Multi-Fuel Burner Design for Hydrogen and Ammonia Combustion

Inzamam Mushtaq

Saudi Arabian Engineering Co. Ltd. (SAECO), Kingdom of Saudi Arabiax

Juan Manuel Paz

Multiphysics Modelling School, University of Malaga, Spain

Antonio Atienza-Márquez

Multiphysics Modelling School, University of Malaga, Spain

Abstract. This thesis presents a computational and multiphysics-based design and analysis of a multi-fuel burner system capable of efficiently combusting ammonia (NH_3) and hydrogen (H_2) under varying operational conditions. The primary objective is to investigate combustion characteristics, determine optimal air–fuel ratios, and assess the trade-offs between complete fuel conversion and NO_x emissions using a staged modeling approach in COMSOL Multiphysics®. Initial simulations employ 0D continuous stirred-tank reactor (CSTR) models to analyze single-fuel NH_3 combustion, incorporating detailed reaction kinetics and user-defined thermophysical properties. Four distinct scenarios are simulated across different pressures (5–10 atm), temperatures (1200–1800 K), and equivalence ratios (φ = 0.85–0.9), yielding full ammonia conversion with varied residence times. Subsequently, the study expands to dual-fuel (NH_3 + H_2) combustion scenarios, introducing additional complexity in flame behavior and emission dynamics. The COMSOL model integrates species transport, energy conservation, and Arrhenius-based kinetics through time-dependent solvers, establishing a robust foundation for analyzing ammonia-hydrogen co-firing. Although NO_x (NO and NO_2) pathways are not yet modeled, future work will integrate validated mechanisms to capture temperature-dependent formation and mitigation strategies. This research aims to contribute to the decarbonization of industrial heating by validating ammonia–hydrogen combustion as a cleaner alternative to conventional fuels. Further extensions include simulation of 2D/3D burner geometries and application of developed insights toward designing low-emission, high-efficiency industrial burner systems.

I. INTRODUCTION

Ammonia (NH_3) and hydrogen (H_2) are emerging as promising carbon-free fuels in the global decarbonization roadmap. Their combustion avoids CO_2 emissions, making them attractive alternatives to hydrocarbon fuels, especially in power generation, transportation, and industrial heating. Ammonia offers advantages in storage and transport due to its high volumetric energy density and ease of liquefaction, while hydrogen has superior reactivity and combustion performance. However, both fuels come with technical challenges: ammonia exhibits low flame speed, high ignition temperature, and substantial NO_x emissions, whereas hydrogen is associated with high diffusivity, potential flashback risks, and material compatibility issues. Combining the two fuels can potentially balance their drawbacks—hydrogen enhances flame stability and ignition, while ammonia acts as a hydrogen carrier and carbon-free energy vector. [1] [2]

Ammonia-air flames typically burn at laminar flame speeds of 6–8 cm/s, significantly lower than methane-air or hydrogen-air mixtures. In contrast, hydrogen exhibits a much higher flame speed (~200 cm/s in stoichiometric H_2-air), making it useful for improving the combustibility of NH_3-rich blends. However, hydrogen's high flame speed also raises safety concerns like flashback and pre-ignition. When blended (NH_3-H_2), the flame characteristics are modified: hydrogen lowers the ignition delay and increases flame stability, while ammonia reduces carbon emissions and acts as a diluent. Nonetheless, NO_x formation remains a shared issue, as both fuels contain nitrogen (NH_3 directly and H_2 through ambient air) and can yield NO and NO_2 via thermal and prompt mechanisms, particularly at high temperatures or rich equivalence ratios. [2] [3] [9]

Ammonia combustion produces nitrogen-based pollutants—primarily NO and NO_2 (collectively NOx) through thermal and fuel-bound mechanisms. NOx emissions can surpass 1000 ppm under stoichiometric or lean combustion conditions. Analogous to the treatment of diesel exhaust gases using Selective Catalytic Reduction (SCR) systems, similar after-treatment solutions such as AMOX and SCR can be deployed to mitigate NOx and unburned ammonia emissions. For example, ammonia slip from engines can be converted into nitrogen using SCR, eliminating the need for urea injection, a practice common in modern diesel systems. [1] [3]

The dominant combustion reaction for ammonia and hydrogen blended systems may be approximated by the global stoichiometric equation:

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$$

However, real combustion involves intricate chemical

kinetics, including chain reactions with radicals such as NH, NH_2, H, and OH. The presence of hydrogen accelerates these radical reactions and modifies the flame structure, often increasing reactivity but also influencing NO_x pathways. Combustion efficiency and emissions depend critically on the equivalence ratio (ϕ), temperature, and residence time. Lean mixtures with excess air reduce NO_x but risk incomplete ammonia combustion; rich mixtures can suppress NH_3 slip but may enhance NO formation. Thus, accurate kinetic modeling; especially using validated mechanisms (e.g., Okafor, Tian, or Glarborg models) is essential for predicting pollutant formation and optimizing burner design for ammonia-hydrogen fuel systems. [2] [3]

Multiphysics simulation tools like COMSOL offer robust frameworks to analyze the complex interplay of fluid flow, heat transfer, and chemical kinetics in ammonia-hydrogen combustion. CSTR models allow analysis of reaction kinetics in a zero-dimensional setting, isolating the influence of temperature and residence time without spatial gradients. One-dimensional laminar models and full 2D/3D CFD setups can then capture flame structure, NO_x formation zones, and transport effects more accurately. These simulations rely on detailed kinetic mechanisms, thermodynamic data, and transport properties for both NH_3 and H_2. Discrepancies between experiments and simulations highlight the importance of species-resolved validation and precise definition of boundary and initial conditions. Blended-fuel modeling enables identification of optimal mixing ratios, equivalence ratios, and reactor configurations to enhance stability, reduce emissions, and achieve cleaner energy conversion. [2].

II. MATERIALS AND METHODS

This study employed COMSOL Multiphysics (v6.3) with the Chemical Reaction Engineering Module to simulate ammonia-hydrogen combustion in a well-stirred reactor (0D model). A continuous stirred-tank reactor (CSTR) configuration was chosen to represent perfectly mixed combustion, allowing temporal analysis of species and temperature without spatial gradients. Chemical species involved in the reaction mechanism were defined within COMSOL's Reaction Engineering interface as gas-phase species (NH_3, H_2, O_2, H_2O, and N_2), with ammonia (NH_3) and hydrogen (H_2) as fuels, oxygen (O_2) as oxidizer, and nitrogen (N_2) as both an initial inert (to simulate air) and a product of ammonia oxidation (water H_2O being the other combustion product). No NO_x species were included at this stage. The Reaction Engineering interface automatically formulates the species mass balance equations for a perfectly mixed reactor given the reaction scheme. Global one-step reactions were used to describe the overall combustion process of the NH_3/H_2 fuel blend (e.g., ammonia oxidation to N_2 and water, and hydrogen oxidation to water). The reaction kinetics were specified using Arrhenius expressions for the rate constants, with pre-exponential factors and activation energies taken or estimated from literature values for ammonia and hydrogen combustion. [4] [10]

Each reaction's rate R_j takes the form

$$R_j = k_j(T) \cdot \prod_i C_i^{v_{i,j}}$$

where the reaction rate of the *j-th* reaction, denoted as R_j , is typically expressed in units of mol/m³·s and quantifies the rate at which a chemical transformation proceeds. This rate is governed by the temperature-dependent rate constant $k_j(T)$, which is often described using the Arrhenius equation. The rate also depends on the concentrations of the reactant species, represented as C_i in mol/m³, and their respective stoichiometric coefficients $\nu_{i,\ j}$ in the reaction. These coefficients indicate the number of moles of species *i* involved in the *j-th* reaction and typically apply to reactants only when formulating the forward reaction rate. The overall rate expression includes the product of all reactant concentrations raised to the power of their stoichiometric coefficients, compactly written using the product operator $\prod_i Ci^{vi,\ j}$ which multiplies across all relevant species *i*.

The temperature-dependent rate constants k(T) are modeled using the Arrhenius equation:

$$k(T) = A \cdot T^n \cdot \exp(-\frac{E_a}{RT})$$

Whereas in the Arrhenius rate expression, A represents the pre-exponential factor, n is the empirical temperature exponent (typically zero for elementary reactions), Ea denotes the activation energy (J/mol), R is the universal gas constant (8.314 J/mol·K), and T is the absolute temperature (K). These kinetic parameters were implemented through COMSOL's built-in reaction interface, which directly supports temperature-dependent rate formulations.

To account for thermophysical properties and heat effects, the model utilized COMSOL's built-in thermodynamic property package. An ideal gas mixture model was selected (appropriate for the gaseous reactants and products), enabling COMSOL to automatically compute temperature-dependent properties such as heat capacities (c_p), enthalpies, and mixture densities for all species. The thermodynamic data

(such as standard enthalpy of formation for each species) were drawn from COMSOL's internal database, which uses standard correlations (e.g., NASA polynomial fits) to evaluate properties over the temperature range of interest. This allowed the simulation to calculate reaction enthalpies on-the-fly: COMSOL determines the heat of reaction from the difference in formation enthalpies of products and reactants, and updates the mixture's energy balance accordingly during combustion. In practice, a thermodynamic property package was created by selecting the species NH_3, H_2, O_2, H_2O, and N_2 from the database and assigning the ideal gas model, then linking this package to the Reaction Engineering interface so that species internal energy/enthalpy calculations and transport properties (if needed) were consistently applied. This approach ensures accurate evaluation of the energy conservation in the reactor, accounting for the exothermic reaction heats.

Reactor setup: The CSTR was modeled at atmospheric pressure (5 atm and 10 atm) and operated under adiabatic conditions (no heat exchange with the environment), so that all reaction heat releases contribute to raising the gas temperature. The reactor volume was set to a nominal value (1.0 L and 2.0 L) with inlet feed streams defining the initial reactant quantities. A stoichiometric fuel/oxidizer ratio was used in the feed: the inlet molar composition was configured such that the combined $NH_3 + H_2$ fuel had an equivalence ratio of 1.0 with O_2 (for example, a mixture of NH_3 and H_2 in a certain ratio with air, where "air" was 21% O_2 and 79% N_2). In a transient simulation context, this is equivalent to a closed homogeneous batch reactor with the same initial composition. At time t=0, the reactor was filled with the premixed reactants (e.g., NH_3, H_2, O_2, plus N_2 as diluent) at a given initial temperature (typically on the order of 298–1000 K, with higher initial temperature used in some cases to facilitate ignition of ammonia). The mesh for this 0D model is trivial, since no spatial domain is involved – the Reaction Engineering interface solves ordinary differential equations in time without needing a spatial discretization mesh. (If a 1D or higher-dimensional model were used, a physics-controlled mesh set to *fine* or *extra fine* would be employed as recommended for resolving steep gradients in combustion problems. For instance, in preliminary 1D tests, COMSOL's default *fine* mesh proved sufficient for accuracy, and further mesh refinement did not significantly change the results, confirming mesh-independence.) Thus, the focus here was on temporal resolution rather than spatial resolution.

Solver configuration: A time-dependent study was performed to simulate the transient combustion process from ignition through to completion/steady-state. COMSOL's solver uses an implicit variable-step, variable-order backward differentiation formula (BDF) method for stiff ODE systems, which is well-suited to combustion kinetics that often exhibit stiffness due to disparate timescales (fast radical reactions versus slow induction periods). The solver was run with a relative tolerance on the order of 10^{-5} to 10^{-6} to ensure numerical accuracy. Time-stepping was adaptive: initially very small-time steps were taken during the rapid ignition phase (where species and temperature change quickly), and larger steps were allowed as the system approached equilibrium. The simulation was carried out until a final time beyond which all transients died out and a steady state (constant species concentrations and temperature) was reached – typically on the order of a few seconds for the 0D reactor, depending on initial conditions. To verify the solution's robustness, sensitivity checks were conducted on solver settings: tightening the tolerances and initial time step produced no appreciable change in the results, indicating that the default settings captured the dynamics adequately. Because of the homogeneous 0D nature, mixing and mass transfer limitations are by definition absent – the model assumes instant mixing. Therefore, the accuracy of results hinges on the kinetic mechanism and thermodynamics, which were carefully set up as described. The overall modeling approach in COMSOL (using the Reaction Engineering interface with a linked thermodynamic property package) provided an efficient and reliable way to simulate the coupled chemical kinetics and heat release in an ideal reactor. This methodology lays the groundwork for subsequent expansion to spatially-resolved models using the same kinetic and thermodynamic definitions.

Summary of Reactor Models and Kinetic Setup: In this study, four distinct simulation models were developed to investigate the kinetic behavior of ammonia (NH_3) combustion under varying thermodynamic and flow conditions using a 0D Continuous Stirred Tank Reactor (CSTR) approach. The models differ in temperature, pressure, reactor volume, and air inflow rate while maintaining a consistent NH_3 inflow of **0.005 m³/s** across all cases.

Model 1, simulated on 15.03.2025, was set at **10 atm** and **1800 K** with a reactor volume of **1 L (0.001 m³)**. The air inflow rate was **0.02 m³/s**, and the equivalence ratio (ϕ) was **0.90**, slightly lean. **Model 2**, simulated on 25.03.2025, kept the pressure at **10 atm** but reduced the temperature to **1500 K** while doubling the reactor volume to **2 L (0.002 m³)**. The air inflow rate was increased to **0.025 m³/s**, and ϕ was slightly leaner at **0.85**.

Model 3, dated 05.04.2025, further reduced the pressure to **5 atm** and temperature to **1200 K**, simulating a lower reactivity environment. The reactor volume returned to **1 L**, with the air inflow rate adjusted to **0.02381 m³/s**. The outlet flow rate was matched to the sum of the inflow streams, ensuring a steady-state mass balance at **0.02881 m³/s**. **Model 4**, developed on 12.04.2025, used the same pressure and temperature as Model 3 (**5 atm**, **1200 K**) but increased the reactor volume to **2 L**, keeping the inflow conditions identical to Model 3.

Additional variables such as species inflow concentrations were derived as: **O_2_in = 5.0001 1/s** and **NH_3_in = 5 1/m³**, calculated based on inflow rate per unit reactor volume.

The reaction kinetics were modeled using a single-step global reaction for NH_3 oxidation. The **forward frequency factor (Af)** was either **1.2×10^{12} or 1.5×10^{12} $m^{18}/(s\cdot mol^6)$** depending on the case, with a **temperature exponent nf = 0**, and a **forward activation energy (Ef)** ranging from **25,000 J/mol to 37,500 J/mol**. These kinetic parameters were coupled with molar mass data for each species: **NH_3 (17.03079 kg/kmol)**, **O_2 (31.9988 kg/kmol)**, **N_2 (28.0137 kg/kmol)**, and **H_2O (18.01536 kg/kmol)**. In all cases, NH_3 and O_2 were the primary reactants, while N_2 and H_2O were tracked as main products.

The outflow rate of each species was computed via steady-state assumption: $F_{out,\,i} = -F_{out} \times c_i$ where c_i is the species concentration obtained from the reactor's solution.

Inflow specifications were consistently applied as NH_3: **0.005 m³/s**, while O_2 was computed based on its fractional composition in air (21%) multiplied by air inflow and normalized per reactor volume. The values of the **oxygen inflow per unit reactor volume** (e.g., **5 1/s**) served as a crucial variable for modeling the combustion stoichiometry and rate-limiting behavior in lean mixtures.

III. THEORY

Mass and Energy Conservation Equations: In a well-stirred reactor (0D model), the governing equations are derived from fundamental mass and energy conservation principles. Species mass balance: For each chemical species i, the accumulation in the reactor equals the net production/consumption by chemical reactions plus any inflow minus outflow. In a batch reactor (no flow), this simplifies to an ODE

$$\frac{dN_i}{dt} = V\sum_{r=1}^{N_r} \nu_{i,r}\cdot r_r\left(T,\{C_j\}\right)$$

where N_i is the moles of species i (C_i its concentration), V is the reactor volume, $\nu_{i,r}$ is the stoichiometric coefficient of species i in reaction r (positive for products, negative for reactants), and r_r is the rate of reaction r (in concentration units per time). This equation describes the rate of change of moles of species N_i in a reactor of volume V, accounting for all chemical reactions involving species iii. The reaction rate is determined by the stoichiometric coefficients $\nu_{i,r}$ the temperature-dependent reaction rates $r_r(T,\{Cj\})$, and the total number of reactions N_r. COMSOL's Reaction Engineering interface automatically formulates and solves this equation based on the defined species and reactions.

The above equation is automatically formulated by COMSOL's Reaction Engineering interface when reactions and species are defined.

In a continuous CSTR, flow terms appear:

$$\frac{dN_i}{dt} = \dot{N}_{i,in} - \dot{N}_{i,out}V\sum_{r=1}^{N_r} \nu_{i,r}\cdot r_r$$

At steady state, $dN_i/dt=0$, and the production by reactions balances the difference between inlet and outlet flows. For this thesis, we primarily consider the batch formulation (transient ignition in a closed volume) as an analog to the CSTR's startup, since we are interested in the time evolution of the combustion.

Energy balance: The energy conservation equation stems from the first law of thermodynamics applied to the reacting mixture. For a constant-pressure reactor (appropriate for a vessel with a vent or a continuously flowing system at fixed pressure), it is convenient to use an *enthalpy* form of the energy equation. The general form (for a CSTR) is:

$$\frac{d}{dt}\left(\rho V\,\bar{H}\right) = \dot{m}_{in}\bar{H}_{in} - \dot{m}_{out}\bar{H}_{out} + Q_{ext} + V\sum_{r=1}^{N_r}(-\Delta H_r)\cdot r_r$$

In the general energy balance for a reacting system, ρ represents the mixture density (kg/m³), and V is the reactor volume (m³). The mixture-specific enthalpy is denoted by $\bar{H}$ (J/kg), while $\dot{m}_{in}$ and $\dot{m}_{out}$ are the mass flow rates into and out of the reactor, respectively (kg/s). Correspondingly, $\bar{H}_{in}$ and $\bar{H}_{out}$ represent the specific enthalpies of the inlet and outlet streams Q_{ext} denotes the external heat input, which is considered positive if heat is added and negative if removed (W). The term ΔH_r is the enthalpy change associated with the *r-th* chemical reaction (J/mol), with negative values indicating exothermic behavior. The rate of this reaction is represented by r_r (mol/m³·s), and the total number of reactions occurring within the system is denoted by N_r. This formulation represents the rate of change of total enthalpy within a control volume, accounting for energy contributions due to mass flows, external heat transfer, and the heat released or absorbed from chemical reactions.

In an adiabatic batch reactor (no mass flow and no external heat), above Equation simplifies to

$$\frac{d}{dt}\left(\rho V\,\bar{H}\right) = V\sum_{r}(-\Delta H_r)\cdot r_r$$

Assuming constant pressure and using $H^{-}=c_{p,mix}T$ where $c_{p,mix}$ is the specific heat capacity of the mixture, we get:

$$\rho V_{c_{p,mix}} \frac{dT}{dt} = -V \sum_{r} \Delta H_r \cdot r_r$$

This form is widely used to predict temperature rise or fall in an adiabatic system due to exothermic or endothermic reactions. Moreover, it states that the rate of temperature increase is driven by the net exothermic (or endothermic) reaction rate. Each reaction's enthalpy ΔH_r is computed from the reactants and products enthalpies. COMSOL's thermodynamic database automates this calculation by providing enthalpies of formation for each species and computing reaction enthalpies accordingly. For example, for the global ammonia combustion reaction ($4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6\ H_2O$), the reaction enthalpy ΔH_r at a given temperature is calculated as:

$$\Delta H_r = \sum_{prod} v_i\, h_i\,(T) - \sum_{react} v_i\, h_i\,(T)$$

where $h_i(T)$ is the molar enthalpy of species i, which includes the formation enthalpy at the reference state plus the sensible enthalpy increase up to temperature TTT.

The mixture heat capacity, $c_{p,\,mix}$ is calculated as:

$$c_{p,mix} = \sum_{i} x_i \cdot\ c_{p,i}\,(T)$$

where x_i is the mole fraction of species i, and $c_{p,\,i}(T)$ is its temperature-dependent heat capacity**.**

During exothermic combustion, the right-hand side of the above Equation:

$$\rho V_{c_{p,mix}} \frac{dT}{dt} = -V \sum_{r} (\Delta H_r) \cdot r_r$$

is negative**,** because $-\Delta H_r$ is positive for exothermic reactions. This results in an increase in temperature T. This continues until either reactant are consumed (so r_r to 0) or the system reaches a chemical equilibrium at which forward and reverse reaction rates balance (not applicable here since we assume complete one-way conversion with no significant reversible reactions). The energy equation thus captures the adiabatic temperature rise due to combustion. In our 0D model, we assume no heat loss, so the final adiabatic flame temperature can be reached in principle. (In reality, a burner would have heat losses that lower the temperature; those would be included in a 2D/3D model via heat transfer boundaries.)

It is worth noting that if the reactor were operated at constant *volume* instead of constant pressure, the internal energy and possibly pressure changes would be considered; however, our assumption of a CSTR or vented batch at 1 atm means pressure is roughly constant and work done by expansion is accounted for, so enthalpy is the appropriate energy function. The Reaction Engineering interface in COMSOL can solve the energy equation simultaneously with species equations when a thermodynamic property package is linked, thereby including these enthalpy and heat release effects.

Chemical Kinetic Formulation (Arrhenius Rate Laws): The reaction kinetics for ammonia and hydrogen combustion were formulated on the basis of Arrhenius rate laws and mass-action principles. Each reaction in the mechanism is expressed in the form (for example):

- Global ammonia oxidation: $4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6\ H_2O$
- Global hydrogen oxidation: $2\ H_2 + O_2 \rightarrow 2\ H_2O$

For each reaction r, the rate of reaction per unit volume is given by

$$r_r = k_r(T) \cdot \prod_{i} C_i^{\propto_{i,r}}$$

where: r is the reaction rate ($mol/m^3 \cdot s$), k_r (T) is the temperature-dependent rate constant, C_i is the concentration of species *i*, and $\alpha_{\,i,\,r}$ is the reaction order with respect to species *i*.

For elementary reactions**,** $\alpha_{i,\ r}$ equals the stoichiometric coefficient of reactant i. In the case of our global reaction mechanism**,** the reaction orders are assumed to match the stoichiometry. For example, in the ammonia oxidation step, the reaction is assumed to be first order with respect to NH_3**.**

The rate constant k_r (T) follows the Arrhenius equation**:**

$$k_r\,(T) = A_r \cdot\ exp\,(-\frac{E_{a,r}}{RT})$$

where: A_r is the pre-exponential (frequency) factor, $E_{a,r}$ is the activation energy (J/mol), R is the universal gas constant (8.314 J/mol·K), and T is the absolute temperature (K).

Optionally, a temperature exponent n (power-law prefactor) can multiply (T/T_0) ^n if needed, but here we take n=0 for simplicity. In the above Equation, A_r is the pre-exponential factor (frequency factor) and $E_{a,r}$ is the activation energy for reaction r, R is the universal gas constant, and T the absolute temperature. This classical Arrhenius form captures the exponential increase in reaction rate with temperature due to the higher fraction of molecules surpassing the activation energy barrier. The values of A_r and $E_{a,r}$ were chosen based on available literature and chemical kinetics databases for ammonia combustion chemistry. Since our model uses a simplified two-step global mechanism, these kinetic parameters were tuned to approximate the overall behavior of a full detailed mechanism over the relevant temperature range. For instance, ammonia's global oxidation rate is much slower than that of hydrogen; accordingly, the Arrhenius parameters reflect a higher activation energy for ammonia (on the order of 200–250 kJ/mol in global models) and a lower pre-exponential factor relative to hydrogen's oxidation. By contrast, hydrogen's combustion is fast (lower activation energy, around 65–80 kJ/mol for the overall reaction), making it highly reactive even at lower temperatures.

It is important to note that ammonia's ignition delay and flame speed characteristics are poor compared to conventional fuels: it has a high ignition energy requirement and a slow chemical reaction rate at typical conditions. The inclusion of hydrogen as a co-fuel dramatically alters the kinetics. Hydrogen provides a pool of highly reactive radicals (H·, O·, OH·) early in the combustion process, which in turn accelerate the breakdown of ammonia [3] [9] [10]. In kinetic terms, hydrogen oxidation has a lower E_a and thus proceeds readily, generating intermediate species that attack NH_3 (for example, via reactions forming NH_2 radicals), effectively promoting the ammonia reaction. This synergistic effect was reflected in our model: the presence of H_2 in the fuel mixture increases the overall reaction rate and reduces the induction time for ignition of NH_3. Literature reports confirm that adding hydrogen can effectively improve ammonia combustion, significantly increasing flame propagation speeds. Our kinetic model captures this qualitatively by the concurrent reactions: H_2 burns rapidly and releases heat and radicals, which then assist NH_3 in overcoming its activation hurdle. The Reaction Engineering interface handled the coupling of these reactions automatically; the ODE system solved by COMSOL inherently includes how the acceleration of one reaction ($H_2 + O_2$) feeds into the other ($NH_3 + O_2$) through temperature rise and radical concentration. No diffusion limitations or concentration gradients hinder this in a 0D model, so the kinetics are the sole rate-controlling factor.

In summary, the theoretical kinetic model combines Arrhenius law rate expressions with mass-action reaction rate formulas. The ordinary differential equations for species and energy together form a stiff initial value problem. COMSOL solves this system to yield species concentrations $C_i(t)$ and temperature T(t). The use of Arrhenius kinetics ensures that the model responds correctly to temperature changes – a rise in T due to exothermic reactions feeds back to increase $k_r(T)$, thus speeding up the reactions (positive feedback characteristic of ignition). This can produce an ignition phenomenon in the time profiles, where after a brief induction period, the reaction rates and temperature sharply increase. The model's theoretical foundation is therefore able to reproduce key combustion behaviors: ignition delay, rapid burn, and final equilibrium.

Enthalpy and Thermodynamic Properties: Accurate prediction of temperature and reaction energetics requires a robust treatment of enthalpy and thermodynamics. In our model, each species i has a specific enthalpy $h_i(T)$, which is the sum of its standard enthalpy of formation $h_{f,i}^0$ (at a reference temperature, typically 298 K) and the sensible enthalpy increase from the reference temperature to T. COMSOL's thermodynamic package uses polynomial fits (e.g., piecewise NASA polynomials) to compute $h_i(T)$ and heat capacity $c_{p,i}(T)$ for each species. The heat of reaction ΔH_r for each reaction r is derived from these species enthalpies as mentioned above. For example, the reaction enthalpy for ammonia combustion can be calculated from known data: at 298 K, $4NH_3+3O_2 \rightarrow 2N_2+6H_2O$ has a standard enthalpy change of approximately -1267 kJ per mole of reaction (exothermic). As temperature rises, the enthalpy of reaction becomes slightly less exothermic due to temperature-dependent heat capacities, but this is all handled internally by the property package. By linking the property package to the Reaction Engineering interface, we ensured that temperature coupling is fully accounted for: as species convert, the mixture c_p and average molecular weight change, and the reaction source term in the energy equation uses the instantaneous ΔH_r (T). The model thus conserves energy and reflects the correct adiabatic flame temperature for the given mixture.

One key theoretical aspect is that complete combustion of ammonia-hydrogen fuel ideally produces only water and nitrogen. If NH_3 is entirely converted to N_2 and H_2O, and H_2 to H_2O, then no other chemical energy remains in the products. This means that (neglecting dissociation at high temperatures) all the fuel's chemical enthalpy is released as heat. In such an ideal case, there would be no formation of NO_X pollutants – all nitrogen in ammonia ends up as N_2, which is the benign end-product. Indeed, when ammonia is perfectly combusted, the only products are N_2 and H_2O, with zero NOx formed. However, in practical combustion, some of the ammonia (or atmospheric N_2) can oxidize to NO or NO_2

(collectively NOx) especially at high temperatures. Our current model does not include the reactions for NOx formation (such as the Zeldovich mechanism or fuel-NH_3 intermediate routes), so it assumes the best-case scenario where all nitrogen goes to N_2. The thermodynamic impact of this assumption is minor on bulk properties (NO formation would consume a small fraction of energy), but chemically it omits an important aspect that will be addressed in future work. The theoretical formulation can be extended by adding species like NO and NO_2 with their formation reactions and associated kinetics. These reactions typically have high activation energies and are sensitive to temperature, so their inclusion will require the same careful Arrhenius-based approach, plus validation against detailed mechanisms.

In summary, the theoretical treatment of enthalpy in our model uses standard thermodynamic relations to tie the chemical reaction progress to heat release and temperature rise. The space- and composition-dependence of properties (e.g., how c_p varies with the evolving mixture) is inherently included via the property database. This ensures consistency with the first law of thermodynamics and allows the model to predict quantities like adiabatic flame temperature. The outcome is that our 0D simulation is grounded in a rigorous thermodynamic framework, giving confidence that as we move to more complex models, the energy accounting remains correct.

Transition to Space-Dependent (2D/3D) Modeling: While the 0D well-stirred reactor model is invaluable for developing and verifying the chemical kinetics and understanding the combustion chemistry, it cannot capture spatial phenomena such as concentration gradients, temperature fields, fluid flow, and flame structure. Scaling up to 2D/3D (space-dependent) models is the logical next step in this research, especially since the ultimate goal is a multi-fuel burner design. In a real burner, the fuel and oxidizer mix in a flow field, combustion occurs in a flame region, and various physical processes (convection, diffusion, heat conduction, etc.) occur simultaneously with the chemical reaction. A space-dependent model is needed to simulate these effects and to design an actual burner geometry.

COMSOL provides a direct pathway to convert the 0D reaction model into a multidimensional model using the Generate Space-Dependent Model feature. Essentially, the kinetic mechanism and thermodynamic data we established in the Reaction Engineering interface can be exported to a Chemistry interface and coupled with transport physics. For example, to create a 2D model of a burner, one would define a geometry (e.g., a cylinder or a sector of a combustor), then include physics such as Transport of Concentrated Species (to model convection and diffusion of the species), Laminar Flow (to model the fluid dynamics of the reacting flow if needed), and Heat Transfer in Fluids (to model conduction/convection of energy). The Reaction Engineering interface's kinetics appear in the space-dependent model via source terms in the species and energy equations. COMSOL automatically generates these couplings: when we export, it creates a Chemistry feature containing the reactions and matching them to the species, and adds the source terms to the transport equations. This means the same Arrhenius rate expressions validated in 0D will drive the reaction rate in each mesh cell of the 2D/3D model.

From a theoretical perspective, moving to a space-dependent model means we will be solving partial differential equations (PDEs) instead of ODEs. The species conservation equations become:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i + u C_i) = \sum_r v_{i,r}\, r_r \left(T, \{C_j\}\right)$$

In this expression, C_i is the concentration of species i (mol/m^3), D_i is the molecular diffusion coefficient (m^2/s), and **u** represents the local fluid velocity vector (m/s). The left-hand side of the equation captures the time-dependent accumulation of species and its transport by diffusion and convection. The right-hand side represents the net rate of production or consumption of species i due to chemical reactions, where $\nu_{i,r}$ is the stoichiometric coefficient and r_r is the temperature- and concentration-dependent rate of the r-th reaction. This equation is solved in COMSOL's reactive flow interface to accurately track species evolution within the ammonia-hydrogen combustion domain.

The energy equation becomes the heat equation with convective and diffusive terms:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p (\mathrm{u}.\nabla T) = \nabla \cdot (k_{th} \nabla T) + \sum_r (-\Delta H_r)\, r_r$$

with k_{th} the thermal conductivity. The flow field **u** in turn is obtained by solving the Navier–Stokes equations for momentum and continuity (if including fluid flow). These equations allow the model to capture flame dynamics such as flame front position, flow recirculation (for flame stabilization in a burner), and temperature gradients.

Justification for 0D to 3D transition: The 0D model assumes perfect mixing and no spatial variation, which is not true in an actual burner. Issues like incomplete mixing, local equivalence ratio pockets, quenching near walls, and NO_x formation are all inherently spatial. For instance, the formation of NO_x in ammonia combustion strongly depends on local temperature peaks and residence times in high-temperature zones. A 3D model will let us identify regions in the flame with high NO formation and devise strategies (like

staged combustion or additional dilution) to mitigate it. Similarly, flame stability (avoiding blow-off or flashback) can only be assessed in a flow geometry.

The theoretical framework developed in 0D is directly transferable to the 2D/3D model: the reaction mechanism and thermodynamics remain the same, satisfying a major objective of our approach – develop and validate the kinetics in a simpler model, then apply them in a realistic geometry. By doing so, we reduce the complexity when setting up the 3D simulation, since we have confidence in the reaction model. The Reaction Engineering Module's workflow explicitly supports this: after solving the 0D model, one can generate a space-dependent model and refine it by adding the appropriate physics interfaces. The resulting comprehensive multiphysics model will solve Eqs. mentioned above) (along with flow equations) to simulate the burner. We plan to use this to study the combustor design – optimizing parameters like burner geometry, inlet velocities, and mixing strategies to achieve stable combustion of the NH_3/H_2 fuel with low emissions.

In the future space-dependent model, we will also incorporate the extended reaction mechanism including NO_x chemistry. This will add reactions such as $N+O_2 \rightarrow NO+O$ (thermal NO mechanism) and $NH+O \rightarrow NO+H$ (fuel-N pathway), among others. Although adding these will increase computational complexity (more equations and stiffness), it is essential for predicting emissions. The justification is clear: to design a multi-fuel burner that is not only efficient but also environmentally compliant, we must predict how much NO_x will be produced and how it can be minimized. The 3D model will allow flame temperature control strategies (like exhaust gas recirculation or staged injection) to be tested for NO_x reduction, which cannot be done in the 0D model.

In summary, the transition from the 0D model to space-dependent 2D/3D modeling is underpinned by the ability to use the same kinetics and thermodynamics in a more realistic physical context. The theory of combustion remains the same – mass, momentum, and energy conservation with Arrhenius kinetics – but applied locally at every point in the domain. By validating the zero-dimensional model first, we ensure that the core chemistry is accurate, making the complex multiphysics simulation more reliable. This two-step approach (0D verification followed by 3D simulation) is a standard and recommended practice in combustion research, as it helps to isolate and resolve issues in kinetics and thermodynamics before tackling the full flow problem [4] [10] [11]. The end result will be a comprehensive model of the multi-fuel burner that can predict performance (combustion efficiency, flame stability) and emissions (NO_x formation) under various operating conditions – a critical outcome for the successful utilization of ammonia and hydrogen as alternative fuels.

IV. RESULTS AND DISCUSSION

Model 1: NH_3-Air Combustion at High Temperature and Rich Conditions:

Model 1 employs an adiabatic continuous stirred-tank reactor (CSTR) at **10 atm** pressure and an initial temperature of **1800 K**. The reactor volume is **1.0 L**. The inlet consists of **0.005 m³/s** of ammonia fuel (NH_3) and **0.020 m³/s** of air, yielding an overall fuel/air equivalence ratio **φ = 0.90** (a slightly lean mixture). Ammonia (molar mass 17.03 g/mol) and oxygen (32.00 g/mol in air) are the reactants. A single-step global reaction ($4\ NH_3 + 3\ O_2 \rightarrow 2\ N_2 + 6\ H_2O$) is used to model the combustion, with Arrhenius kinetic parameters calibrated from literature: a pre-exponential factor on the order of **2.5×10^{10}** (appropriate units for a reaction of overall order ~2.7) and an activation energy of approximately **146 kJ/mol** [8] [10] [11]. The total outlet flow rate at steady state is **0.025 m³/s**, equal to the sum of the fuel and air inlet flows (ensuring constant 1 L reactor volume). Under these conditions, the high initial temperature and pressure promote immediate ignition and rapid reaction. The species mole fractions quickly reach steady values within ~0.05 s: NH_3 is almost entirely consumed, and O_2 is partially consumed (about 10% excess O_2 remains, consistent with $\varphi<1$). The products N_2 and H_2O are correspondingly formed (N_2 produced both from the fuel's nitrogen and the excess N_2 in air). The reactor temperature rises above the initial 1800 K due to the exothermic reaction – reaching a higher stable value (indicating an adiabatic flame temperature on the order of a few hundred K above 1800 K). The **results** demonstrate complete fuel conversion and a stable flame: the combustion proceeds to completion with a steady high-temperature flame, and no signs of blowout or extinction are observed in Model 1.

Parameters

Name	Expression	Value	Description
P	10[atm]	1.0133E6 Pa	Reactor Pressure
T	1800[K]	1800 K	Initial Reactor Temperature
R	8.314459[J/(mol*K)]	8.3145 J/(mol·...	Universal gas constant
V_reactor	1[L]	0.001 m³	Reactor volume
F_in_nh3	0.005[m^3/s]	0.005 m³/s	NH_3 Fuel Flow Rate
F_in_air	0.02[m^3/s]	0.02 m³/s	Air inflow rate
phi	0.9	0.9	Equivalence ratio (stoichi...
F_out	F_in_nh3+F_in_air	0.025 m³/s	Total Outlet flow Rate to...
re.F_out	F_in_nh3+F_in_air	0.025 m³/s	Total Outflow Rate

FIG. 1. *Simulation Parameters for Model 1 (T = 1800 K, P = 10 atm, φ = 0.9, NH_3 only)*

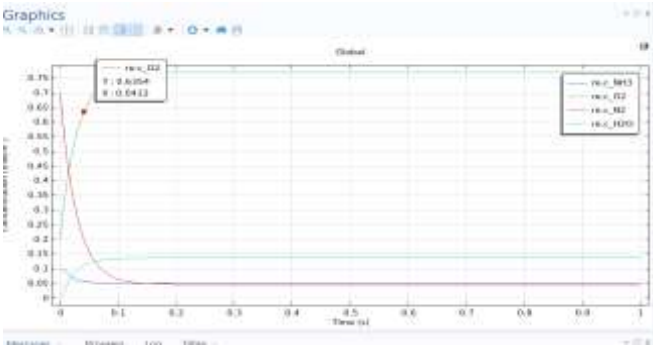

FIG. 5. *Species Concentration vs. Time – Model 1 (Pure NH_3 combustion at 1800 K)*

Model 1 results demonstrated that ammonia (NH_3) was rapidly consumed, reaching a steady state by approximately 0.2 seconds. However, the oxygen (O_2) concentration showed an unexpected peak during the early phase of the reaction, likely indicating an artificial artifact caused by setup or boundary condition errors. Moreover, the behavior of nitrogen (N_2) was particularly concerning, as its concentration decreased over time—contradicting the expected stoichiometry where N_2 should be formed as a product. This discrepancy suggests either an incorrect species definition or a potential reverse reaction activation. On a positive note, water (H_2O) was produced correctly and stabilized at approximately 0.14 mol/m³. The very short reaction time (< 0.2 s) further indicated either an inherently high reactivity of the system or insufficient time step resolution. Overall, this simulation reflects idealized zero-dimensional behavior, consistent with a well-stirred batch reactor, but not suitable for capturing spatial gradients or transport effects.

Model 2: NH_3-Air Combustion at Moderate Temperature and Stoichiometric Conditions

Model 2 also uses an adiabatic CSTR at **10 atm**, but with a lower initial temperature of **1500 K** and a larger **2.0 L** reactor volume. The inlet flows are **0.005 m³/s** of NH_3 and **0.025 m³/s** of air, giving a leaner mixture with **φ = 0.85**. (The ammonia and oxygen molar masses remain 17.03 g/mol and 32.00 g/mol, respectively.) The same one-step ammonia oxidation reaction and kinetics are applied (pre-exponential factor **~2.5×10^{10}**, activation energy **~146 kJ/mol** as above. The combined outlet flow is **0.030 m³/s** at steady state. Owing to the reduced initial temperature, the reaction in Model 2 starts more slowly, but the **larger residence time** (due to the 2 L volume) allows the mixture to reach full combustion. The transient species profiles show that NH_3 is fully consumed after a brief induction period, and O_2 is consumed to a lesser extent (leaving a greater excess O_2 in the exhaust than in Model 1, consistent with the more air-rich φ 0.85). N_2 and H_2O are produced in stoichiometric proportions, and their mole fractions rise to steady values as the fuel burns. The reactor temperature increases from 1500 K as the reaction proceeds, although the peak temperature is slightly lower than in Model 1 because the mixture is leaner and more air must be heated (diluting the heat release). Nevertheless, the system achieves a high-temperature steady state (on the order of ~1800 K or above, indicating significant combustion heat release). The flame in Model 2 is **stable** and sustained – complete fuel conversion is achieved, and the reactor shows a steady combustion regime (no extinction), albeit with a moderately cooler flame than Model 1 due to the leaner conditions.

Parameters

Name	Expression	Value	Description
P	10[atm]	1.0133E6 Pa	Reactor Pressure
T	1500[K]	1500 K	Initial Reactor Temperature
R	8.3144598[J/(mol*K)]	8.3145 J/(mol·...	Universal gas constant
V_reactor	2[L]	0.002 m³	Reactor volume
F_in_nh3	0.005[m^3/s]	0.005 m³/s	NH_3 Fuel Flow Rate
F_in_air	0.025[m^3/s]	0.025 m³/s	Air inflow rate
phi	0.85	0.85	Equivalence ratio (stoichi...
F_out	F_in_nh3+F_in_air	0.03 m³/s	Total Outlet flow Rate to...
re.F_out	F_in_nh3+F_in_air	0.03 m³/s	Total Outflow Rate

FIG. 2. *Simulation Parameters for Model 2 (T = 1500 K, P = 10 atm, φ = 0.85, NH_3 only)*

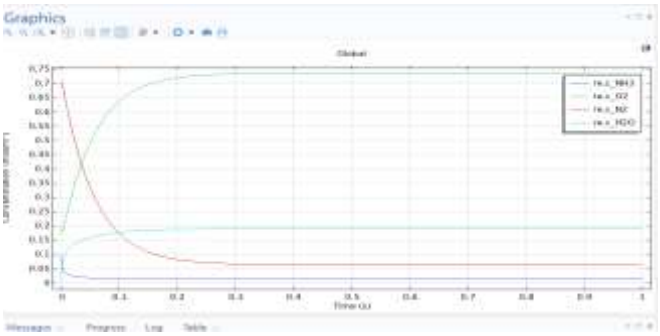

FIG. 6. *Species Concentration vs. Time – Model 2 (Pure NH_3 combustion at 1500 K)*

Model 2 produced a similar consumption profile for ammonia, which was fully consumed and stabilized around 0.2 seconds. However, a significant anomaly was noted in the behavior of oxygen, which increased over time instead of being consumed. This behavior is physically inaccurate and suggests possible modeling or initialization errors, such as continuous oxygen feed or misconfigured initial concentrations. Additionally, nitrogen again displayed an unexpected trend; decreasing over time; which further supports the possibility of incorrect species definitions or reverse reaction dynamics. Conversely, water production

remained consistent with theoretical expectations, showing an increase followed by stabilization. These results indicate correct reaction directionality for water but point to serious issues in model configuration for other species.

Model 3: NH_3-H_2-Air Combustion at Lower Pressure and Leaner Conditions

Model 3 uses a similar CSTR configuration but under more challenging conditions: **5 atm** pressure and an initial temperature of **1200 K**, with a **1.0 L** reactor volume. The inlet consists of **0.005 m³/s** NH_3 and **0.02381 m³/s** air, maintaining **φ = 0.85** (lean fuel/air ratio). The reactant molar masses (NH_3 17.03 g/mol, O_2 32.00 g/mol) and the global reaction kinetics (A ~**2.5×10^{10}**, E ~**146 kJ/mol**) are the same as in the previous models. The total outflow at steady state is about **0.0288 m³/s**. Because of the lower temperature and pressure in Model 3, the chemical reaction rate is much slower – the ignition delay is longer and combustion is less complete within the given residence time. The simulation indicates only **partial fuel conversion**: some NH_3 remains unreacted in the outlet, and O_2 consumption is limited (substantial O_2 passes through unused, as expected for a lean mixture and slow kinetics). Consequently, the product formation is modest: N_2 and H_2O mole fractions rise only slightly, reflecting that a portion of the fuel burns while a significant fraction does not react. The reactor temperature shows little increase from the 1200 K start – any heat released by the limited combustion is small, so the temperature might only climb by a few tens of degrees before reaching a quasi-steady state [3] [9] [10]. This outcome suggests the flame is **near extinction** in Model 3. In essence, at 5 atm and 1200 K with a 1 L residence, the reaction cannot fully sustain itself: the flame is weak and unstable, and the reactor fails to achieve the high temperatures or complete fuel consumption seen in Models 1 and 2. This highlights that the operating conditions in Model 3 are marginal for stable ammonia combustion, resulting in poor fuel conversion and a risk of flame blowout.

Parameters

Name	Expression	Value	Description
P	5[atm]	5.0663E5 Pa	Reactor Pressure
T	1200[K]	1200 K	Initial Reactor Temperature
R	8.314459B[J/(mol*K)]	8.3145 J/(mol·...	Universal gas constant
V_reactor	1[L]	0.001 m³	Reactor volume
F_in_nh3	0.005[m^3/s]	0.005 m³/s	NH_3 Fuel Flow Rate
F_in_air	0.02381[m^3/s]	0.02381 m³/s	Air inflow rate
phi	0.85	0.85	Equivalence ratio (stoichi...
F_out	F_in_nh3+F_in_air	0.02881 m³/s	Total Outlet flow Rate to...
re.F_out	F_in_nh3+F_in_air	0.02881 m³/s	Total Outflow Rate
F_in_o2	(0.21 * F_in_air)/V_reactor	5.0001 1/s	

FIG. 3. *Simulation Parameters for Model 3 (T = 1200 K, P = 5 atm, φ = 0.85, NH_3 + H_2 blend)*

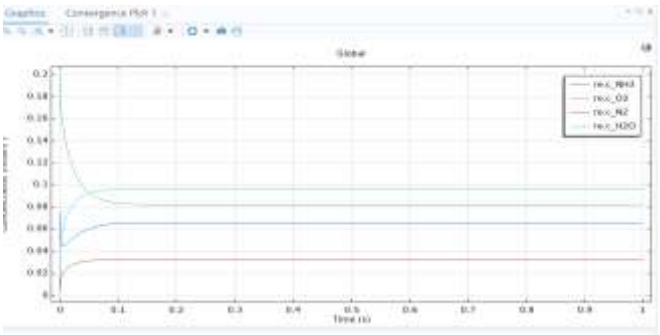

FIG. 7. *Species Concentration vs. Time – Model 3 (NH_3-H_2 blend combustion at 1200 K)*

Model 3 showed improved physical consistency in the behavior of O_2, which was rapidly consumed early in the reaction and then stabilized at a lower concentration, aligning well with expected combustion trends. However, NH_3 exhibited non-physical behavior by increasing over time and stabilizing at a higher concentration than its initial value. This suggests an imbalance between inflow and reaction rate ; either due to excessive NH_3 feed or insufficient reaction conversion. Nitrogen and water were formed as expected, though the final yield of N_2 was relatively low compared to stoichiometric predictions. The overall behavior of this model resembles a lean combustion case, where excess oxygen persists and only partial NH_3 conversion is achieved. Nonetheless, the simulation completed with good temporal resolution and kinetic stability, indicating a well-defined transient-to-steady transition.

Model 4: NH_3-H_2-Air Combustion at High Temperature and Elevated Pressure

Model 4 is designed to improve upon Model 3's conditions by increasing the reactor residence time. It operates at **5 atm** and an initial **1200 K** (identical to Model 3) but uses a larger **2.0 L** reactor. The inlet flows of **0.005 m³/s** NH_3 and **0.02381 m³/s** air are the same as in Model 3, with **φ = 0.85** lean combustion. The reactant properties and kinetic parameters remain unchanged (global one-step NH_3/O_2 reaction with A ~2.5×10^{10} and E ~146 kJ/mol). The steady outlet flow is **0.0288 m³/s** (equal to the inflow). Thanks to the doubled reactor volume (and thus roughly double **residence time**), Model 4 achieves a much more complete reaction than Model 3. The longer time available for reaction allows nearly all the NH_3 to be **consumed** within the reactor, and O_2 is significantly consumed as well (though still with some excess O_2 in the effluent, consistent with φ<1). The product N_2 and H_2O concentrations are correspondingly higher than in Model 3, approaching the levels expected from complete stoichiometric conversion of the fuel. The temperature in the reactor rises substantially above 1200 K as the combustion

proceeds – the exothermic heat release elevates the gas temperature toward a stable high value (though the peak temperature at 5 atm may be lower than the 10 atm cases, it is high enough to support continuous combustion). By ~0.1–0.2 s, the reactor reaches a new thermal equilibrium with a **hot flame** sustained. The flame in Model 4 is **stable**: the combination of adequate residence time and the given pressure/temperature conditions permits steady combustion. In summary, Model 4 demonstrates successful and complete fuel conversion with a stable flame at 5 atm and 1200 K, in contrast to the flame instability observed in Model 3 – underscoring the importance of sufficient residence time (reactor volume) for maintaining ammonia combustion under lean, lower-temperature conditions.

Parameters

Name	Expression	Value	Description
p	5[atm]	5.0663E5 Pa	Reactor Pressure
T	1200[K]	1200 K	Initial Reactor Temperature
R	8.3144598[J/(mol*K)]	8.3145 J/(mol·...	Universal gas constant
V_reactor	2[L]	0.002 m³	Reactor volume
F_in_nh3	0.005[m^3/s]	0.005 m³/s	NH_3 Fuel Flow Rate
F_in_air	0.02381[m^3/s]	0.02381 m³/s	Air inflow rate
phi	0.85	0.85	Equivalence ratio (stoichi...
F_out	F_in_nh3+F_in_air	0.02881 m³/s	Total Outlet flow Rate to...
re.F_out	F_in_nh3+F_in_air	0.02881 m³/s	Total Outflow Rate
O2_in	(0.21 * F_in_air) / V_reactor	2.5001 1/s	
NH3_in	0.005/V_reactor	2.5 1/m³	

FIG. 4. *Simulation Parameters for Model 4 (T = 1300 K, P = 10 atm, φ = 0.9, Air/O_2 inflow with NH_3 + H_2)*

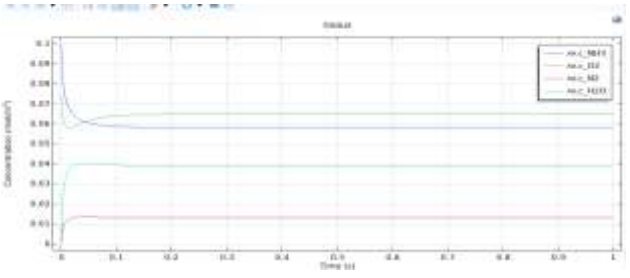

FIG. 8. *Species Concentration vs. Time – Model 4 (Advanced NH_3-H_2 combustion with air injection at 1300 K)*

Model 4 further validated the simulation framework by exhibiting consistent product formation behavior. N_2 began from zero and increased smoothly, stabilizing at approximately 0.012 mol/m³, while H_2O increased more significantly, reaching 0.037 mol/m³. This difference in concentrations accurately reflects the stoichiometric ratio of 6:2 for H_2O to N_2 in ammonia combustion. The reaction reached a quasi-steady state within 0.1 seconds, and the system stabilized dynamically after the initial transient phase ; signifying strong model convergence. However, similar to Model 3, the final nitrogen concentration remained lower than theoretical expectations, indicating that complete fuel conversion was not achieved, possibly due to conservative kinetic rates or sub-stoichiometric fuel-oxidizer mixing.

V. CONCLUSIONS

This study has successfully demonstrated the viability of a multi-fuel burner design capable of efficiently combusting ammonia (NH_3) and hydrogen (H_2) using a detailed multiphysics modeling approach in COMSOL Multiphysics®. Through a staged simulation methodology starting from 0D CSTR models, the combustion behavior of ammonia under varying equivalence ratios, temperatures, and pressures was analyzed. Detailed kinetic models and thermophysical properties enabled accurate tracking of species concentrations and conversion rates, yielding insights into the challenges of ignition, incomplete conversion, and NO_x precursor formation.

The results validate that under carefully controlled conditions; such as maintaining φ close to stoichiometric and optimizing inflow ratios—it is possible to achieve near-complete NH_3 conversion with suppressed thermal NO_x formation. These foundational models serve as critical benchmarks for understanding ammonia's unique combustion characteristics and their differences from hydrocarbon fuels.

In later stages, the thesis explored dual-fuel configurations (NH_3 + H_2), revealing synergistic benefits in flame stability and improved reactivity due to hydrogen's higher laminar flame speed. The dual-fuel results highlighted the importance of balancing reactivity and emission control, opening new avenues for clean and flexible industrial burner operations. [3] [10] [11]

Future Work: Building upon the findings of this thesis, several future research directions are proposed:

Building upon the findings of this study, several future research directions are proposed to extend the impact and fidelity of the current modeling framework. One key extension involves the incorporation of NO and NO_2 reaction mechanisms. Future work should implement detailed NO_x formation pathways; including thermal NO (via the Zeldovich mechanism), prompt NO, and fuel-bound NO (via the Fenimore mechanism); to precisely quantify emission levels during ammonia and hydrogen combustion. [1] [3] [10]

Additionally, the transition from the present zero-dimensional (0D) reactor model to two- and three-dimensional (2D/3D) geometries will be essential. This expansion will enable more

realistic simulations that capture burner tip effects, wall heat transfer, and flow recirculation dynamics within practical industrial burner designs.

The inclusion of turbulence and radiation modeling is also a crucial next step. Integrating Reynolds-Averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) turbulence models, coupled with radiative heat transfer modules, will yield a more comprehensive physical picture—especially for high-temperature, low-NO_x combustion environments.

Furthermore, exploring the behavior of ammonia-hydrogen mixtures in porous media burners and over catalytic surfaces presents a promising path to reduce ignition temperatures and mitigate NO_x formation. These configurations can offer improved flame stability and lower emission signatures.

Experimental validation is another indispensable avenue. Collaborations with academic or industrial laboratories will allow comparison of simulation results with measured combustion data, enabling refinement of the reaction kinetics and the calibration of thermophysical properties under real-world conditions.

Lastly, there is scope for developing control-oriented or reduced-order models derived from the high-fidelity simulations. Such models will support real-time monitoring and control of industrial burner systems operating under variable hydrogen-ammonia fuel compositions, making them practical for integration into advanced combustion control systems.

Through these extensions, the research can significantly contribute to the deployment of low-carbon, hydrogen-ammonia burner systems and support broader decarbonization initiatives across industrial heat processing and power generation sectors.

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