibly results in inefficient combustion and reduced total efficiency [5]. Hydrogen-rich syngas can achieve higher temperatures for better efficiency however material damage from thermal stress requires proper management of the combustion chamber. The best combustion performance requires deciding the correct ratio of H_2 to CO that exists in syngas.

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Higher ratios of hydrogen to carbon monoxide led to decreased carbon dioxide emissions in the process [6]. The complete combustion of high hydrogen content in syngas reduces both CO2 and particulate matter emissions because it is an environmentally beneficial fuel [7]. The stability of industrial boiler flames depends on hydrogen presence because it keeps consistent combustion performance. The H_2/CO ratio needs adjustment to reach best combustion while keeping high thermal efficiency and reducing pollutant emissions [8].

Syngas use delivers added environmental benefits which transcend emission mitigation [9]. The carbon footprint of energy generation decreases using syngas since its production stems from renewable biomass and waste sources [10]. Syngas waste-to-energy operations follow circular economy principles since they transform waste materials into valuable energy while solving waste disposal problems [11]. Syngas allows integration with carbon capture systems to boost the environmental sustainability of energy systems that employ it [12].

The rising importance of syngas in industrial energy generation receives added support from improved gasification and combustion technology because of its many benefits [13]. The detailed analysis of syngas combustion behavior especially concerning H_2/CO ratios and inlet air temperatures needs added research.

The analysis of syngas combustion uses computational methods primarily because they provide more value through lower expenses and deeper analysis than traditional experimental methods [14]. The intricate combustion processes can be simulated through Computational Fluid Dynamics (CFD) models which generate detailed information about flame behaviors along with heat transfer and chemical kinetic data [15]. The composition variations of syngas (hydrogen to carbon monoxide ratios) benefit from this computational approach because the fuel shows complex combustion behaviors. Computational models analyze different heat release patterns and flame stability through varying equivalence ratio and fuel composition according to research findings [16]. Scientists use computational approaches to change parameters including pressure temperature and flow rate because physical experiments create operational limitations [17]. Exploration occurs on multiple operating conditions and fuel compositions due to flexible computational models. Simulations decide ignition delay times alongside flame stability under different conditions based on modifications to syngas composition [18]. The analysis of syngas combustion through physical experiments becomes costly and time-consuming since it requires specialized equipment along with strict safety protocols [19]. Through computational analysis companies can minimize their costs because they can virtually test different scenarios. The method provides significant value during investigations of new combustor design approaches and existing system optimization efforts. Computational models implement refined algorithms that foresee how combustion reacts when subjected to diverse scenarios which cannot be examined through experimental testing. Designing efficient combustion systems that must run under various conditions depends on predictive capabilities which help reduce emissions [20].

Academic methods enable the combination of syngas combustion studies with plasma-assisted combustion techniques and hybrid energy systems [21]. The work delivers an extensive breakdown of efficient syngas use strategies applicable to power generation and industrial processes. The article investigates what happens when the hydrogen-to-carbon monoxide ratio in syngas changes along with its effect on combustion performance and energy emissions stability optimization. The investigation investigates syngas combustion factors in detail to help create efficient sustainable energy systems which satisfy current industrial requirements.

2. Methodology

The present study employs a computational fluid dynamics approach to investigate the combustion characteristics of syngas in a can-type combustor. The simulations are performed using the commercial software COMSOL Multiphysics, which offers robust modelling capabilities for turbulent reacting flows. The computational domain is designed to closely be the experimental setup described in the literature, allowing for a direct comparison of the numerical results with the available experimental data. The governing equations for the fluid flow and combustion processes are solved using the finite element method.

2.1. Governing equations

The governing equations for the fluid flow and combustion processes are the conservation of mass, momentum, energy, and species transport.

The mass conservation equation is given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

where ρ is the density and u is the velocity vector.

Momentum Equations:

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot \tau + \rho g \quad (2)$$

where p is the pressure, τ is the viscous stress tensor, and g is the gravitational acceleration vector.

Energy Equation:

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho uH) = \nabla \cdot (\lambda \nabla T) + \dot{Q} + \rho u \cdot g \quad (3)$$

where E is the total energy, H is the total enthalpy, λ is the thermal conductivity, T is the temperature, and $\dot{Q}$ is heat sources or sinks due to chemical reactions.

Species Transport Equations:

$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho u Y_i) = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{\omega}_i \quad (4)$$

where Y_i is the mass fraction of species , i, D_i is the diffusion coefficient of species i, and $\dot{\omega}_i$ is the rate of production or consumption of species i due to chemical reactions.

Eddy-Dissipation Model

$$R_{ij} = \nu_{ij} M_i \min\left(\frac{r_{MVC,j}}{M_r}, r_{ED,j}\right) \quad (5)$$

where R_{ij} is the reaction rate of species i in reaction j, ν_{ij} is the stoichiometric coefficient of species i in reaction j, M_i is the molar mass of species i, $r_{MVC,j}$ is the rate of the reaction based on the mean volumetric concentration, and $r_{ED,j}$ is the rate of the reaction based on the eddy-dissipation model. The mixing time scale τ_T is a key parameter in the eddy-dissipation model. It is the characteristic time for turbulent mixing [22].

The chemical kinetics of the syngas combustion are modeled using a reduced mechanism, which includes the most important reactions for the oxidation of CO and H_2 [23].

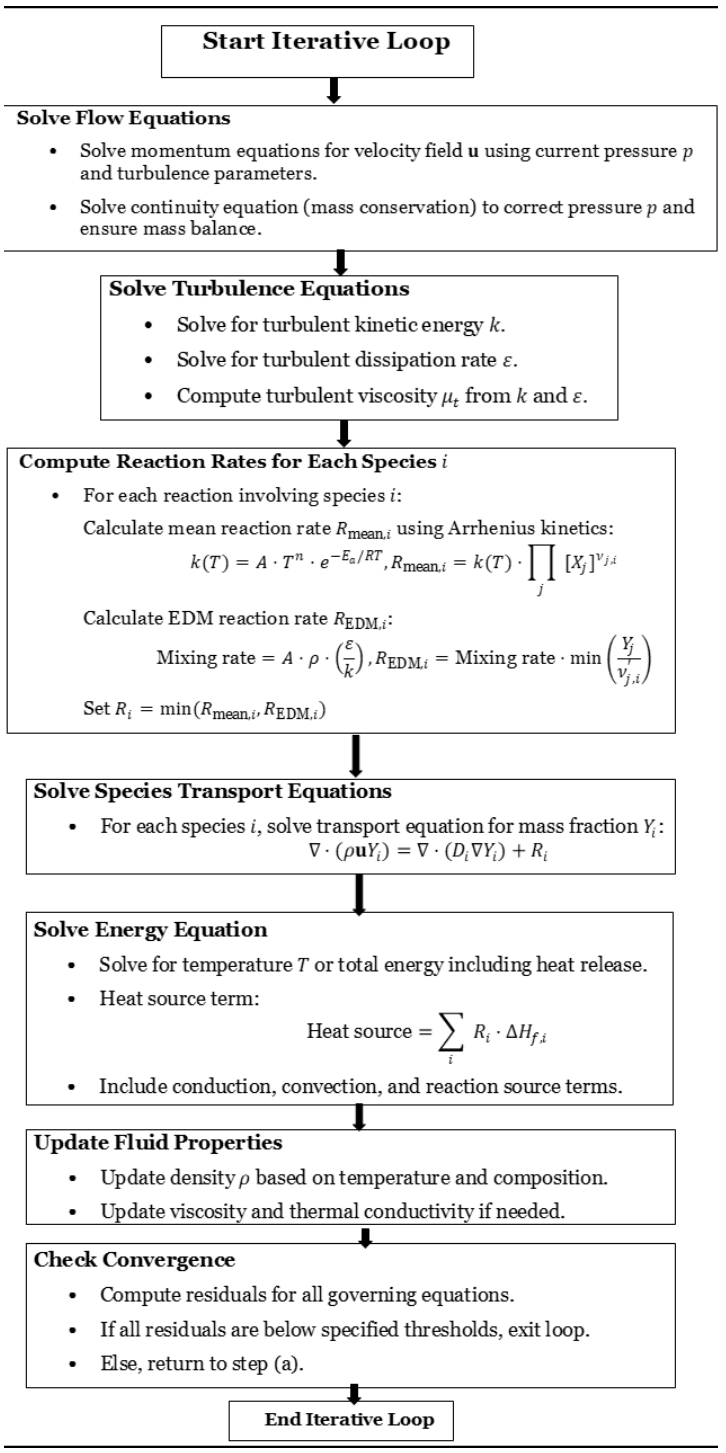
In turbulent combustion, the turbulent reaction rate plays a crucial role in accurately being the complex interaction between turbulence and chemical reactions. specifically employs the Eddy Dissipation Model to calculate this rate.[24]

Turbulence-Chemistry Interaction: Turbulence enhances the mixing of reactants, leading to faster reaction rates compared to laminar flames. The turbulent reaction rate captures this effect by accounting for the increased mixing and transport of reactants due to turbulent eddies.[25]

Eddy Dissipation Model: The EDM assumes that reactions occur within small, turbulent structures called "fine scales." These fine scales are characterized by high strain rates and rapid mixing. The EDM calculates the reaction rate based on the time scales of turbulent mixing and chemical reaction. The turbulent reaction rate is modeled as the minimum of the mean-value closure rate and the EDM rate. This ensures that the reaction rate is limited by either the chemical kinetics or the turbulent mixing, whichever is slower.[26]

Damköhler Number: The Damköhler number is a dimensionless quantity that compares the time scales of turbulent mixing (τT) and chemical reaction (τc). For low Da (τT << τc), the reaction is slow compared to mixing, and the mean-value closure rate is sufficient. For high Da (τT >> τc), the reaction is fast compared to mixing, and the EDM rate becomes dominant.

Modeling Accuracy: Accurately capturing the turbulent reaction rate is essential for predicting flame characteristics such as flame speed, temperature distribution, and pollutant formation. EDM, while simplified, provides a reasonable approximation of the turbulent reaction rate in many practical combustion applications. The detail flowchart for numerical investigation as per above method is presented below.



Flowchart 1. Flowchart of computational process

2. Model geometry

The model geometry consists of following sections.

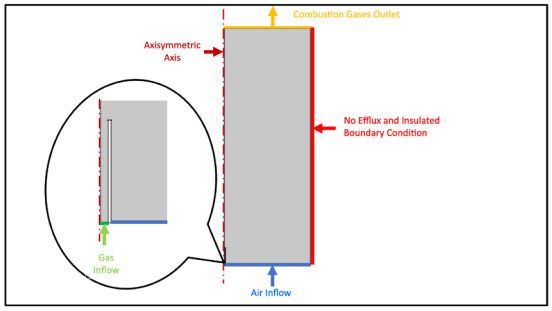


Figure 1. 2D axisymmetric model geometry considered for analysis

Inlet section includes the fuel inlet and the surrounding co-flow air inlet. The dimensions of these inlets are specified in the document, with Di being the inner diameter of the fuel inlet and do being the outer diameter of the co-flow air inlet. Combustion Chamber is the region where the fuel and air mix and burn. The boundary conditions applied to the model are as, fuel inlet is specified with values for velocity, temperature, and species mass fractions. Co-flow air inlet specified with values for velocity and temperature. Out-flow boundary condition, allowing the flow to exit the combustion chamber. The remaining boundaries of the computational domain are treated as walls.

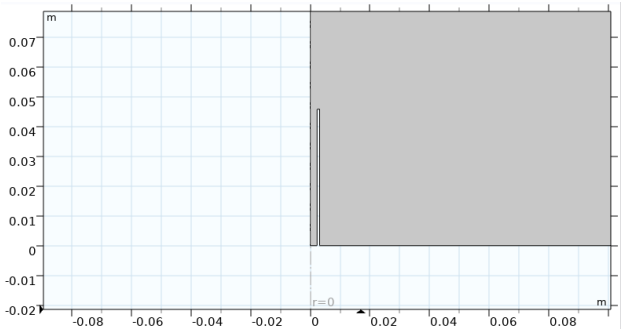


Figure 2. 2D axisymmetric model geometry focusing gas inlet region

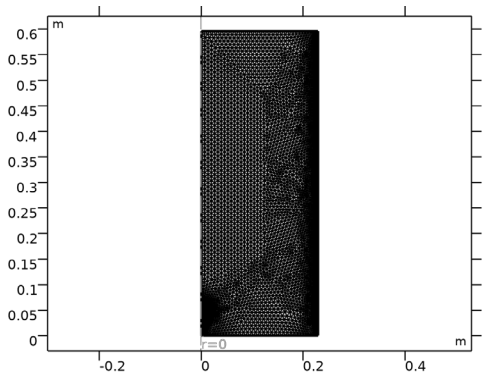


Figure 3. Discretization of 2D axisymmetric geometry with mesh

Mesh Statistics

Table 1. Mesh Statistics for grid independence test

Sr.No.	Mesh Type	Number of Elements	Maximum Element Size [m]	Minimum Element Size [m]
1.	Fine	695	0.0316	1.79E-4
2.	Finer	1090	0.022	7.44E-5
3.	Extra Fine	2844	0.0119	4.47E-5
4.	Extremely Fine	10518	0.00595	1.19E-5

Table 1 provides mesh details for various computational grids used in the analysis of syngas combustion. The numerical investigation uses combustion chamber as illustrated in figure 1 as the physical model, non-premixed diffusion combustion and ideal gas behavior for the products of combustion. Numerical simulations were conducted by varying inlet temperature, H_2/CO ratio with same jet velocity, co-flow velocity, and inlet volume fractions of N_2. The resulting, temperature, and reaction rate values were analyzed at different gas concentrations. A linear regression equation was developed to predict the maximum flame temperature based on numerical results.

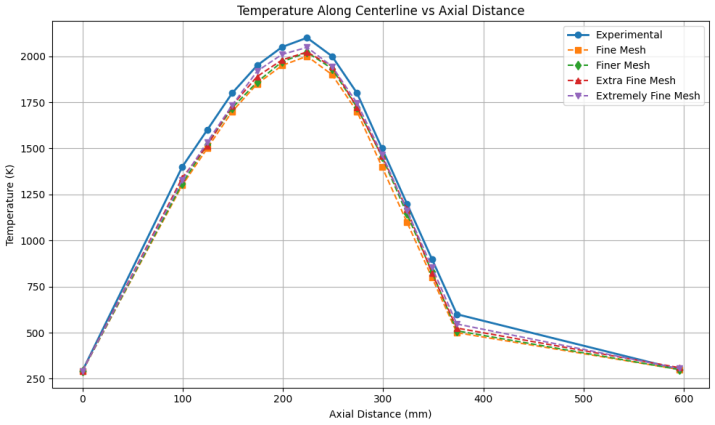


Figure 4. Validation for grid convergence test

The numerical simulation is conducted and reported by changing inlet temperature from 292 K to 400 K. The H_2/CO ratio as 0.2, 0.5, 1, 1.4 and 5. Fuel jet velocity considered as 100 m/s and co-flow velocity as 1 m/s. The inlet volume fraction for N_2 maintained at 0.4. After simulation, the pressure was found, temperature and mass fraction were obtained. The parameters such as temperature, pressure and mass fractions were analyzed at different concentration of gases.

3. Results

Temperature Distribution

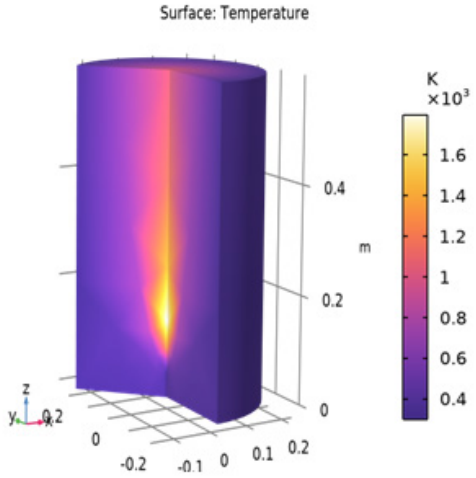


Figure 5. Temperature distribution in combustion chamber for H2/CO ratio of 0.2 at 298 K

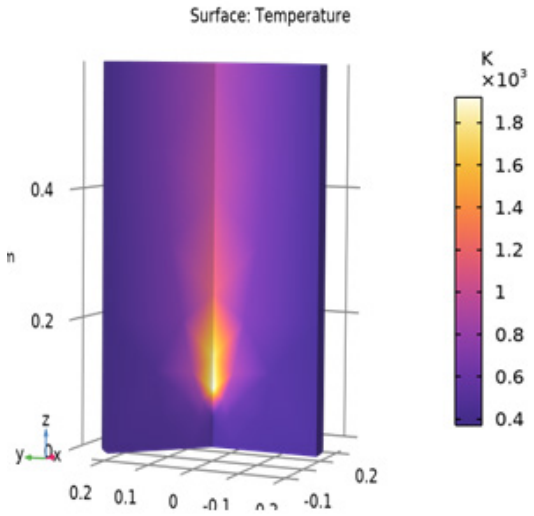


Figure 6. Temperature distribution in combustion chamber for H2/CO ratio of 5 at 400 K

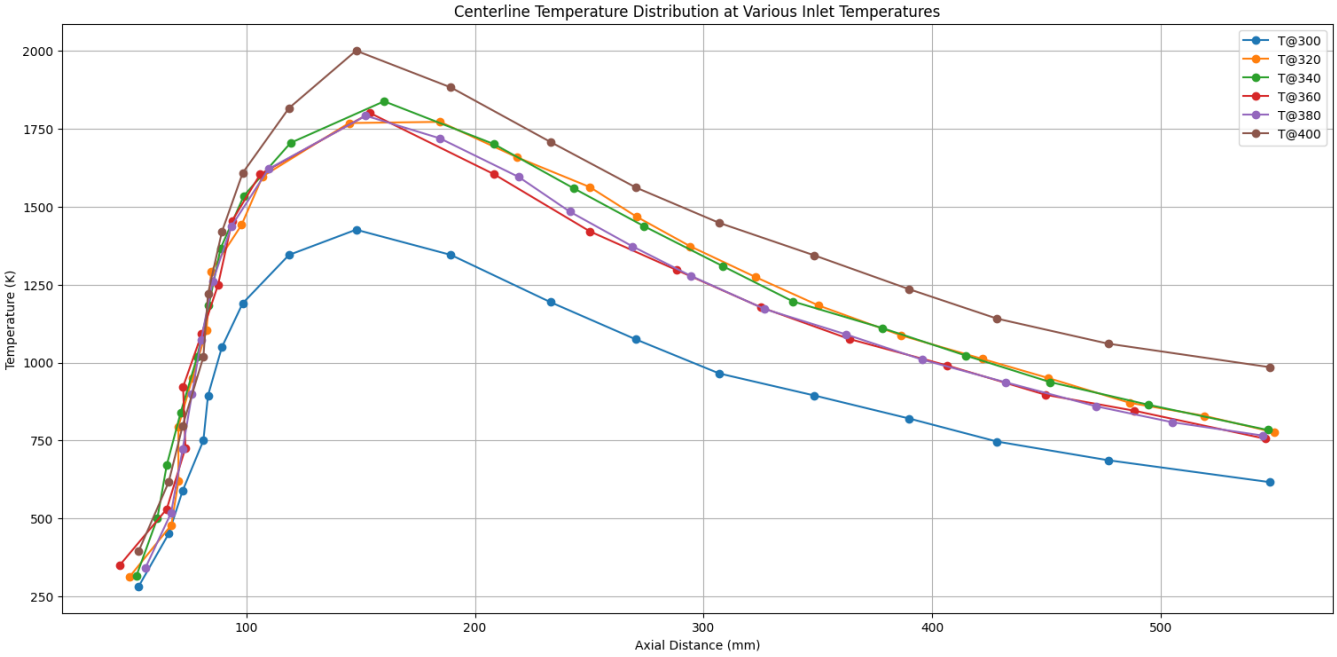


Figure 7. Inlet air temperature vs combustion chamber temperature for H2/CO ratio 0.2

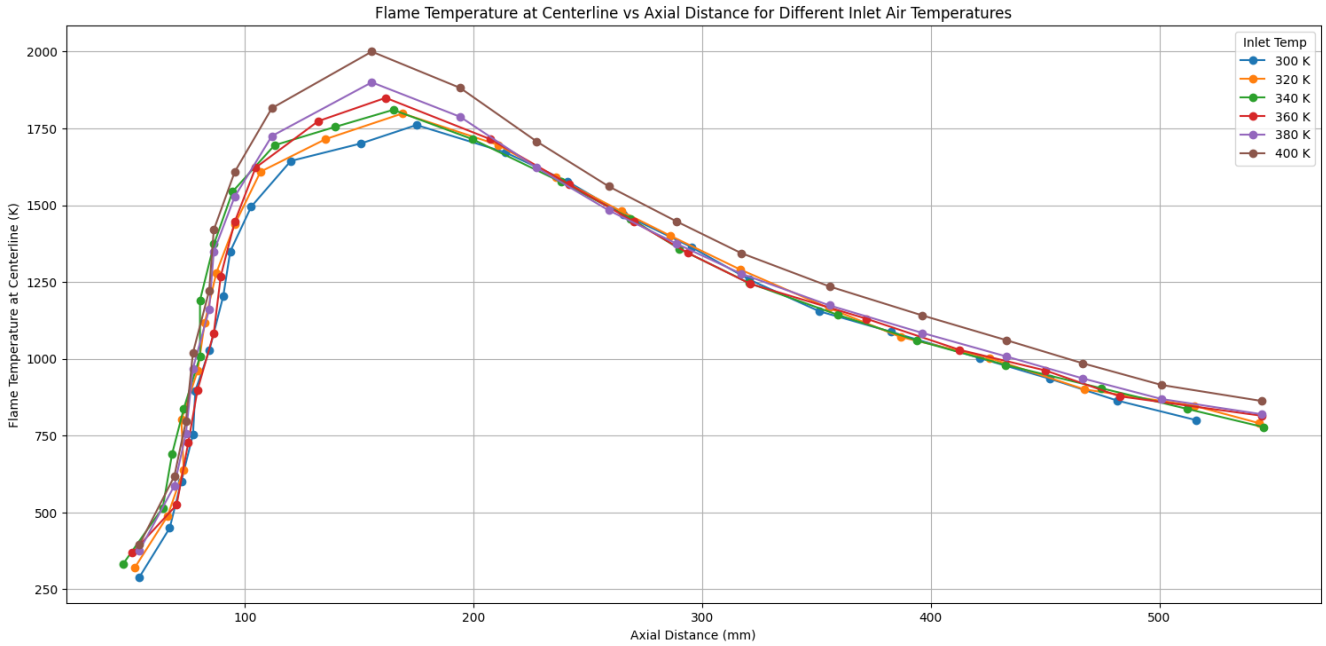


Figure 8. Inlet air temperature vs combustion chamber temperature for H2/CO ratio 0.5

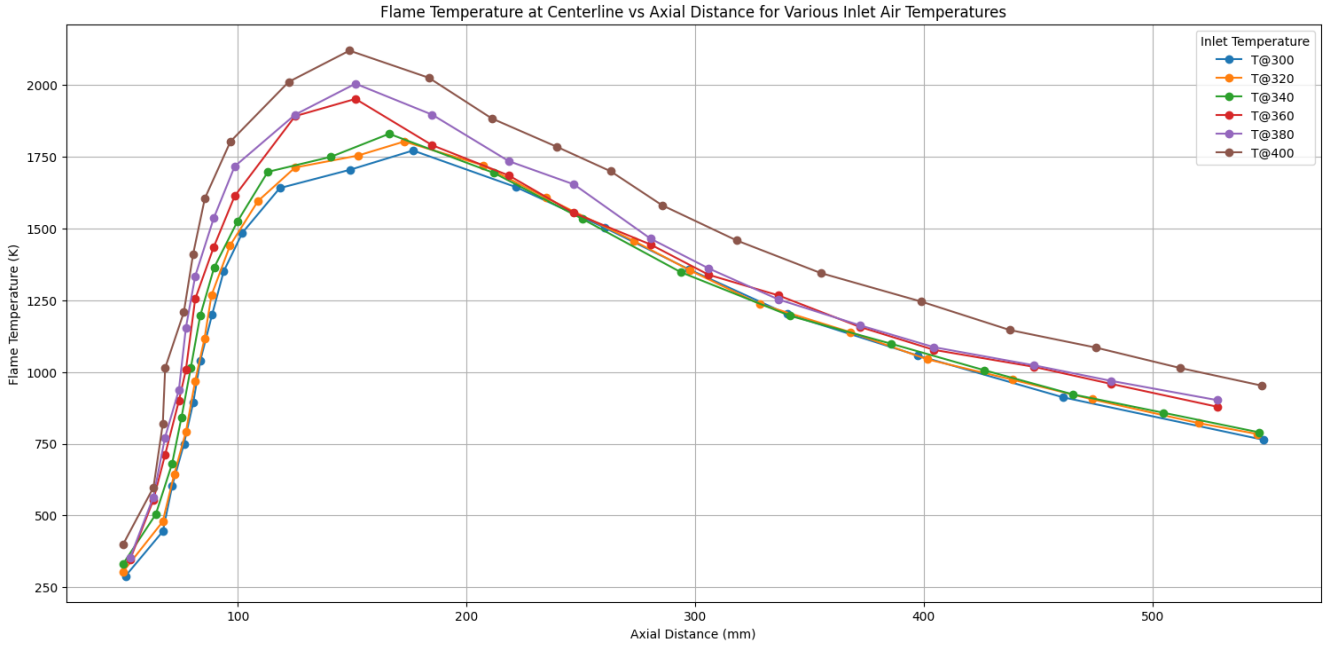


Figure 9. Inlet air temperature vs combustion chamber temperature for H2/CO ratio 1

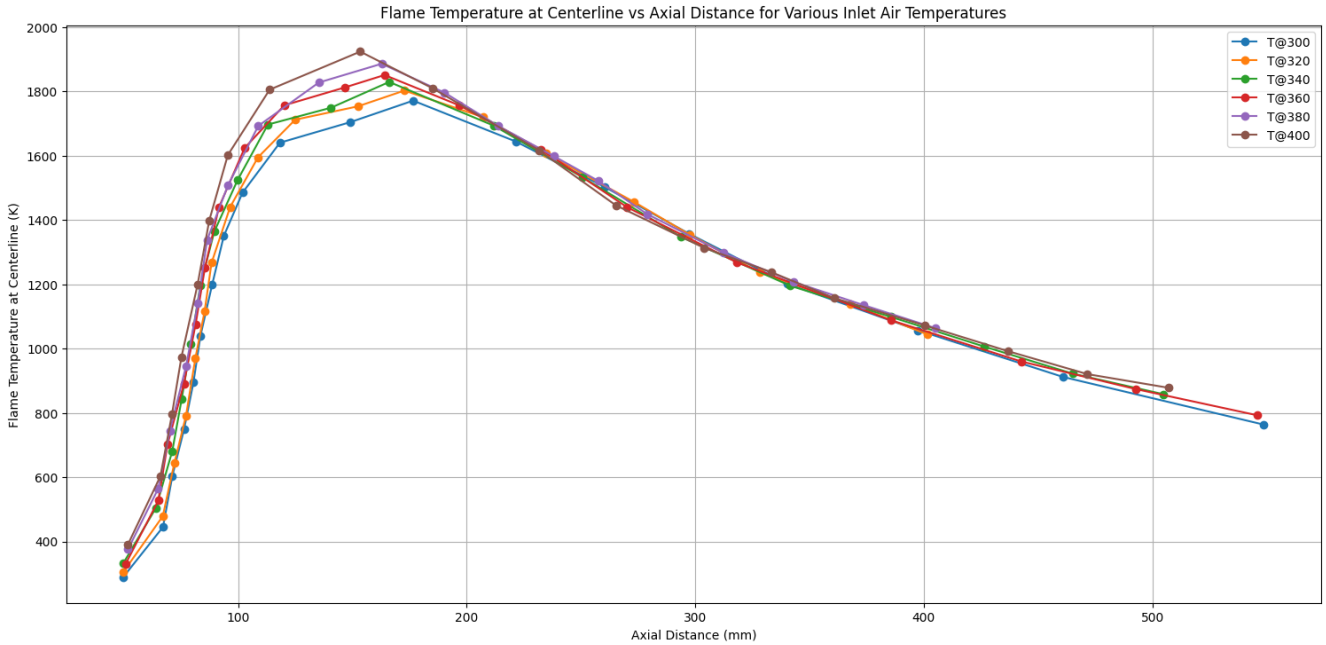


Figure 10. Inlet Air Temperature Vs Combustion Chamber Temperature for H2/CO ratio 1.4

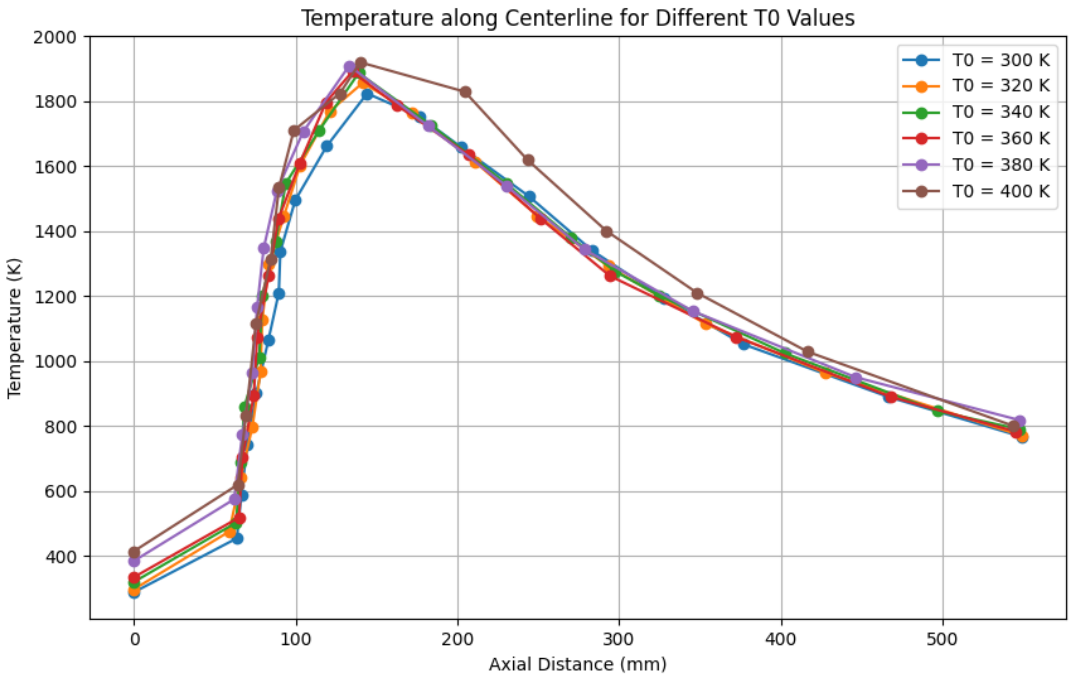


Figure 11. Inlet Air Temperature Vs Combustion Chamber Temperature for H2/CO ratio 2

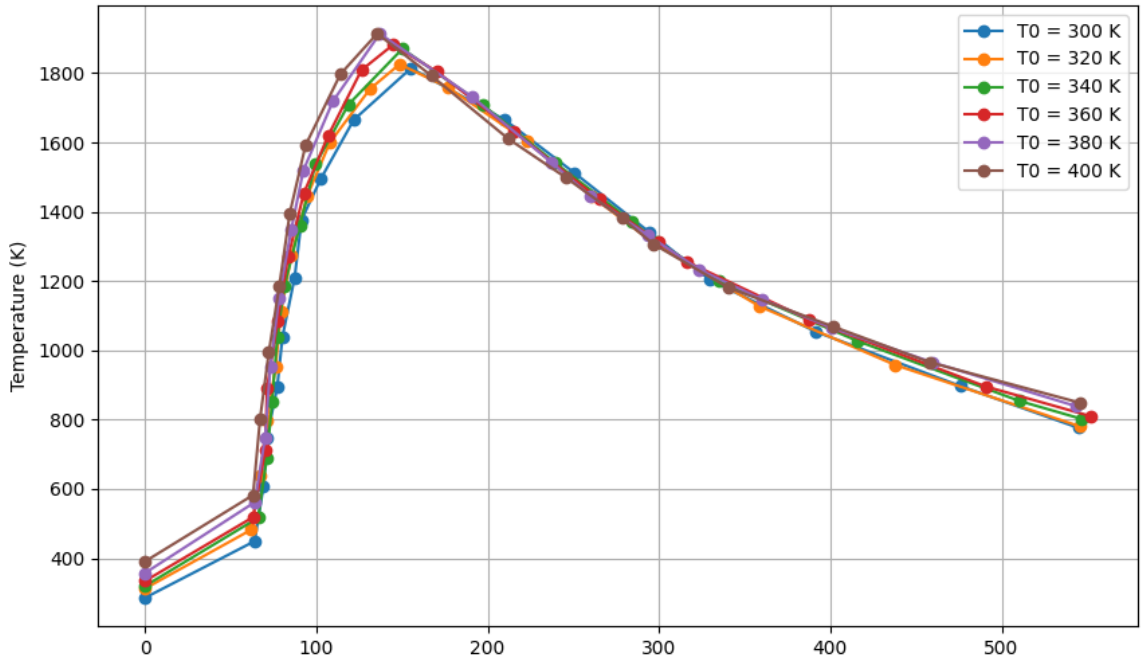


Figure 12. Inlet Air Temperature Vs Combustion Chamber Temperature for H2/CO ratio 5

Many researchers have worked to develop methods that increase heat generation from syngas with low heating value. By adding extra hydrogen to the syngas mix the combustion efficiency improves. The inlet air heating technique serves to raise the reaction rate which results in higher heat production. An air preheater serves as an effective solution to increase inlet air temperature. The simulations of combustion dynamics for inlet air temperatures between 298 K and 400 K were performed. Results show improved heat release rates when inlet air temperature increased so the method proves successful for combustion efficiency improvement. Investigation illustrates that improving low-calorific-value syngas heat release performance can possibly be achieved by perfecting inlet air temperature. The variations of inlet air temperature on adiabatic flame temperature become visible through Figures 7 -12 that examine H2/CO molar ratios kept constant alongside N2 composition uniformity. The presented figures reveal how rising inlet air temperature leads to greater adiabatic flame temperatures. Figure 7 presents the variation of combustor temperature with inlet air temperature for a low H_2/CO ratio of 0.2, showing a CO-dominant syngas mixture. The temperature rise within the combustor is relatively modest and nearly linear, reflecting the slower combustion kinetics and lower heating value of carbon monoxide. The limited hydrogen content leads to subdued combustion intensity, resulting in lower flame temperatures across the entire inlet air temperature range. As shown in Figure 8, increasing the H_2/CO ratio to 0.5 enhances the combustor temperature profile compared to Figure 7. The presence of more hydrogen accelerates the combustion process and increases the thermal energy release. While the trend stays linear, the slope is slightly steeper, showing improved combustion efficiency due to the synergistic effect of hydrogen addition. Figure 9 depicts the combustor temperature for an equimolar H_2/CO mixture. The temperature rise becomes significantly more pronounced, showing the combined influence of hydrogen's high reactivity and the thermal contribution from CO. The combustor exhibits more intense and uniform heating, highlighting the transition from CO-dominant to balanced fuel combustion behavior. With a further increase in hydrogen content (H_2/CO = 1.4), Figure 10 shows a marked improvement in combustor temperature response. The temperature gradient with respect to inlet air temperature becomes steeper, signifying faster combustion and higher flame temperatures. This hydrogen-rich mixture promotes enhanced ignition characteristics and more complete combustion. Figure 11 illustrates the combustor performance for a high H_2/CO ratio of 2.0. A significant increase in combustor exit temperature is seen, with a sharp temperature rise corresponding to increasing inlet air temperature. The elevated hydrogen content ensures rapid flame propagation and high heat release, making such mixtures highly effective for high-performance combustion systems. Figure 12 shows the extreme case of a hydrogen-rich mixture (H_2/CO = 5.0). This configuration results in the steepest temperature increase among all cases, confirming hydrogen's dominant role in enhancing combustion intensity. The combustor runs at the highest thermal output for any given inlet air temperature, emphasizing the potential of hydrogen-rich syngas in advanced combustion applications requiring high efficiency and reduced carbon emissions.

Variation in Peak Temperature Location Along the Axial Distance in a Can Combustor: In syngas-fueled can combustors, the location of peak temperature along the axial distance depends strongly on the H_2/CO ratio of the fuel mixture, as well as the inlet air temperature and mixing characteristics.

Low H_2/CO Ratios (e.g., 0.2–0.5): For fuel mixtures with low hydrogen content, combustion initiation is relatively slower due to the lower flame speed and higher ignition delay of CO-rich syngas. As a result, the flame stabilizes further downstream, and the peak temperature is typically seen at a greater axial distance from the burner inlet. The combustion process is more gradual, and the heat release zone is extended.

Intermediate H_2/CO Ratios (e.g., 1.0–1.4): As hydrogen content increases, the ignition delay shortens, and combustion becomes more intense. This shifts the peak temperature closer to the inlet region. The flame becomes more compact, and the region of maximum thermal energy release moves upstream, reducing the flame length and increasing thermal gradients near the combustor's entrance.

High H_2/CO Ratios (e.g., 2.0–5.0): At high hydrogen levels, the combustion process is very rapid and often begins almost at once after fuel–air mixing. In such cases, the peak temperature is found very close to the inlet or primary zone of the combustor. This upstream shift can result in very high local heat loads near the combustor walls, which has implications for thermal management and material selection.

Table 2. Effect of H_2/CO ratio on combustion intensity, peak temperature location, flame length

H_2/CO Ratio	Combustion Intensity	Peak Temperature Location	Flame Length
0.2	Slow, delayed	Downstream (farther axial)	Long
0.5	Moderate	Mid-axial region	Moderate
1.0–1.4	Fast	Closer to inlet	Short
2.0–5.0	Very fast	Near-inlet (primary zone)	Very short

Reaction rates:

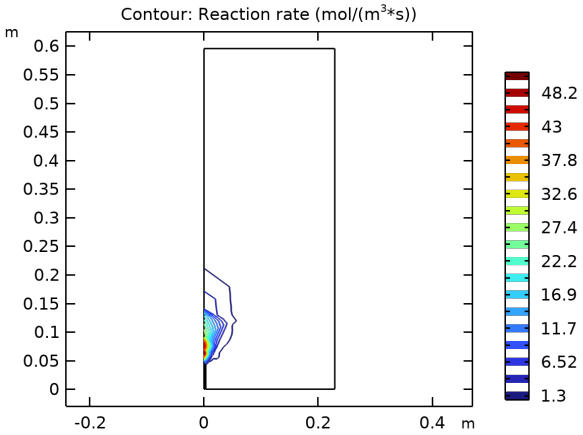


Figure 13. CO reaction rate in combustion chamber for H2/CO ratio of 1.4 at 298

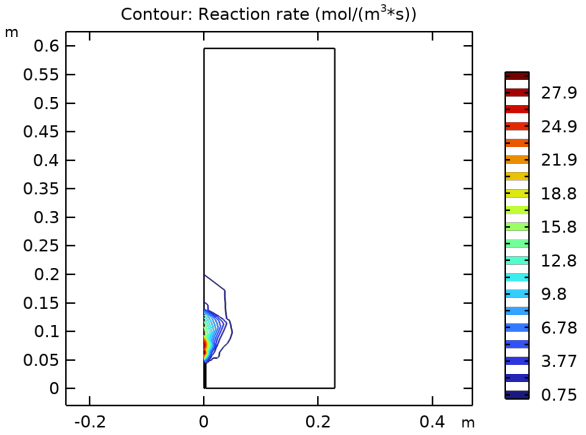


Figure 14. CO reaction rate in combustion chamber for H2/CO ratio of 1.4 at 400 K

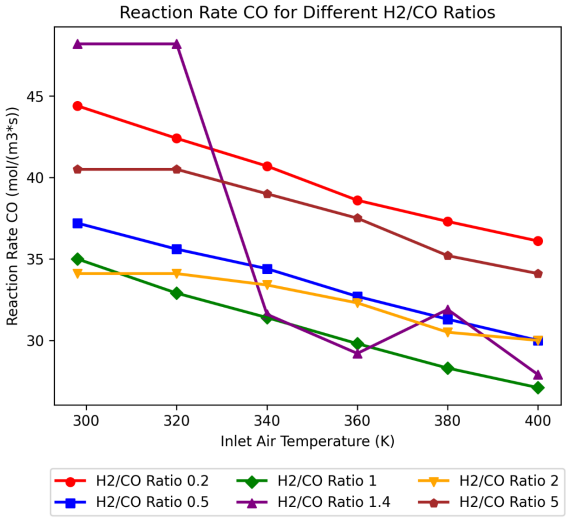


Figure 15. CO reaction Rate for various H2/CO Ratios at different temperatures

The reaction rate of carbon monoxide for different hydrogen-to-carbon monoxide (H_2/CO) ratios at distinct environment is presented in Figure 15. These phenomena give the impression that as the H_2/CO ratio increases, the reaction rate of CO decreases. Therefore, a higher concentration of hydrogen leads to slower oxidation of carbon monoxide. The increase in inlet air temperature reduces the reaction rate of CO due to the decrease in oxygen concentration needed for reaction as most oxygen is spontaneously used for hydrogen oxidation. Also, a higher concentration of hydrogen may be inhibiting the reaction between CO and other molecules. These facts are crucial for perfecting reaction conditions in industrial processes involving these gases. The hydrogen presence seems to set up an obstacle which reduces CO reaction efficiency through a competitive oxidation mechanism. The study of these chemical reactions requires fundamental knowledge to develop optimized burners and chemical processes that use CO oxidation. The conversion rate of CO in combustion processes reaches peak efficiency through H2/CO ratio control along with monitored inlet air temperature.

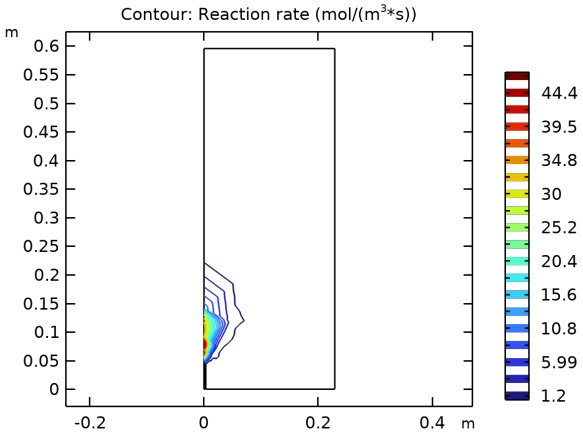


Figure 16. H2 reaction rate in combustion chamber forH2/CO ratio of 0.2 at 298 K

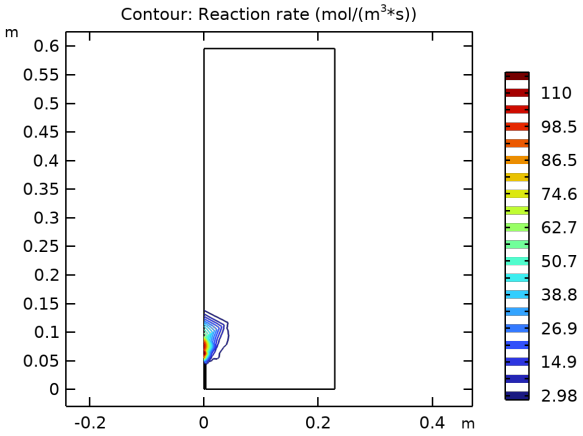


Figure 17. H2 reaction rate in combustion chamber for H2/CO ratio of 5 at 400 K

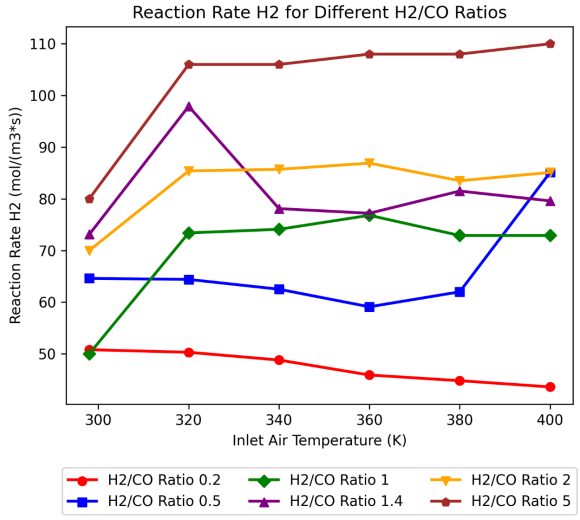


Figure 18. H2 Reaction rate for various H2/CO Ratios at different temperatures

Figure 18 shows the reaction rate of hydrogen (H2) when inlet air temperature rises at various H2/CO molar ratios. H2 reaction rates increase in parallel with increasing values of H2/CO molar ratio. The reaction rate of H2 shows substantial growth when temperature levels increase. The average kinetic energy of reactants defines temperature as a measurement. Higher temperatures generate greater kinetic energy among reactants which leads to their increased particle motion speed. A higher speed of molecular collisions at increased temperatures produces more energetic interactions between molecules for improved reaction rates. The required activation energy needed to start the reaction becomes more accessible at elevated temperatures allowing the reaction rate to accelerate further. Simulation data reveals that temperature together with molar ratios powerfully affects the reaction speed of H2. The reaction rate for H2 is slower when H2/CO molar ratios stay low according to the graph data. The successful optimization of reaction rates depends heavily on adjusting the molar ratio according to this evidence.

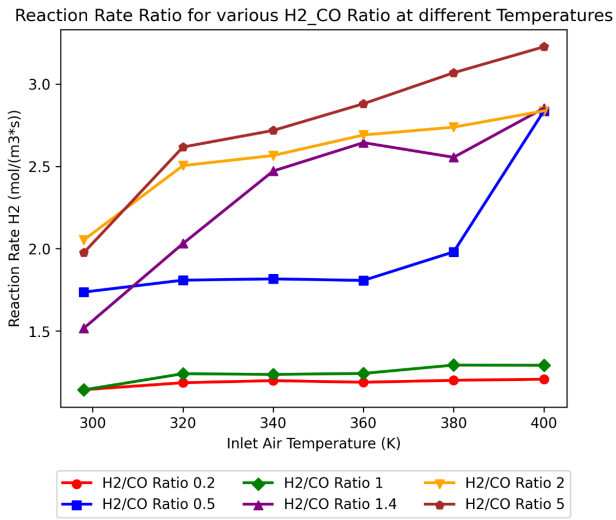


Figure 19. Reaction Rate ratio for various H2/CO Ratios at different temperatures

The research shows in Figure 19 how different temperatures affect the reaction rates when changing the H2/CO molar ratios. The experimental findings show that the H2/CO molar ratio directly affects the reaction speed. The documented information proves useful for perfecting combustion reaction conditions. The presence of higher amounts of H2 in the mixture enhances reaction speed but such conditions could trigger uncontrollable spontaneous fire. A suitable best H2/CO molar ratio must be set up to achieve stable combustion. High hydrogen content in syngas can lead to temperatures exceeding 1200 K which may increase NOx emissions. The visual data in the graph presents the relationships between H2/CO molar ratio and reaction rate with temperature so researchers better understand combustion dynamics. H2/CO molar ratio monitoring and regulation enables efficient stable combustion operations that prevent spontaneous combustion and minimize the formation of excessive NOx emissions.

Heat of reaction

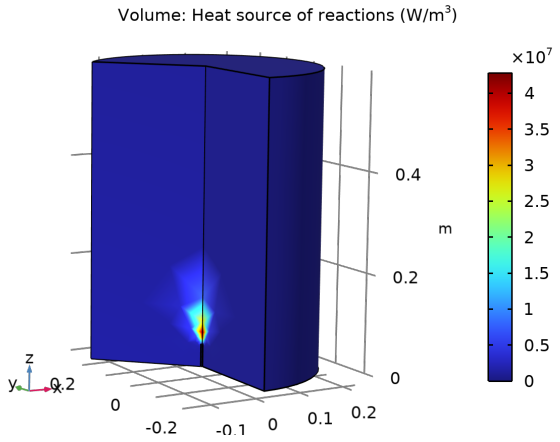


Figure 20. Heat of reaction in combustion chamber for H2/CO ratio of 0.2 at 298 K

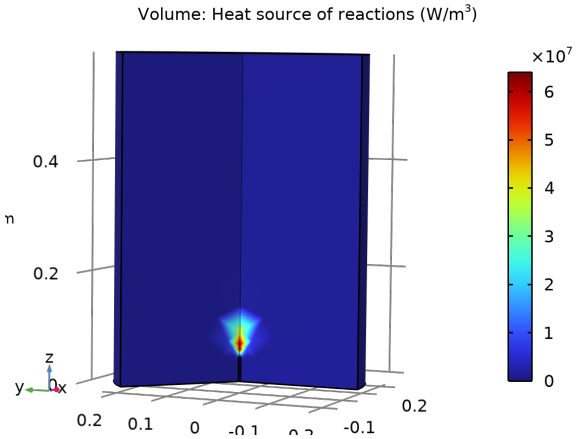


Figure 21. Heat of Reaction in combustion chamber for H2/CO ratio of 5 at 400 K

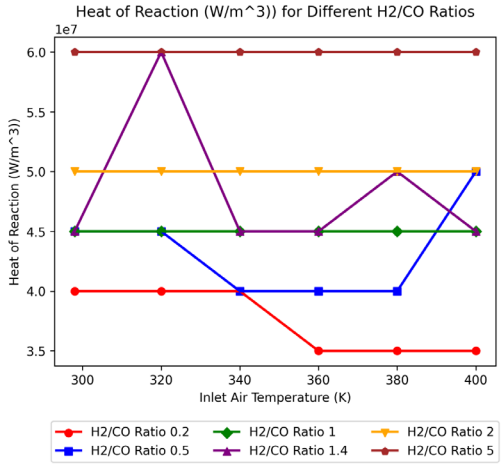


Figure 22. Heat of Reaction (W/m^3) for various H2/CO ratio at different temperatures

The Figure 22 displays the reaction heat (W/m^3) for various H_2/CO molar ratios measured at different temperatures. The reaction heat becomes stable when the H2/CO ratio exceeds 1. Research shows that the heat of reaction depends on H2/CO molar ratios instead of inlet air temperature variations. The data reveals that elevating the H2/CO molar ratio leads to increased heat release in the process because the reaction becomes more exothermic. The H2/CO ratio needs precise control because it directly influences heat production during the process.

4. Conclusion

Numerical study of syngas combustion in a round-jet burner produces essential findings about various characteristics of the process. The adiabatic flame temperature receives substantial impact from the H2:CO ratio found in syngas. The H2/CO ratio of samples decides the maximum achievable adiabatic flame temperature because it underlines the vital impact composition has on combustion behavior. Carbon monoxide reaction rate together with hydrogen rate show important influence from both the input air temperature and the H2/CO ratio. Higher ratios of hydrogen to carbon monoxide cause carbon monoxide reactions to slow down as hydrogen reactions simultaneously accelerate. The syngas's H2/CO ratio causes greater sensitivity changes to reaction heat than the inlet air temperature does. Syngas compositions affect heat generation optimization through changes of the H2/CO ratio because the reactions become more exothermic. Minimizing heat generation differences and perfecting reaction speed requires engineers to keep precise control of H2/CO ratio together with inlet air temperature in syngas-powered systems. The research-based numerical findings from this study create essential knowledge for engineering, the development and maintenance of power generation systems and industrial processes and transportation systems through syngas-based combustion.

Author contributions statement

Seema Borde and Amogh Sambare: Conceptualization, method, software, formal analysis, writing – original draft, and writing – review & editing. Aniruddh Nikalje: Supervision, review and editing.

Declaration of interests

The authors have no competing financial or personal interests related to this work.

Data availability

Generated data will be available from corresponding author with reasonable requests.

Declaration of generative AI and AI-assisted technologies in the writing process

No generative AI or AI-assisted technologies were used in the writing process.

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