

Article

SI and RCCI Quasi-Dimensional Combustion Modeling of Ammonia-Fueled Engines with Fuel-NO_x Formation

Alberto Ballerini ¹, Gianluca D'Errico ^{1,*}, Christine Mounaïm-Rousselle ² and Pierre Brequigny ²

¹ Dipartimento di Energia, Politecnico di Milano, Via Raffaele Lambruschini 4/A, 20156 Milano, Italy; alberto.ballerini@polimi.it

² PRISME, Université d'Orléans, INSA-CVL, EA 4229, F45072 Orléans, France; christine.rousselle@univ-orleans.fr (C.M.-R.); pierre.brequigny@univ-orleans.fr (P.B.)

* Correspondence: gianluca.derrico@polimi.it

Abstract

The increasing interest in carbon-free fuels has positioned ammonia as a promising energy carrier for Internal Combustion Engines (ICEs), particularly in hard-to-abate sectors such as Heavy-Duty (HD) transport and maritime applications. However, its low reactivity, narrow flammability limits, and intrinsic nitrogen content pose significant challenges for stable combustion and emissions control. This work presents a predictive Quasi-Dimensional (QD) combustion model applied to simulate ammonia-fueled engines operating under both Spark Ignition (SI) and Reactivity Controlled Compression Ignition (RCCI) modes. The proposed framework couples a turbulent premixed combustion sub-model with a diffusive combustion sub-model, including a dedicated fuel-NO_x mechanism to capture nitrogen oxide formation pathways associated with fuel-bound nitrogen. The model accounts for key physical and chemical processes governing combustion, such as ignition delay, mixture stratification, and heat release dynamics, while maintaining computational efficiency suitable for parametric studies. The model is validated against experimental data from a Single-Cylinder Engine (SCE) over a wide range of operating conditions, including variations in equivalence ratio, spark timing, Ammonia Energy Fraction (AEF), and injection strategy. Results demonstrate good agreement in terms of in-cylinder pressure evolution, Apparent Heat Release Rate (AHRR), and NO_x emissions, with peak-pressure errors below 4 bar and peak-pressure locations predicted within 2 crank angle degrees. Notably, the dedicated fuel-NO_x sub-model substantially improves emission predictions, revealing that fuel-bound nitrogen is the dominant source of NO_x in ammonia combustion. Overall, the proposed QD model represents a robust and efficient tool for the analysis and optimization of ammonia-fueled engines, supporting the development of low-carbon combustion strategies for future energy systems.



Academic Editors: Steven Begg and Nwabueze Emekwuru

Received: 26 May 2026

Revised: 22 June 2026

Accepted: 22 July 2026

Published: 30 July 2026

Copyright: © 2026 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

Keywords: ammonia combustion; internal combustion engine modeling; fuel-NO_x; alternative fuels; low-carbon energy

1. Introduction

Ammonia (NH₃) has emerged as an attractive alternative fuel for Internal Combustion Engines (ICEs), owing to its high hydrogen (H₂) content (17.8% by weight) and the absence of carbon in its molecular structure [1]. Ammonia is being actively explored for its role in reducing greenhouse gas emissions and decreasing dependence on fossil fuels, both as an energy carrier and a direct fuel [2,3].

The primary characteristic of ammonia as an engine fuel lies in its environmental benefits. Unlike conventional hydrocarbon fuels, ammonia combustion produces no carbon dioxide (CO₂) emissions, making it a compelling option for climate change mitigation [4]. Moreover, ammonia can be easily stored as compressed gas or as a liquid at moderate pressure and temperature (10 bar, 25 °C), resulting in a relatively high energy density, and eliminating the need for complex storage systems [5,6]. However, ammonia's chemical properties present significant challenges for direct use in ICEs. Its high autoignition temperature (651 °C), low Laminar Flame Speed (LFS) (approximately 0.07 m/s at stoichiometric conditions), and narrow flammability limits complicate combustion in conventional engine configurations [6–8]. Despite these limitations, substantial progress has been made in adapting engine technologies to enable reliable ammonia utilization.

In recent years, several experimental studies demonstrated the feasibility of pure ammonia operation in ICEs. For example, Lhuillier et al. [9] tested a retrofitted Spark Ignition (SI) gasoline engine with a moderate Compression Ratio (CR), finding comparable performance levels with respect to those obtained with methane in near-stoichiometric lean conditions. Jespersen et al. [10] investigated the influence of spark energy and discharge characteristics on the lean-burn behavior of ammonia in a premixed SI engine, demonstrating that combustion stability is strongly dependent on both the ignition system configuration and spark timing.

The requirement of stable and predictable engine operations motivated the investigation of different strategies to promote ammonia ignition and combustion. Mounaïm-Rousselle et al. [11] and Reggeti et al. [12] explored the Spark Assisted Compression Ignition (SACI) mode, where the premixed air-ammonia charge is first ignited by a spark, then autoignition is promoted in the end-gas by flame expansion and high CR. A significantly faster burn process was observed with respect to a traditional turbulent flame propagation, which extended the engine operating range, especially at low loads.

Hydrogen enrichment has also proved to be a significant combustion enhancer. The study by Lhuillier [13] showed that hydrogen addition improves the ammonia combustion efficiency and helps reduce ammonia slip in the exhaust. Other experimental studies estimated the optimal hydrogen enrichment to be approximately 10–20% by volume [7,14], implying that hydrogen has to be supplied either by an additional storage tank or reformed onboard from ammonia [15,16].

Reactivity Controlled Compression Ignition (RCCI) has emerged as a promising strategy to enhance and regulate combustion in ammonia-fueled engines. RCCI belongs to the class of Dual-Fuel (DF) combustion strategies, in which a homogeneous air-Low Reactivity (LR) fuel mixture (e.g., ammonia or natural gas) is ignited through the Direct Injection (DI) of a small quantity of a High Reactivity (HR) fuel into the combustion chamber. Similarly to conventional Compression Ignition (CI) engines, the HR fuel undergoes autoignition following an Ignition Delay (ID) period. The subsequent ignition of the premixed air-ammonia charge occurs simultaneously at multiple locations, from which turbulent flame fronts propagate until the mixture is fully consumed. This approach holds particular promise for reducing carbon-based emissions in large-bore marine engine applications, where ammonia can displace a substantial fraction of the diesel fuel [17]. Dupuy et al. [18] examined RCCI operation on a Single-Cylinder Engine (SCE) across an extensive range of air-ammonia equivalence ratios, exploring various diesel pilot injection durations and energy fractions. Their findings indicate that minimizing carbon emissions requires a simultaneous optimization of both the diesel energy fraction and the premixed air-ammonia equivalence ratio. Hiraoka et al. [19] investigated RCCI operation and reported that raising the Ammonia Energy Fraction (AEF) results in a prolonged ammonia-diesel ID. Imamori et al. [20] conducted a comparison between diesel-ammonia RCCI and conventional diesel

combustion, demonstrating that an AEF of 94% yields an 82% reduction in greenhouse gas emissions. The influence of diesel injection parameters was addressed by Liu et al. [21], who showed that higher injection pressures and advanced injection timing both contribute to increased chemical reactivity of the in-cylinder charge, thereby shortening the ID. Conversely, Mounaïm-Rousselle et al. [22] and Mi et al. [23] explored a split diesel injection strategy, dividing the fuel delivery into a pilot and a main injection event. This approach demonstrated improvements in the reactivity of the diesel-air-ammonia mixture, accompanied by lower emissions of nitrogen oxides, carbon monoxide (CO), and unburned ammonia.

In this expanding experimental Research & Development (R&D) context, numerical modeling plays a crucial role in enhancing the understanding of various aspects that influence the combustion process and pollutant emission formation. Several works available in the literature focus on Three-Dimensional (3D) Computational Fluid Dynamics (CFD) simulations of ammonia and hydrogen-ammonia blends in SI or DF engines [24–28]. These studies offer valuable insights into the distinctive aspects of ammonia combustion, albeit at the cost of high computational demand and long simulation times.

At the opposite end of the modeling spectrum, reduced-order models aim to achieve comparable accuracy with a more favorable trade-off between computational demand and predictive fidelity. Such approaches have been applied to estimate the possible outcomes due to the conversion of a gasoline SI engine to ammonia-fueled operation [29], as well as to explore the variation of key engine performance metrics across different operating conditions [30]. However, few works in the literature apply these modeling approaches to support experimental R&D, particularly for RCCI combustion. Motivated by these considerations, the objective of the present work is to develop Quasi-Dimensional (QD) combustion models and apply them to simulate ammonia-fueled engines in both SI and RCCI configurations. The models are validated against experimental data acquired over a range of operating conditions, spanning Spark Advance (SA), equivalence ratio, and AEF. In addition, a novel fuel-NO_x sub-model is introduced to improve the accuracy of pollutant emission predictions.

The main novelty of the present work lies in the development and validation of a unified QD combustion framework able to describe both SI and RCCI ammonia-fueled engine operation within the same modeling environment. Compared with previous QD and 0D/1D combustion models, the proposed approach introduces: (i) a dedicated fuel-NO_x source term for ammonia combustion, derived from One-Dimensional (1D) laminar flame calculations and coupled with the in-cylinder burned-zone NO evolution; (ii) an extension of the tabulated ID methodology to account for ammonia/diesel fuel-fuel interactions in RCCI operation; (iii) a coupled premixed/diffusive combustion formulation capable of reproducing the transition from diesel-pilot-triggered ammonia combustion to turbulent flame propagation. The objective is not to replace detailed 3D CFD simulations, but to provide a computationally efficient tool suitable for preliminary engine design, operating-condition screening, and parametric optimization.

The remainder of the paper is structured as follows. Section 2 describes the experimental setup for the ammonia-fueled engine tested under SI and RCCI operating conditions. Section 3 introduces the combustion modeling framework, first presenting the two combustion sub-models governing SI and CI combustion separately, and then detailing their coupling for the simulation of RCCI operation; the fuel-NO_x sub-model is also described. Section 4 presents the validation of the proposed models, addressing SI operation first, followed by RCCI conditions. Finally, Section 5 summarizes the conclusions of the study and outlines potential directions for future research.

2. Experimental Setup

The experimental data analyzed in this study were acquired at the Laboratoire PRISME of the University of Orléans. A DW10F four-cylinder Light-Duty (LD) engine was converted into a 500 cm³ SCE [18,24]. Its main geometric characteristics are summarized in Table 1, while a schematic view of the experimental setup is shown in Figure 1.

Table 1. Characteristics of the ammonia SCE.

Bore [mm]	85.0
Stroke [mm]	88.0
CR [-]	16.42
Connecting-rod length [mm]	141
Exhaust Valve Opening (EVO) [° aTDC]	134
Exhaust Valve Closing (EVC) [° aTDC]	−324
Intake Valve Opening (IVO) [° aTDC]	344
Intake Valve Closing (IVC) [° aTDC]	−117
Main/LR fuel	NH ₃
HR fuel	Diesel

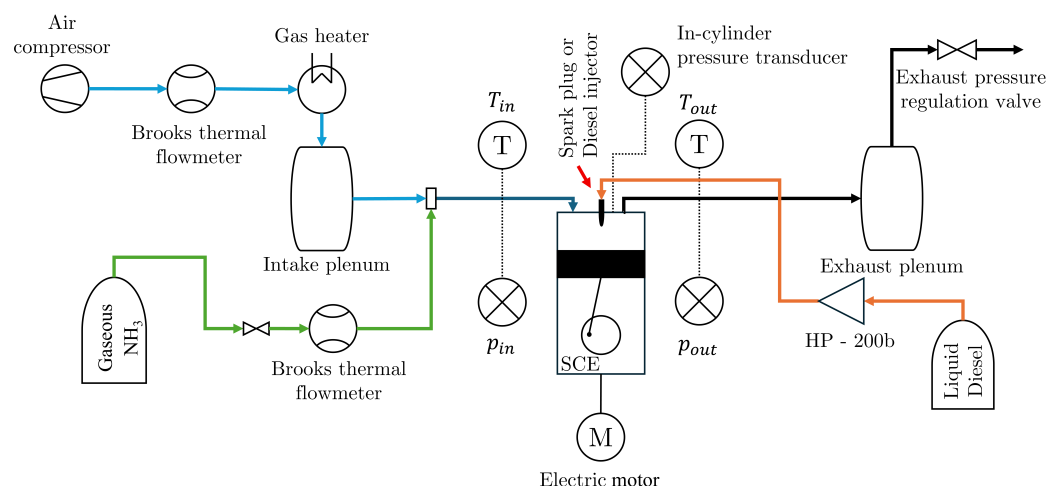


Figure 1. Schematic of the experimental ammonia SCE.

The engine can operate in both SI and RCCI modes by replacing the central spark plug with a direct injector. Diesel was selected as HR fuel for the RCCI operation.

In-cylinder pressure was acquired at a resolution of 0.1 Crank Angle (CA) using a Kistler 6045A relative quartz pressure transducer (Kistler Instrumente AG, Winterthur, Switzerland) connected to a LabView data acquisition system. Intake and exhaust manifold temperatures and pressures were monitored by means of K-type thermocouples and resistive absolute pressure transducers, respectively. Ammonia was stored in the liquid phase in a dedicated tank and vaporized prior to mixing with air. Ammonia and air mass flow rates were measured using Brooks thermal flow-meters. For RCCI operation, fuel was delivered via a Bosch 7-hole common rail injector, with the diesel injection pressure ($p_{die, inj}$) held constant at 200 bar to ensure adequate flexibility in adjusting the injection duration.

All experimental tests were carried out at a fixed engine speed of 1000 rpm. The investigated parameters included the air-ammonia equivalence ratio (ϕ) and ignition timing, defined in terms of SA for the SI mode or Start Of Injection (SOI) and Duration Of Injection (DOI) for the RCCI mode. Intake temperature and pressure (T_{in} and p_{in} , see Figure 1) were regulated by the gas heater and air compressor, respectively. These were kept constant at 80 °C and 1 bar across all test points. The average pressure trace for each operating condition was obtained by averaging 200 consecutive engine cycles.

The measured operating conditions for the SI and RCCI modes are reported in Table 2. The AEFs are computed with the following equation:

$$AEF = \frac{m_{\text{NH}_3} \cdot LHV_{\text{NH}_3}}{m_{\text{NH}_3} \cdot LHV_{\text{NH}_3} + m_{\text{die}} \cdot LHV_{\text{die}}} \quad (1)$$

where m_{NH_3} is the trapped ammonia mass at IVC, m_{die} is the injected diesel mass, and LHV is the Lower Heating Value of the corresponding fuel.

Table 2. Experimental engine operating conditions analyzed in this study for the SI and RCCI configurations.

ϕ_{NH_3} [-]	SI Operating Conditions			RCCI Operating Conditions				
	SA [° aTDC]	IMEP [bar]	CoV _{IMEP} [%]	SOI [° aTDC]	DOI [μs]	AEF [%]	IMEP [bar]	CoV _{IMEP} [%]
0.85	−24	5.8	4.9	−11	400	98.6	6.8	1.8
	−30	6.2	2.7		450	97.8	6.7	1.8
	−33	6.3	2.2		500	96.9	6.9	1.9
	−35	6.4	2.5		550	95.7	7.3	1.6
0.90	−18	6.6	5.3	−12	400	98.7	6.7	4.0
	−26	6.7	2.2		450	97.9	7.4	1.6
	−29	6.6	2.3		500	97.0	7.5	1.7
	−31	6.6	2.2		550	96.0	7.5	1.3
0.95	−19	6.9	3.4	−13	425	98.5	7.5	1.6
	−25	7.0	2.2		475	97.6	7.4	1.1
	−27	6.8	2.0		525	96.7	7.6	1.0
	−29	6.7	2.0		575	95.5	7.5	0.8
1.00	−18	7.3	2.7	−11	450	98.7	7.1	2.3
	−22	7.2	1.9		500	97.3	7.5	0.9
	−24	7.1	1.8		550	96.3	7.6	0.6
	−25	7.2	1.7		600	94.9	7.6	0.6

As can be observed, the small quantities of injected diesel confirm the main feature of the RCCI operation, namely a premixed combustion of ammonia and air which is triggered by the autoignition of a small diesel-air-ammonia mixture. This differs from typical DF mode, where the directly injected fuel contributes a larger fraction of the total in-cylinder energy.

3. Combustion Models

This Section describes the main characteristics of the combustion model proposed in this work and implemented in Gasdyn [31], the ICE simulation software developed by the ICE Group at Politecnico di Milano. First, the turbulent premixed flame model, characteristic of SI engines, is described. Then, the diffusive combustion model is introduced. These two sub-models are then coupled to model RCCI combustion, highlighting key aspects specific to DF combustion modeling such as ID estimation and flame area evolution. Finally, the fuel-NO_x emission sub-model is presented.

3.1. Turbulent Premixed Flame Combustion Model

Combustion in SI engines is modeled assuming a turbulent flame propagating hemispherically from the spark plug location. The presence of a coherent flame front divides the

cylinder into two distinct zones: an *unburned* zone (subscript *u*), containing the fresh charge, and a *burned* zone (subscript *b*), resulting in a two-zone thermodynamic description.

The burning rate is described through a modified version of the Eddy Burn-Up model, originally proposed by Tabaczynski [32] and subsequently revised by the authors in [33]. The model assumes that unburned mass is first entrained by the flame front (subscript *e*) and subsequently consumed over a characteristic burn-up time τ_b . The main governing equations are:

$$\frac{dm_e}{dt} = \rho_u S_t A_l \quad (2)$$

$$\frac{dm_b}{dt} = \frac{m_e - m_b}{\tau_b} \quad (3)$$

$$\tau_b = \frac{0.15}{C_e} \cdot \frac{L_i}{u'} \quad (4)$$

where ρ_u is the unburned charge density, S_t is the turbulent flame speed, A_l is the geometric laminar flame surface, L_i is the integral length scale, u' is the turbulence intensity, and C_e is a tuning parameter with a default value equal to 1.

Turbulence quantities (L_i , u') are computed using the *K-k-ε* model of [34]. The turbulent flame speed is evaluated through a modified form of the correlation proposed by Gülder [35]:

$$S_t = 1.3 \cdot C_t \cdot S_l \cdot \left[1 + 0.60 \cdot f_{trans} \cdot \left(\frac{u'}{S_l} \right)^{1/2} \left(\frac{L_i u'}{\nu_u} \right)^{1/4} \right] \cdot f_w \quad (5)$$

where ν_u is the kinematic viscosity of the unburned zone, S_l is the LFS, and C_t is a tuning parameter with a default value of 1. The factors f_{trans} and f_w account for the early and late phases of combustion, respectively. The transition factor f_{trans} varies between 0 (laminar) and 1 (fully turbulent) and follows the formulation proposed by Herweg and Maly [36], subsequently modified by Sforza [37]:

$$f_{trans} = \left[1 - \exp \left(- \frac{r_K - S_{tay}}{C_{delay} L_i} \right) \right]^{1/2} \cdot \left[1 - \exp \left(- \frac{u' + S_l}{L_i} \cdot t_{ign} \right) \right]^{1/2} \quad (6)$$

where r_K is the flame kernel radius, C_{delay} is a tuning parameter with a default value of 0.1, and t_{ign} is the time elapsed since spark timing. The Taylor microscale S_{tay} is given by:

$$S_{tay} = \frac{\sqrt{15} L_i}{\left(\frac{L_i u'}{\nu_u} \right)^{1/2}} \quad (7)$$

The phenomenological correction factor f_w captures the effect of flame-wall interaction and the eventual quenching of the flame near the walls. It is described by an S-shaped formulation:

$$f_w = \begin{cases} 1 & Y_b \leq Y_{b,50} \\ \exp \left(-2.908 \cdot \left(\frac{Y_b - Y_{b,50}}{1 - Y_{b,50}} \right)^{5/2} \right) & Y_b > Y_{b,50} \end{cases} \quad (8)$$

where Y_b is the instantaneous burned mass fraction and $Y_{b,50}$ is the burned mass fraction at which the flame surface in contact with the cylinder walls reaches 50% of the total flame front area.

3.2. Diffusive Combustion Model

The diffusive combustion model used in this work was originally developed in [38,39] and later extended by the present authors [40]. The model adopts a multi-zone representation of the air-fuel mixture, designed to capture the spatial heterogeneity characteristic of conventional CI combustion and to predict pollutant formation. DI is explicitly modeled, as it is the primary process governing air-fuel stratification. The model further accounts for the chemical and physical phenomena governing autoignition, and incorporates the geometry of the combustion chamber and injection system, both of which influence the overall combustion process.

The model can be conceptually divided into two sub-models: a multi-zone Zero-Dimensional (0D) combustion sub-model, and a 1D sub-model for spray evolution and charge stratification.

3.2.1. Multi-Zone 0D Combustion Model

The multi-zone combustion model subdivides the air-fuel mixture into distinct zones, each characterized by a fixed equivalence ratio (ϕ). Zone masses are initialized using the instantaneous mass distribution predicted by the spray model, which is discussed later. The iso- ϕ zones are treated as open thermodynamic systems, allowing mass transfer between adjacent zones as the richest zones are depleted and the charge progressively approaches a homogeneous composition. Mass conservation is enforced through a cascading mixing scheme, assuming that fuel mass is transferred sequentially from richer zones to adjacent leaner ones.

Each iso- ϕ zone is further subdivided into three sub-zones based on the thermodynamic state of the mixture: ‘liquid’, ‘unburnt vapor’, and ‘burnt vapor’, as depicted in Figure 2.

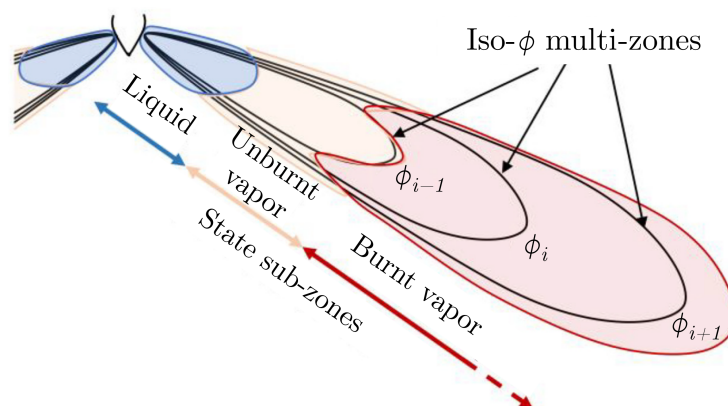


Figure 2. Schematic representation of the iso- ϕ multi-zones with the distinction into ‘liquid’, ‘unburnt vapor’, and ‘burnt vapor’ sub-zones.

The mass fraction allocated to each sub-zone is governed by the evaporation and ignition sub-models embedded within the charge stratification framework. Thermodynamic properties—such as temperature (T), pressure (p), and volume (V)—are evaluated for each k -th sub-zone within every iso- ϕ zone.

The standard Woschni model [41] is used to determine the global heat transfer to the walls, based on the average cylinder temperature. This is then distributed among the different sub-zones, weighted by the zonal temperature.

In addition to the thermodynamic properties, the multi-zone combustion model is also responsible for providing information on pollutant formation, particularly regarding NO_x . This is achieved by applying the Extended Zel’dovich thermal mechanism proposed

by Lavoie [42] to each iso- ϕ sub-zone. The concentrations of the other species are assumed to be at chemical equilibrium.

3.2.2. 1D Spray and Charge Stratification Model

The spray model is based on the jet momentum theory developed by Musculus and Kattke [43]. A 1D Eulerian framework is employed to track the evolution of key spray parameters, including spray tip penetration and the axially averaged air-fuel distribution. The axially averaged distribution is then used to generate a Two-Dimensional (2D) representation of the air-fuel distribution inside the spray, by imposing the radial profile proposed by Abramovich [44], obtaining the following relation:

$$\frac{\bar{X}_f}{\bar{X}_{f,c}} = (1 - \xi^\alpha)^2 \quad (9)$$

where the local fuel concentration ($\bar{X}_f$) relates to the centerline value ($\bar{X}_{f,c}$) based on the dimensionless radial coordinate ($\xi = r/R$, with R being the Control Volume (CV) radius). The parameter α is an adjustable coefficient used to match the velocity distribution observed experimentally, and is equal to 1.5 for fully developed jets.

By applying this distribution, each CV of the 1D spray is subdivided into radial contours, based on their equivalence ratio value. The air-fuel mass contained in each iso- ϕ contour volume is summed axially and subsequently passed to the combustion model as initial zone mass distributions. A schematic of the 1D model with the assumed radial distribution is shown in Figure 3.

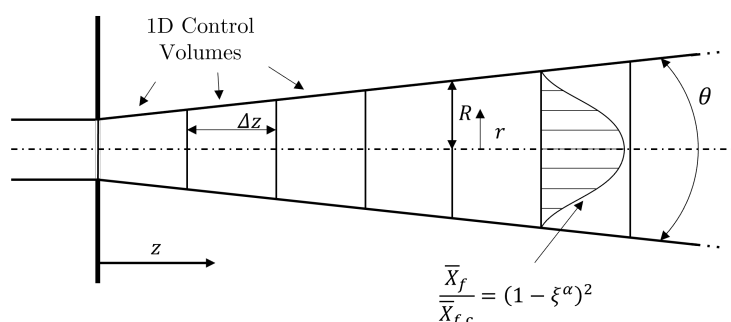


Figure 3. Representation of the 1D discretization of the fuel spray in CV of equal length (Δz). The axial (z) and radial (r) coordinates are highlighted, with the assumed radial distribution (from [44]) and the cone spray angle (θ).

The spray model provides the mass distribution across the different iso- ϕ zones, as well as the physical subdivision into the three physical sub-regions: ‘liquid’, ‘unburnt vapor’, and ‘burnt vapor’ (see Figure 2).

To do so, an evaporation sub-model is included to determine the Liquid Length (LL), after which the fuel is assumed to be in the ‘unburnt vapor’ sub-state, implying that fuel is fully mixed with air (at different ϕ , maintaining the stratification) and ready to react. After the ID period, combustion begins and the ‘burnt vapor’ sub-region of the spray is populated with mass from either the ‘unburnt vapor’ (if already evaporated) or ‘liquid’ sub-regions.

The spray model is initialized at the Start Of Injection (SOI), with a fixed spray angle (θ) determined with the correlation proposed by Naber et al. [45]:

$$\theta = 2 \cdot \arctan \left[C_\theta \left(\left(\frac{\rho_a}{\rho_f} \right)^{0.19} - 0.0043 \left(\frac{\rho_f}{\rho_a} \right)^{0.5} \right) \right] \quad (10)$$

where C_θ is a tuning parameter called spray angle coefficient, ρ_f is the fuel liquid density, and ρ_a is the air density, both evaluated at SOI.

The influence of real engine geometry on the spray evolution is accounted for by modifying two parameters beyond the Point Of Impact (POI), defined as the location on the spray grid where the spray impinges on the piston crown. The POI is a tunable parameter proportional to bore/4:

$$d_{POI} = C_{POI} \cdot b/4 \quad (11)$$

Beyond the POI, the cone spray angle is reduced, together with a change in the radial distribution profile. This is controlled by two tunable parameters, the angle coefficient after wall (C_w) and the distribution after wall (α_w) respectively. Overall, these changes result in reduced air entrainment in the spray, which inherently lowers the combustion rate.

3.3. Construction of the Dual-Fuel Combustion Model

Prior to SOI, the cylinder is modeled as a single homogeneous zone composed of an air-LR fuel mixture, under the assumption that the LR fuel is introduced during the intake stroke through Port Fuel Injection (PFI). This formulation enables an accurate estimation of the in-cylinder pressure throughout the compression stroke.

Upon reaching the SOI, the multi-zone combustion and charge stratification models (cf. Sections 3.2.1 and 3.2.2) are activated. Consistent with the homogeneous air-LR fuel mixture assumption, the iso- ϕ multi-zones incorporate the LR fuel in their composition, which consequently affects the evaluation of the thermodynamic properties and the composition of the corresponding burned zones. It should be noted that the equivalence ratio assigned to each zone is defined exclusively with respect to the HR fuel and oxygen (O_2). As a result of this assumption, a larger fresh charge mass is required to achieve the same HR fuel equivalence ratio, since the available oxygen is proportionally reduced.

The ID can be estimated through two distinct approaches: a Tabulated Kinetics of Ignition (TKI) method, as described in [38], or through the Livengood-Wu integral [46]. In the context of DF operation, both methods must account for the effect of the LR fuel on the autoignition process to reliably predict the ID. In the present work, the TKI approach was extended to capture fuel-fuel interactions by initializing constant-pressure homogeneous reactors with mixtures of both fuels and oxidizer. The resulting lookup tables are indexed by initial pressure, temperature, HR fuel mixture fraction, LR fuel mixture fraction, and Exhaust Gas Recirculation (EGR).

The mixture fraction (Z) is defined as the fuel mass fraction in the mixture. For the HR fuel:

$$Z_{HR} = \frac{m_{fuel,HR}}{m_{fuel,HR} + m_{fuel,LR} + m_{air}} \quad (12)$$

with an analogous definition for the LR fuel. Note that introducing this additional variable increases table size proportionally to the LR fuel mixture fraction range, resulting in higher computational cost and longer table generation time compared to single-fuel tables.

Following the Start Of Combustion (SOC), the charge stratification model supplies the information required to characterize the premixed and mixing-controlled combustion of the HR fuel spray. To account for the turbulent flame contribution, an additional zone containing no HR fuel is included alongside the iso- ϕ zones. The evolution of this zone is governed exclusively by the combustion of the air-LR fuel mixture surrounding the spray, as described by Equations (2)–(4). Since this zone is free of HR fuel, its thermodynamic properties—and in particular the LFS—are independent of the HR fuel composition.

Combustion inside and outside the spray occurs simultaneously, with both processes contributing to the overall Heat Release Rate (HRR). The turbulent air-LR fuel flame is assumed to originate as an infinitesimally thin brush enclosing the HR fuel spray.

In DF engines, the spherical flame assumption no longer holds; instead, conical flames are observed, as experimentally reported in [47,48]. To capture this behavior in the evaluation of the laminar flame surface (A_l in Equation (3)), the flame front model developed by Frerichs [49] is adopted. This model assumes a pancake combustion chamber geometry with the spray origin at the center. The flame front evolves in two distinct phases: an initial and mainly axial propagation until a critical length ($l_{cone,cr}$) is reached, followed by spreading in all directions perpendicular to the flame surfaces. A numerical root-finding algorithm is applied to evaluate the flame surface area accounting for the interaction with the cylinder walls and adjacent flames, as illustrated in Figure 4.

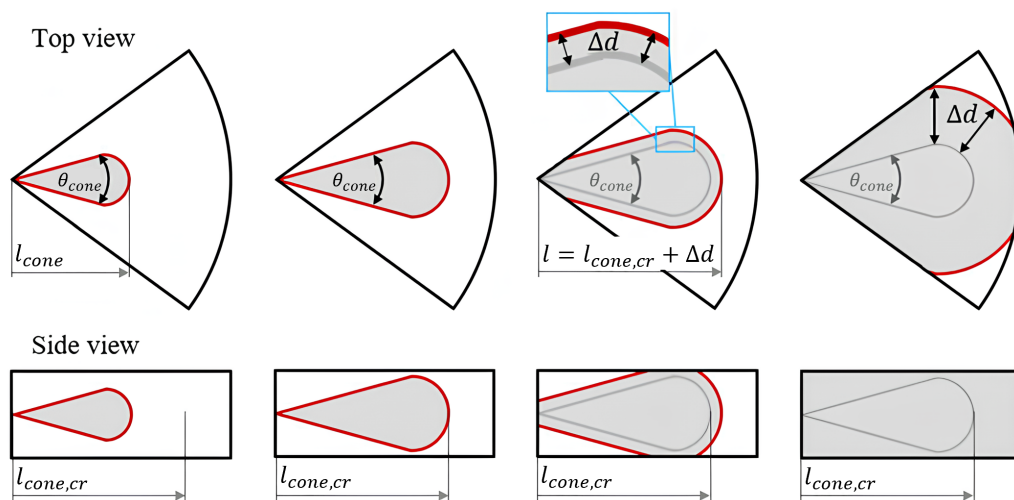


Figure 4. Representation of the conical flame front propagation seen from a top view (upper row) and from a side view (bottom row).

3.4. Fuel- NO_x Model

In the context of combustion simulation, the evaluation of pollutant emission is of great importance, given the stringent regulations that engine manufacturers and end-users have to comply with. This is especially relevant for NO_x emissions, due to their high impact on ecosystems and human health. Accurate estimation of this pollutant is necessary in early engine development phases, to introduce proper mitigation strategies.

For conventional fuels (e.g., gasoline and diesel), the thermal formation pathway is considered the main source of NO_x , typically addressed by the Extended Zel'dovich model [42]. However, ammonia combustion poses a new challenge in NO_x estimation due to the presence of nitrogen in the fuel, resulting in the necessity to account for fuel-derived NO_x . Recent studies have used numerical simulations to distinguish the specific thermal and fuel contributions to total NO_x emissions. Yang et al. [50] proposed a method to decouple fuel- and thermal- NO_x by dividing the source of elemental nitrogen, which could derive from fuel or air. The former was assigned to the ammonia oxidation sub-mechanism, while the latter was used in the Zel'dovich mechanism. With this approach, applied to a 3D CFD simulation of a pure-ammonia SI engine, they found comparable levels of fuel- and thermal- NO in stoichiometric conditions. The study by Ma et al. [51] proposed a similar virtual decoupling method to separate fuel and thermal pathways. They consistently observed a dominance of thermal- NO in an ammonia/hydrogen marine engine, under different operating conditions.

From these studies, it is clear that fuel- NO_x plays a significant role in overall pollutant emissions. As such, a simplified model is proposed in this work to account for this aspect. In this model, a fuel- NO_x source term is introduced, proportional to the burning rate (dm_b) and to the mass fraction of NO inside the flame brush ($Y_{\text{NO},fl}$).

Fuel-NO_x is initialized in the flame brush and then moves into the burnt region, where it evolves with the Extended Zel'dovich mechanism together with the thermal-NO. This model can be summarized in the following equation:

$$\frac{dm_{\text{NO}}}{dt} = \frac{d[\text{NO}]}{dt} \cdot MM_{\text{NO}} \cdot V_b + \frac{dm_b}{dt} \cdot Y_{\text{NO},fl}(p, T, \phi, EGR) \quad (13)$$

The first term of the RHS of Equation (13) represents the contribution due to thermal-NO, computed as the variation of NO volumetric concentration multiplied by the burned volume and the molar mass of NO (MM_{NO}), while the second is the source term from the flame brush attributed to fuel-NO.

The quantity $Y_{\text{NO},fl}$ represents the NO mass fraction associated with ammonia oxidation inside the propagating flame structure. It is extracted from steady 1D freely propagating premixed flame simulations by evaluating the NO mass fraction in the post-flame region, immediately downstream of the main heat-release layer. In this way, the tabulated value accounts for the nitrogen-containing intermediate chemistry resolved by the detailed kinetic mechanism, while avoiding the direct integration of the full ammonia oxidation mechanism during the engine-cycle simulation. The tabulated variable therefore represents an effective fuel-NO contribution generated by the flame brush, which is subsequently transported into the burnt zone and further evolved through the thermal-NO mechanism.

This formulation is intentionally simplified. It does not explicitly solve the temporal evolution of individual nitrogen-containing intermediates such as NH, NH₂, HNO, NNH, NO₂, or N₂O during the engine simulation. Their effect is included only indirectly through the detailed-chemistry flame calculations used to generate the lookup table. As a consequence, the model is expected to reproduce the main trends of fuel-bound NO formation in premixed ammonia combustion, but local deviations may occur when strong stratification, incomplete mixing, or interaction with hydrocarbon pilot-fuel products becomes relevant.

In the present implementation, the emission model directly predicts NO formation. Since NO is expected to represent the dominant fraction of total NO_x under the high-temperature in-cylinder conditions considered here, the computed NO concentration is compared with the experimentally measured NO_x concentration. This approximation is commonly adopted in engine combustion modeling, although it can introduce additional uncertainty during the expansion and exhaust phases, where the conversion of NO-to-NO₂ can occur.

4. Results and Discussion

First, the SI operating conditions were analyzed. A complete 1D engine scheme representing the experimental setup (Figure 1) was simulated in Gaseodyn. The numerical model included the different geometrical aspects that characterize the intake and exhaust systems, to faithfully reproduce the experimental SCE. The Gaseodyn scheme is reported in Figure 5.

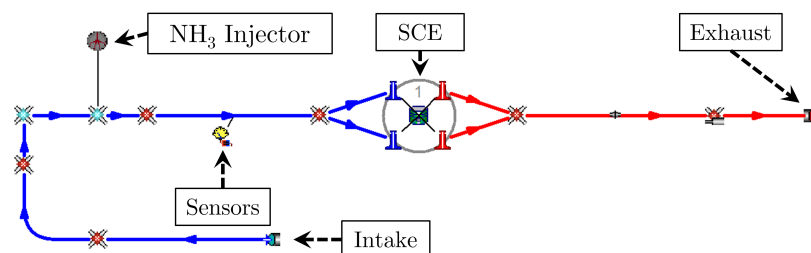


Figure 5. 1D model schematic of the ammonia-fueled SCE reproduced in Gaseodyn pre-processor.

Boundary conditions were varied for each operating condition to match the experimental pressure and temperature measured before the engine (p_{in} and T_{in} in Figure 1). Computed and measured air and ammonia mass flow rates were compared to assess the quality of the simulations. Across the 16 operating conditions, the average absolute error on the simulated air mass flow rate is 0.83% relative to the experimental value. For the fuel mass flow rate, this is equal to 0.55%.

Regarding combustion, the SA values were set equal to the experimental ones reported in the left side of Table 2. The combustion model was tuned through a trial-and-error procedure, owing to the limited number of operating conditions. Default values were adopted for the tuning parameters, except for C_{delay} , which was increased as reported in Table 3.

Table 3. Tuning parameters of the turbulent premixed flame model identified for the ammonia SI SCE simulations.

Tuning Parameter	Value
C_t	1.00
C_{delay}	0.68
C_e	1.00

The LFS and fuel- NO_x were obtained from tabulated data generated by solving a steady, 1D freely propagating premixed flame using Cantera [52], with the chemical mechanism of Stagni [53] (31 species, 203 reactions). The thermodynamic conditions considered are summarized in Table 4.

Table 4. Range of pressure, temperature, equivalence ratio, and EGR for the ammonia LFS and fuel- NO_x tables generation.

	Range	Number of Values
Pressure [bar]	1–90	11
Temperature [K]	300–1200	25
Equivalence ratio [-]	0.7–1.1	7
EGR [-]	0–0.05	2

Figure 6 shows the comparison of the average experimental (Exp., in black) and computed (QD CFD, in red) in-cylinder pressure. Vertical colored dashed lines represent the experimental SA, whose value (measured in ° aTDC) is reported in the upper-right corner of each operating condition. The same colors will be used in subsequent figures to identify the same operating condition. Each column represents the SA sweep performed at a given equivalence ratio (reported as the title of the column), moving from most to least advanced SA (i.e., further from TDC). The gray-shaded areas identify the individual pressure cycles. These are reported in five of the sixteen cases, since they are provided only for these operating conditions.

Overall, a good agreement between experimental and computed values is observed. The model captures the influence of the different equivalence ratios and SA values. Larger discrepancies are present in the cases with lower values of SA (i.e., more advanced). However, it is worth noting that these operating conditions are characterized by high values of Coefficient of Variation (CoV), as reported in Table 2, which may lead to a skewed average in-cylinder pressure cycle. The average absolute error relative to peak (maximum) pressure is below 3 bar. In terms of peak pressure location, the error is contained within 2°. A consistent overestimation of the pressure is visible for the stoichiometric cases ($\phi = 1$,

right-most column of Figure 6), suggesting that the laminar-to-turbulent flame transition occurs too early in the model, or that the LFS is overestimated.

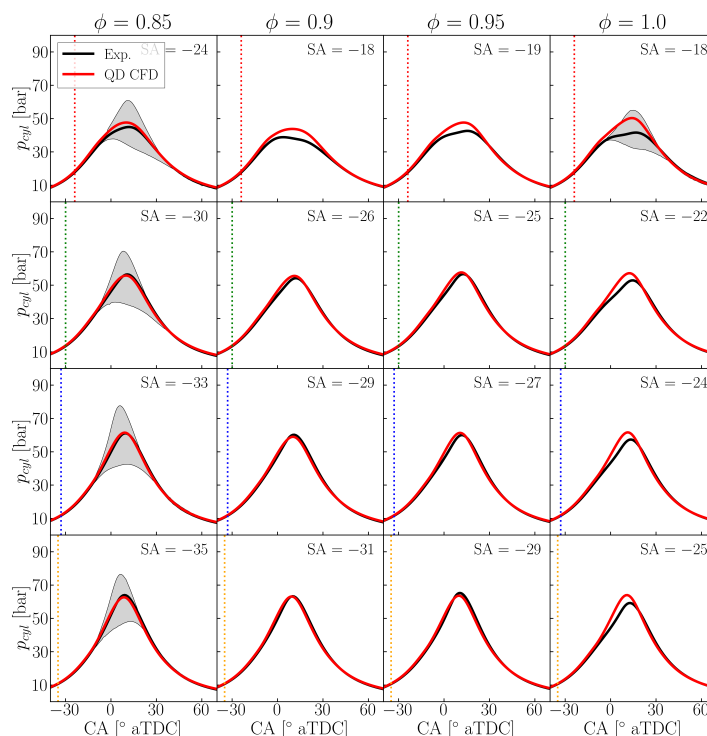


Figure 6. Comparison of the average experimental (black) and calculated QD CFD (red) in-cylinder pressure traces for all operating points of the ammonia SI SCE. Gray-shaded areas represent the raw pressure measurements of 200 consecutive engine cycles. Vertical colored dashed lines represent the SA location. SA values are reported in the upper-right corner of each graph in ° aTDC.

To delve more deeply into the combustion analysis, the experimental and calculated AHRR are compared in Figure 7.

From this comparison it appears that the overestimation of the LFS may be the cause of these higher peak pressures observed in the calculated results. In fact, the rise in AHRR starts at the same CA, but is sharper for the QD CFD traces. Specifically, the rising slope of the calculated AHRR is on average 20% steeper with respect to the experimental one. This evidence favors the overestimation of LFS over transition timing, since this quantity directly influences the AHRR. This is also supported by Liu et al. [54], where they showed that the chemical mechanism proposed by Stagni et al. tends to provide LFS slightly higher than the experimental one.

A discrepancy between the experimental and computed AHRR trends is visible in the final phase of combustion across all operating conditions. This discrepancy is related to the f_w correction factor (Equation (8)), whose influence grows as more of the flame comes into contact with the cylinder walls. This results in a change in the slope of the AHRR, after which the experimental and calculated values nearly realign.

Figure 8 shows the comparison of the computed and experimental combustion durations, obtained by measuring the difference between the CA at which a specific Burned Mass Fraction (BMF) is reached. The BMF is defined as:

$$\text{BMF}(\text{CA}) = \frac{m_b(\text{CA})}{m_{\text{cyl}}} \quad (14)$$

Specifically, three phases are analyzed:

- CA0–10, characterizing the initial flame kernel formation and transition from laminar to turbulent combustion (Figure 8a);
- CA10–50, which identifies the rapid and turbulent flame propagation inside the combustion chamber (Figure 8b);
- CA50–90, representing the final combustion phase, including the reduction in burning rate due to flame-wall interactions and extinction of the flame (Figure 8c).

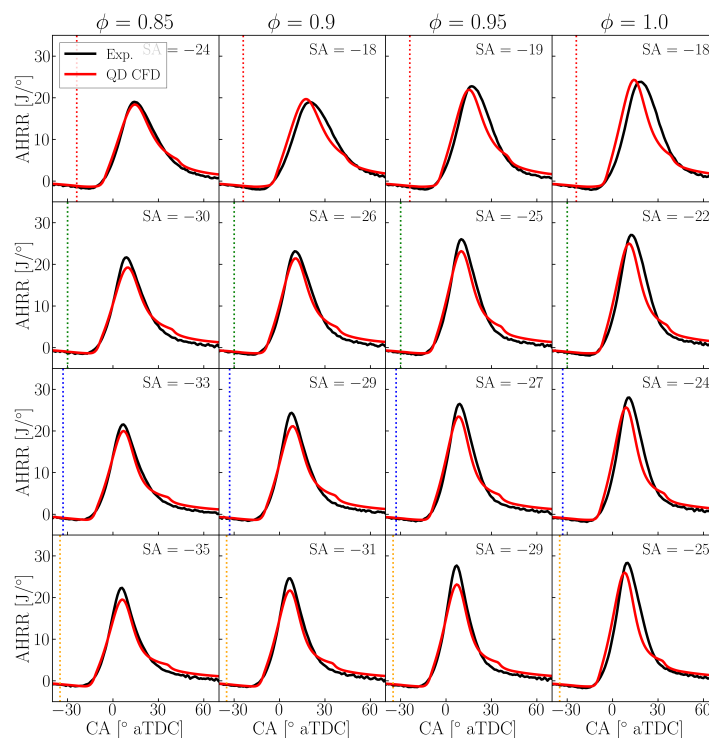


Figure 7. Comparison of the average experimental (black) and calculated QD CFD (red) AHRR for all operating points of the ammonia SI SCE. Vertical colored dashed lines represent the SA location. SA values are reported in the upper-right corner of each graph in ° aTDC.

These scatter plots show that the initial and rapid combustion phases are well captured by the model, with most of the computed results falling in the $\pm 3^\circ$ range with respect to the experimental values. The average error for the CA0–10 is -2.5° , while for the CA10–50 it is 1.2° .

In contrast, the model overestimates the final combustion phase duration, as the average difference between computed and experimental values increases to 10° . The highest errors are observed for the operating conditions with a high CoV, namely those with the least advanced SAs (red symbols) and lean mixtures (circle and square symbols). This discrepancy should be interpreted in light of the measured ammonia slip. Across the SI operating conditions, the engine exhibited significant unburned NH_3 concentrations in the exhaust, of the order of 10^4 ppm. This indicates that a non-negligible fraction of the injected ammonia does not participate in the main combustion process. Possible causes include near-wall flame quenching, incomplete oxidation in low-temperature regions, and fuel trapped in crevice volumes. The last of these appears to be the major source of unburned ammonia, as reported in both numerical and experimental studies [11,55,56]. The present QD model does not include a dedicated crevice or unburned-ammonia sub-model; therefore, the full trapped ammonia mass is assumed to remain available for combustion according to the turbulent flame formulation. This assumption can affect the predicted late heat-release tail, combustion efficiency, and pollutant formation. The development of a crevice/ammonia-slip model is therefore identified as a priority for future work.

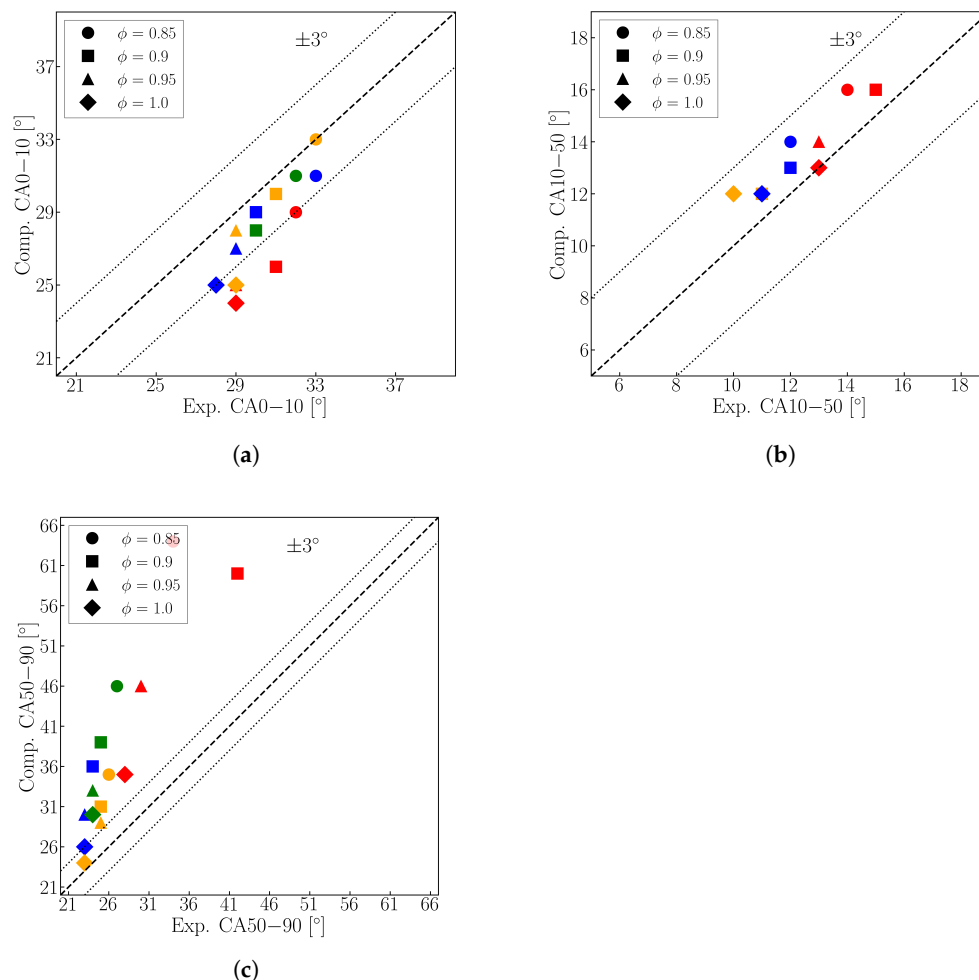


Figure 8. Comparison of the combustion parameters CA0–10 (a), CA10–50 (b) and CA50–90 (c) for the ammonia SI SCE. Symbols identify the equivalence ratio of the operating conditions. The red–green–blue–yellow colors identify the SA, from least advanced to most advanced value, as reported in Figures 6 and 7. Dotted black lines represent the $\pm 3^\circ$ bands. Experimental vs. computed.

Finally, Figure 9 shows the computed NO_x against the experimental measurements of the DW10F ammonia-fueled engine. The different symbols refer to the equivalence ratio of the operating condition analyzed, while the color is linked to the SA values reported in Figures 6 and 7. The black dashed line represents perfect agreement (i.e., the bisector), while dotted lines represent the $\pm 15\%$ error lines.

The computed values of NO_x well approximate the experimental ones, as most conditions are contained between the error lines. An underestimation is observed for the stoichiometric cases, particularly for the ones characterized by the most advanced SAs (blue and yellow diamonds, -33° aTDC and -35° aTDC, respectively). Nonetheless, the effect of varying the equivalence ratio on NO_x emissions—lower values as ϕ increases—is well captured. The value of SA does not appear to greatly influence NO_x emissions, which is also backed up by the model results.

To focus more deeply on the effect of the fuel- NO_x model proposed, Figure 10 presents the evolution of this pollutant during combustion in four different operating conditions covering the equivalence ratio sweep. Dashed lines represent the experimental values at Exhaust Valve Opening (EVO), continuous lines show the computed NO_x concentration including the fuel- NO_x model, while dotted ones do not consider it. The same color-coding is used as in previous Figures.

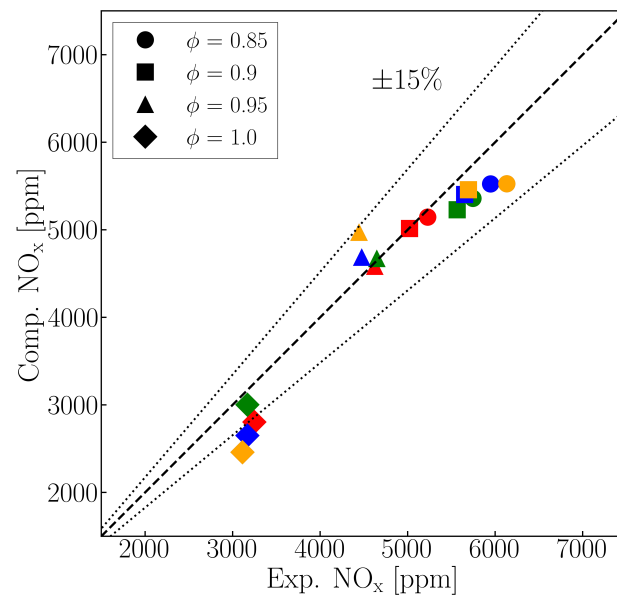


Figure 9. Scatter plot of the NO_x emissions for the ammonia SI SCE operating conditions. Symbols identify the equivalence ratio of the operating conditions. The red-green-blue-yellow colors identify the SA, from least advanced to most advanced value, as reported in Figures 6 and 7. Dotted black lines represent $\pm 15\%$ error lines. Experimental vs. computed values.

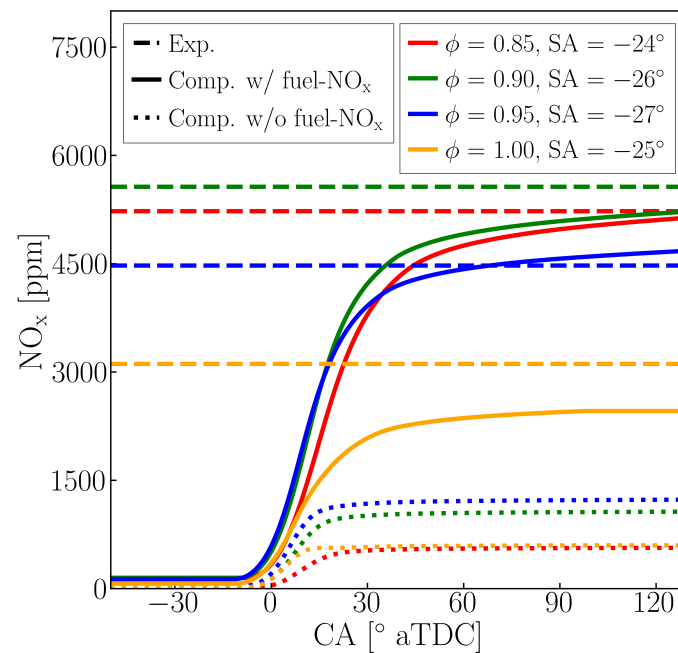


Figure 10. Trends of in-cylinder NO_x concentration computed with (continuous lines) and without (dotted lines) the fuel- NO_x model for the ammonia SI SCE. Experimental values are reported as horizontal dashed lines.

It is clear that the fuel- NO_x term substantially improves the prediction capabilities of the combustion model, and the results suggest that most of the NO_x is produced during fuel combustion, in addition to the thermal contribution.

Reactivity Controlled Compression Ignition Operating Conditions

The RCCI operating conditions were then analyzed. As for the SI configurations, the boundary conditions at IVC were obtained from simulations of the complete engine scheme.

Given the lack of data regarding the injection law, a square-shaped law was imposed for the diesel pilot injection such that the injected mass matches the experimental value. The choice of a square-shaped injection law was considered appropriate given the short injection duration and mass of fuel injected. Moreover, the results were comparable to those obtained with a triangular injection law. A set of tuning parameters for the diffusive combustion model was identified, as reported in Table 5.

Table 5. Tuning parameters of the diffusive combustion model identified for the ammonia RCCI SCE simulations.

Tuning Parameter	Value
C_θ	0.20
C_{POI}	0.50
C_w	1.00
α_w	2.30

Regarding the turbulent premixed flame combustion, the same model parameters were maintained as reported in Table 3, together with the LFS and NO_x lookup tables.

A preliminary assessment of the model indicated a systematic underestimation of the ID when the influence of ammonia on the diesel autoignition process was disregarded. This behavior is consistent with experimental observations from rapid compression machine studies on ammonia/diesel mixtures [57–59], which collectively document an increase in ID with rising AEF, attributed to the chemical inhibition exerted by ammonia. To account for this effect, the modified TKI methodology outlined in Section 3.3 was adopted. The corresponding TKI tables were produced using Cantera, by simulating constant-pressure homogeneous reactor autoignition over the thermodynamic ranges of Table 4, with the addition of diesel to the mixture. All simulations relied on the ammonia/diesel kinetic mechanism validated by Zhang et al. [58].

Figure 11 presents the comparison of the average experimental (Exp., in black) and calculated (QD CFD, in red) in-cylinder pressure for all sixteen RCCI operating conditions. Each column represents the DOI sweep performed at a fixed equivalence ratio (ϕ) and SOI. The value of the DOI is reported in the upper-right corner of each subgraph in μs , while the colored line represents the SOI.

The model responds well to the DOI variation at fixed LR fuel equivalence ratio. Indeed, as the DOI increases, a sharper increase of in-cylinder pressure is observed in both experimental and calculated trends. The larger quantity of diesel leads to a stronger premixed combustion, which translates to an overall shorter combustion duration. This aspect is clearly visible from the comparison of the experimental and computed AHRR, reported in Figure 12.

In particular, as the DOI increases, the AHRR profiles shift to the left and become narrower. This indicates a shorter ID, whose trend is indeed well captured by the DF TKI approach used for these simulations. The latter aspect shows that the model is sensitive to the increased quantity of that evaporates and penetrates further into the air-LR fuel mixture, resulting in a faster combustion overall since more of the trapped mass is ignited simultaneously.

A slight overestimation of the ID is observed for the leanest operating conditions ($\phi = 0.85$) analyzed in this study. This results in a delayed combustion onset, which translates into a reduced peak pressure. On the other hand, at stoichiometric air-LR fuel mixtures ($\phi = 1.0$), the model overestimates the burning rate, leading to a sharper rise in AHRR. This is consistent with the results obtained for the SI configuration in similar operating conditions, and it is expected since the same LFS table was used for the RCCI

cases. In general terms, the average absolute error of the peak pressure is below 4 bar, and the peak pressure location is contained within 2° .

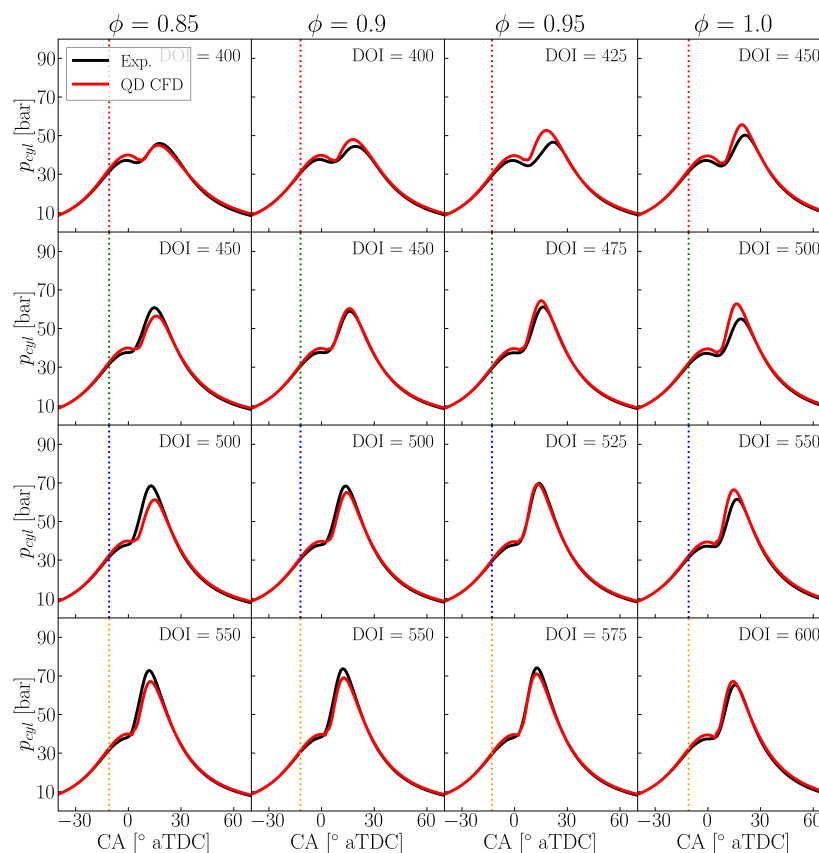


Figure 11. Comparison of the average experimental (black) and calculated QD CFD (red) in-cylinder pressure traces for all operating points of the ammonia RCCI SCE. Vertical colored dashed lines represent the SOI location. DOI values are reported in the upper-right corner of each graph in μs .

For a more detailed analysis of the combustion parameters, the comparisons of experimental and computed CA0–10, CA10–50 and CA50–90 are reported in Figures 13a, 13b and 13c, respectively.

A higher degree of accuracy for the CA0–10 is observed with respect to the SI simulations. The average error is equal to 0° . This, however, becomes 1° in absolute terms. Regarding CA10–50, an almost perfect agreement is visible between the computed and experimental data, with an average error of -0.25° . On the other hand, results for the CA50–90 show a larger discrepancy, with an average error equal to 4° . This is consistent with that observed for the SI cases (Figure 8c), although it presents a better match between the numerical and experimental values. It is also worth noting that the operating conditions with shorter DOIs (red symbols) are the ones that present the largest error.

Nonetheless, the model is able to capture the reduced combustion duration (CA0–90) that characterizes RCCI combustion relative to SI operation. Experimentally, the average combustion duration is 49° for the RCCI cases, while for the SI ones it is 69° . The computed results yield 52° for RCCI conditions and 78° for the SI ones.

Lastly, Figure 14 presents the comparison of computed and measured NO_x emissions for the RCCI cases being analyzed. The same color-symbol combinations in previous Figures are used in this figure to identify the corresponding operating condition.

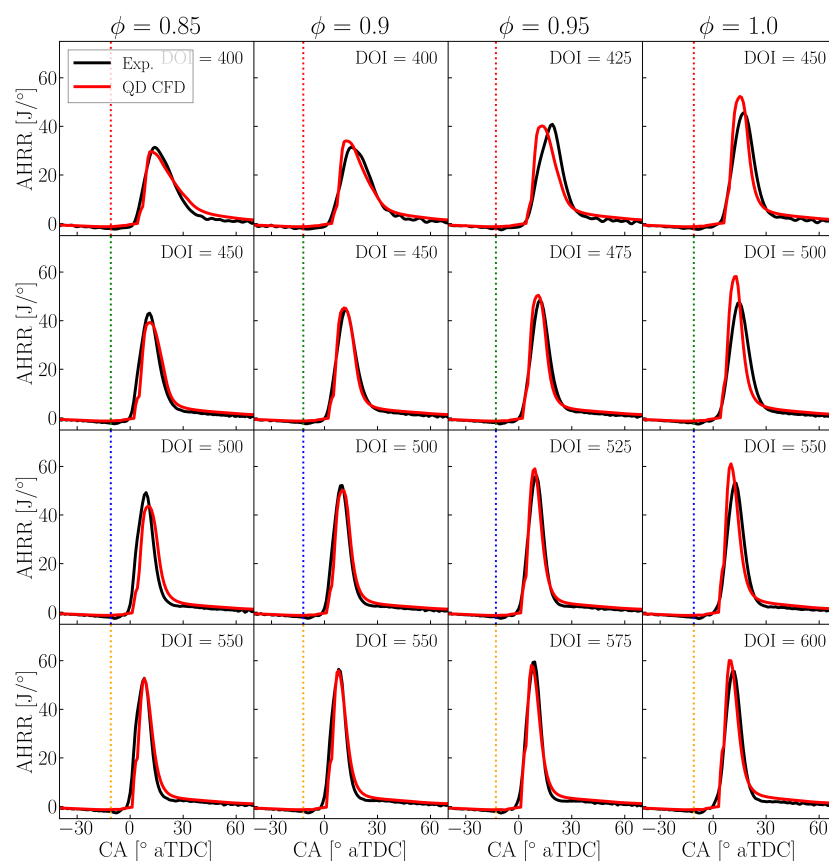


Figure 12. Comparison of the average experimental (black) and calculated QD CFD (red) AHRR for all operating points of the ammonia RCCI SCE. Vertical colored dashed lines represent the SOI location. DOI values are reported in the upper-right corner of each graph in μs .

In these cases, the model clearly tends to overestimate the experimental values. In particular, the experimental data show a decreasing trend when the DOI is increased at a fixed equivalence ratio, identified by the red-green-blue-yellow color pattern (see columns of Figure 11). The closest match between experimental and computed results is obtained at the lowest DOI conditions across all equivalence ratios, suggesting that the presence of the HR fuel influences the fuel- and thermal- NO_x formation. In fact, due to how it is constructed, the model assumes a complete separation between the zones containing (of the original CI model) and the additional air-LR fuel one. Since these are not allowed to mix, the formation of NO_x in the air-LR fuel zone is not influenced by carbon-containing compounds such as CO , CO_2 and hydrocarbon fragments. The suppression of NO by carbon-containing species occurs via two complementary pathways. First, the presence of CO_2 lowers NO formation both thermally, by reducing the peak flame temperature, and chemically, by depleting the O/H radical pool, as reported in the study regarding coal-ammonia combustion by Qiao et al. [60]. They suggested that in the presence of identical temperature and quantity of ammonia, a higher CO_2 concentration yields lower NO generation. However, it has to be highlighted that they considered an O_2/CO_2 atmosphere for part of this study. Nonetheless, a general conclusion regarding the inhibitory effect of CO_2 on NO formation can be drawn from their analysis. Furthermore, the study by Frassoldati et al. [61] showed how hydrocarbon fragments reduce NO to HCN and ultimately to N_2 through the reburn mechanism. Both effects act to lower NO only when the carbon-containing species and the ammonia-derived nitrogen chemistry are allowed to interact, which is not currently considered in the model.

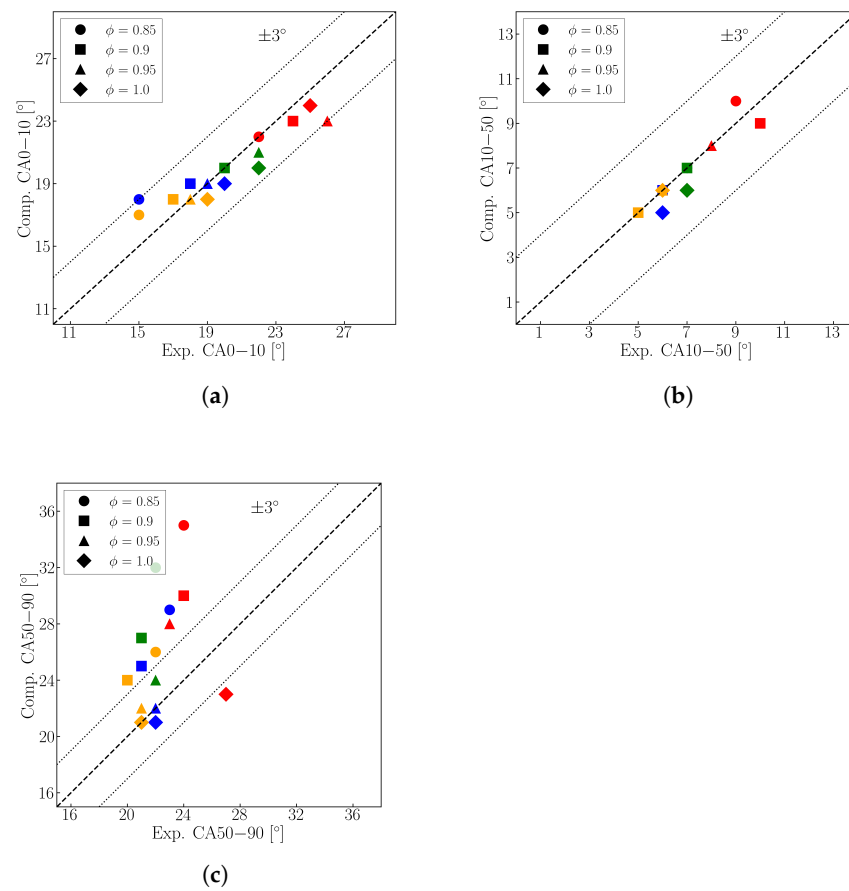


Figure 13. Comparison of the combustion parameters CA0-10 (a), CA10-50 (b) and CA50-90 (c) for the ammonia RCCI SCE. Symbols identify the equivalence ratio of the operating conditions. The red-green-blue-yellow colors identify the DOI, from minimum to maximum value, as reported in Figures 11 and 12. Dotted black lines represent the $\pm 3^\circ$ bands. Experimental vs. computed.

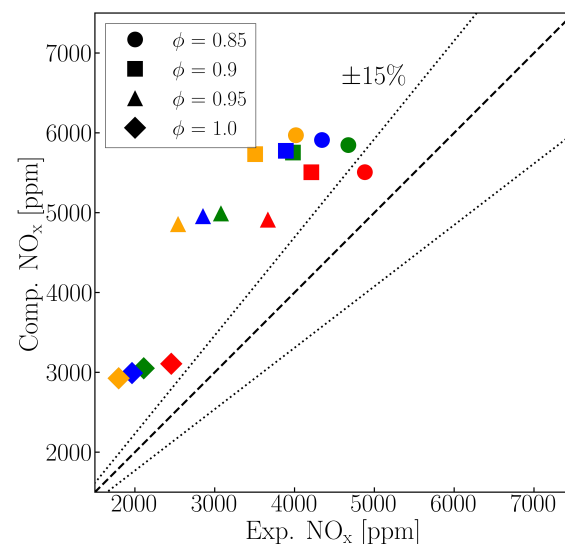


Figure 14. Scatter plot of the NO_x emissions for the ammonia RCCI SCE operating conditions. Symbols identify the equivalence ratio of the operating conditions. The red-green-blue-yellow colors identify the DOI, from minimum to maximum value, as reported in Figures 11 and 12. Dotted black lines represent $\pm 15\%$ error lines. Experimental vs. computed values.

5. Conclusions

The objective of this work was to present a QD combustion framework and apply it to an ammonia-fueled SCE operating in both SI and RCCI modes. A key contribution was the introduction of a fuel- NO_x sub-model, which accounts for nitrogen-bound NO_x produced during ammonia oxidation within the flame brush via a source term proportional to the burning rate. Fuel- NO concentrations inside the flame are retrieved from a lookup table generated through 1D laminar flame simulations, initialized in the flame brush, and subsequently evolve alongside thermal NO via the Extended Zel'dovich mechanism in the burnt zone.

Validation against SI experimental data, covering equivalence ratio and SA sweeps, demonstrated good predictive accuracy, with mass flow rate errors below 1%, peak pressure errors below 3 bar, location errors within 2° , and combustion phasing parameters CA_{0-10} and CA_{10-50} reproduced within a $\pm 3^\circ$ band. A systematic overestimation of the CA_{50-90} duration was attributed to unburned ammonia trapped in crevice volumes, which are not accounted for in the current model. The fuel- NO_x sub-model substantially improved emission predictions, correctly capturing the dominant role of fuel-bound nitrogen and the decreasing NO_x trend with increasing equivalence ratio. A remaining limitation is the absence of a dedicated ammonia-slip and crevice-trapping model, which will be developed and tested in future works. This affects mainly the late combustion phase and may partly explain the overprediction of CA_{50-90} duration in SI operation.

For RCCI operation, the ammonia inhibition effect on diesel autoignition was addressed through a modified TKI approach using validated ammonia/diesel kinetic tables. The model reproduced ID and combustion rate trends as functions of DOI and equivalence ratio, with peak pressure errors below 4 bar and location errors within 2 CA. A systematic NO_x overestimation at higher DOI values was attributed to the assumption of complete zone separation, which precludes interaction between NO_x pathways and carbon-containing species. The inhibitory effect of CO_2 on NO formation, reported in recent literature, represents a priority for future model development.

Overall, the proposed framework provides a computationally efficient and physically consistent tool for simulating ammonia combustion across SI and RCCI operating conditions, suitable for early-stage engine development and optimization studies. Future studies will include its application to simulate a more vast dataset, including the variation of engine speed, boundary conditions, and diesel injection strategy, strengthening its predictive capabilities.

Author Contributions: A.B.: conceptualization, methodology, formal analysis, visualization, software, validation, writing—original draft preparation, and review and editing. G.D.: conceptualization, resources, supervision, and writing—review and editing. C.M.-R.: investigation, writing—review and editing. P.B.: investigation, writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: The authors declare no conflicts of interest.

Definitions and Acronyms

Definitions

α	Radial distribution shape parameter
ϕ	Equivalence ratio

ν	Kinematic viscosity
ρ	Density
θ	Spray angle
ξ	Dimensionless radial coordinate
A_l	Laminar flame surface
b	Bore
m	Mass
MM	Molar mass
L_i	Integral length
p	Pressure
r	Radius
t	Time
T	Temperature
u'	Turbulence intensity
V	Volume
X_f	Fuel volumetric fraction
Y	Mass fraction
S_l	Laminar flame speed
S_t	Turbulent flame speed
S_{tay}	Taylor microscale
Z	Mixture fraction

Subscripts

a	Air
b	Burned
e	Entrainment
f	Fuel
l	Laminar
t	Turbulent
u	Unburned
w	Wall

Acronyms

0D	Zero-Dimensional
1D	One-Dimensional
2D	Two-Dimensional
3D	Three-Dimensional
AEF	Ammonia Energy Fraction
AHRR	Apparent Heat Release Rate
aTDC	after Top Dead Center
BMF	Burned Mass Fraction
CA	Crank Angle
CFD	Computational Fluid Dynamics
CI	Compression Ignition
CR	Compression Ratio
CoV	Coefficient of Variation
CV	Control Volume
DF	Dual-Fuel
DI	Direct Injection
DOI	Duration Of Injection
EGR	Exhaust Gas Recirculation
EVC	Exhaust Valve Closing
EVO	Exhaust Valve Opening
HD	Heavy-Duty
HR	High-Reactivity

HRR	Heat Release Rate
ICE	Internal Combustion Engine
ID	Ignition Delay
IMEP	Indicated Mean Effective Pressure
IVC	Intake Valve Closing
IVO	Intake Valve Opening
LD	Light-Duty
LFS	Laminar Flame Speed
LHV	Lower Heating Value
LL	Liquid Length
LR	Low-Reactivity
PFI	Port Fuel Injection
POI	Point Of Impact
QD	Quasi-Dimensional
RCCI	Reactivity Controlled Compression Ignition
R&D	Research & Development
RHS	Right-Hand Side
SA	Spark Advance
SACI	Spark Assisted Compression Ignition
SI	Spark Ignition
SCE	Single-Cylinder Engine
SOC	Start Of Combustion
SOI	Start Of Injection
TDC	Top Dead Center
TKI	Tabulated Kinetics of Ignition

References

1. Tornatore, C.; Marchitto, L.; Sabia, P.; De Joannon, M. Ammonia as Green Fuel in Internal Combustion Engines: State-of-the-Art and Future Perspectives. *Front. Mech. Eng.* **2022**, *8*, 944201. [\[CrossRef\]](#)
2. Hasan, M.H.; Mahlia, T.M.I.; Mofijur, M.; Fattah, I.M.R.; Handayani, F.; Ong, H.C.; Silitonga, A.S. A Comprehensive Review on the Recent Development of Ammonia as a Renewable Energy Carrier. *Energies* **2021**, *14*, 3732. [\[CrossRef\]](#)
3. Madheswaran, D.K.; Vengatesan, S.; Jegadheeswaran, S.; Thangamuthu, M.; Togun, H.; Duraisamy, B.; Ouyang, C.; Khan, M.W. Ammonia as a hydrogen carrier: A comprehensive analysis of electrolysis efficiency and its potential in sustainable energy systems. *Renew. Sustain. Energy Rev.* **2025**, *221*, 115915. [\[CrossRef\]](#)
4. Proniewicz, M.; Petela, K.; Szlek, A. Life cycle assessment of ammonia as carbon-free fuel in internal combustion engine-driven orchard vehicle. *Fuel* **2025**, *400*, 135809. [\[CrossRef\]](#)
5. Cheng, Q.; Muhammad, A.; Kaario, O.; Ahmad, Z.; Martti, L. Ammonia as a sustainable fuel: Review and novel strategies. *Renew. Sustain. Energy Rev.* **2025**, *207*, 114995. [\[CrossRef\]](#)
6. Aziz, M.; Wijayanta, A.T.; Nandiyanto, A.B.D. Ammonia as Effective Hydrogen Storage: A Review on Production, Storage and Utilization. *Energies* **2020**, *13*, 3062. [\[CrossRef\]](#)
7. Mounaïm-Rousselle, C.; Bréquigny, P.; Dumand, C.; Houillé, S. Operating Limits for Ammonia Fuel Spark-Ignition Engine. *Energies* **2021**, *14*, 4141. [\[CrossRef\]](#)
8. Hayakawa, A.; Goto, T.; Mimoto, R.; Arakawa, Y.; Kudo, T.; Kobayashi, H. Laminar burning velocity and Markstein length of ammonia/air premixed flames at various pressures. *Fuel* **2015**, *159*, 98–106. [\[CrossRef\]](#)
9. Lhuillier, C.; Brequigny, P.; Contino, F.; Rousselle, C. Combustion Characteristics of Ammonia in a Modern Spark-Ignition Engine. In *Conference on Sustainable Mobility*; Technical Report; SAE International: Warrendale, PA, USA, 2019. [\[CrossRef\]](#)
10. Carsten Jespersen, M.; Østerby Holst Rasmussen, T.; Ivarsson, A. Widening the operation limits of a SI engine running on neat ammonia. *Fuel* **2024**, *358*, 130159. [\[CrossRef\]](#)
11. Mounaïm-Rousselle, C.; Mercier, A.; Brequigny, P.; Dumand, C.; Bouriot, J.; Houillé, S. Performance of ammonia fuel in a spark assisted compression Ignition engine. *Int. J. Engine Res.* **2022**, *23*, 781–792. [\[CrossRef\]](#)
12. Reggeti, S.; Kane, S.; Northrop, W. Experimental Investigation of Spark-Assisted Compression-Ignition with Ammonia-Hydrogen Blends. *J. Ammon. Energy* **2023**, *1*, 91–105. [\[CrossRef\]](#)

13. Lhuillier, C.; Brequigny, P.; Contino, F.; Rousselle, C. Performance and Emissions of an Ammonia-Fueled SI Engine with Hydrogen Enrichment. In *14th International Conference on Engines & Vehicles*; Technical Report; SAE International: Warrendale, PA, USA, 2019. [\[CrossRef\]](#)
14. Frigo, S.; Gentili, R. Analysis of the behaviour of a 4-stroke Si engine fuelled with ammonia and hydrogen. *Int. J. Hydrogen Energy* **2013**, *38*, 1607–1615. [\[CrossRef\]](#)
15. Koike, M.; Suzuoki, T.; Takeuchi, T.; Homma, T.; Hariu, S.; Takeuchi, Y. Cold-start performance of an ammonia-fueled spark ignition engine with an on-board fuel reformer. *Int. J. Hydrogen Energy* **2021**, *46*, 25689–25698. [\[CrossRef\]](#)
16. Kane, S.P.; Northrop, W.F. Thermochemical Recuperation to Enable Efficient Ammonia-Diesel Dual-Fuel Combustion in a Compression Ignition Engine. *Energies* **2021**, *14*, 7540. [\[CrossRef\]](#)
17. Dimitriou, P.; Javaid, R. A review of ammonia as a compression ignition engine fuel. *Int. J. Hydrogen Energy* **2020**, *45*, 7098–7118. [\[CrossRef\]](#)
18. Dupuy, A.; Brequigny, P.; Schmid, A.; Frapolli, N.; Mounaïm-Rousselle, C. Experimental study of RCCI engine—Ammonia combustion with diesel pilot injection. *J. Ammon. Energy* **2023**, *1*, 11–20. [\[CrossRef\]](#)
19. Hiraoka, K.; Matsunaga, D.; Kamino, T.; Honda, Y.; Toshinaga, K.; Murakami, Y.; Nakamura, H. Experimental and Numerical Analysis on Combustion Characteristics of Ammonia and Diesel Dual Fuel Engine. *SAE Int. J. Adv. Curr. Pract. Mobil.* **2024**, *6*, 1441–1458. [\[CrossRef\]](#)
20. Imamori, Y.; Takahashi, T.; Ueda, H.; Yamada, S.; Tanaka, T.; Kogure, R. Experimental and Numerical Investigations of Emission Characteristics from Diesel-Ammonia-Fueled Industry Engines. In *2023 JSAE/SAE Powertrains, Energy and Lubricants International Meeting*; Technical Report; Society of Automotive Engineers of Japan: Tokyo, Japan, 2023.
21. Liu, J.; Wang, X.; Zhao, W.; Sun, P.; Ji, Q. Effects of ammonia energy fraction and diesel injection parameters on combustion stability and GHG emissions characteristics in a low-loaded ammonia/diesel dual-fuel engine. *Fuel* **2024**, *360*, 130544. [\[CrossRef\]](#)
22. Rousselle, C.M.; Brequigny, P.; Dupuy, A. Impact of Splitting n-Dodecane Pilot Injection on Ammonia RCCI Engine. In *16th International Conference on Engines & Vehicles*; Technical Report; SAE International: Warrendale, PA, USA, 2023. [\[CrossRef\]](#)
23. Mi, S.; Wu, H.; Pei, X.; Liu, C.; Zheng, L.; Zhao, W.; Qian, Y.; Lu, X. Potential of ammonia energy fraction and diesel pilot-injection strategy on improving combustion and emission performance in an ammonia-diesel dual fuel engine. *Fuel* **2023**, *343*, 127889. [\[CrossRef\]](#)
24. Sforza, L.; Ballerini, A.; Ramognino, F.; Schirru, A.; Lucchini, T.; D’Errico, G.; Dupuy, A.; Rabello de Castro, R.; Brequigny, P.; Mounaïm-Rousselle, C. A numerical study of ammonia combustion in spark-ignition and reactive-fuel pilot-ignition engines. *J. Ammon. Energy* **2024**, *2*, 73–84. [\[CrossRef\]](#)
25. Novella, R.; Pastor, J.; Gomez-Soriano, J.; Sánchez-Bayona, J. Numerical study on the use of ammonia/hydrogen fuel blends for automotive spark-ignition engines. *Fuel* **2023**, *351*, 128945. [\[CrossRef\]](#)
26. Shin, J.; Park, S. Numerical analysis for optimizing combustion strategy in an ammonia-diesel dual-fuel engine. *Energy Convers. Manag.* **2023**, *284*, 116980. [\[CrossRef\]](#)
27. Yao, N.N.; Chen, Y.F.; Wei, L.M.; Xu, Q.Y.; Pan, W.G. Progress in CFD simulation for ammonia-fueled internal combustion engines and gas turbines. *J. Energy Inst.* **2025**, *119*, 101951. [\[CrossRef\]](#)
28. Serrano, J.R.; Novella, R.; Climent, H.; Arnau, F.J.; Calvo, A.; Thorsen, L. Computational Analysis of an Ammonia Combustion System for Future Two-Stroke Low-Speed Marine Engines. *J. Mar. Sci. Eng.* **2024**, *13*, 39. [\[CrossRef\]](#)
29. D’Antuono, G.; Lanni, D.; Galloni, E.; Fontana, G. Comparison of the Performance and Operation Limits of an S.I. Engine Fueled with Neat Ammonia and Hydrogen-Ammonia Blends. In *16th International Conference on Engines & Vehicles*; Technical Report; SAE International: Warrendale, PA, USA, 2023. [\[CrossRef\]](#)
30. Zhao, D.; Gao, W.; Li, Y.; Fu, Z.; Hua, X.; Zhang, Y. Simulation Study on Combustion Performance of Ammonia-Hydrogen Fuel Engines. *Energies* **2024**, *17*, 2337. [\[CrossRef\]](#)
31. Marinoni, A.; Tamborski, M.; Cerri, T.; Montenegro, G.; D’Errico, G.; Onorati, A.; Piatti, E.; Pisoni, E.E. 0D/1D Thermo-Fluid Dynamic Modeling Tools for the Simulation of Driving Cycles and the Optimization of IC Engine Performances and Emissions. *Appl. Sci.* **2021**, *11*, 8125. [\[CrossRef\]](#)
32. Tabaczynski, R.J.; Ferguson, C.R.; Radhakrishnan, K.B. A Turbulent Entrainment Model for Spark-Ignition Engine Combustion. In *Proceedings of the SAE 1977 Transactions-V86-A*, Tulsa, OK, USA, 6–9 June 1977.
33. Ballerini, A.; D’Errico, G.; Nodi, A.; Buttitta, M.; Marmorini, L. Quasi-Dimensional Simulation of a Turbulent Jet Ignition Combustion in High-Performance High-Speed Motorcycle Engine. In *SETC2025: 29th Small Powertrains and Energy Systems Technology Conference*; Technical Report; SAE International: Warrendale, PA, USA, 2025. [\[CrossRef\]](#)
34. Fogla, N.; Bybee, M.; Mirzaeian, M.; Millo, F.; Wahiduzzaman, S. Development of a K-k- ϵ Phenomenological Model to Predict In-Cylinder Turbulence. *SAE Int. J. Engines* **2017**, *10*, 562–575. [\[CrossRef\]](#)
35. Gülder, O.L. Turbulent premixed flame propagation models for different combustion regimes. *Symp. (Int.) Combust.* **1991**, *23*, 743–750. [\[CrossRef\]](#)

36. Herweg, R.; Maly, R.R. A Fundamental Model for Flame Kernel Formation in S. I. Engines. In *Proceedings of the International Fuels & Lubricants Meeting & Exposition*; SAE International: Warrendale, PA, USA, 1992. [\[CrossRef\]](#)
37. Sforza, L.; Lucchini, T.; Gianetti, G.; D'Errico, G. Development and Validation of SI Combustion Models for Natural-Gas Heavy-Duty Engines. In *Proceedings of the 14th International Conference on Engines & Vehicles*, Napoli, Italy, 15–19 September 2019. [\[CrossRef\]](#)
38. Tamborski, M.; D'Errico, G.; Lucchini, T.; Cerri, T.; Onorati, A. A Constant Equivalence Ratio Multi-Zone Approach for a Detailed and Fast Prediction of Performances and Emission in CI Engines. *SAE Int. J. Adv. Curr. Pract. Mobil.* **2022**, *4*, 1815–1827. [\[CrossRef\]](#)
39. Tamborski, M.; D'Errico, G.; Lucchini, T.; Onorati, A. Detailed prediction of HRR and NO_x emissions in CI engines via a novel thermodynamic model with constant equivalence ratio zones. *Int. J. Engine Res.* **2023**, *24*, 2315–2337. [\[CrossRef\]](#)
40. Ballerini, A.; D'Errico, G.; Onorati, A.; Tamborski, M. Extension and Validation of a Constant Equivalence Ratio Multi-Zone Approach to DME Combustion in Vessels and CI Engines. In *Proceedings of the WCX SAE World Congress Experience*, Detroit, MI, USA, 18–20 April 2023. [\[CrossRef\]](#)
41. Woschni, G. A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in the Internal Combustion Engine. In *Proceedings of the National Fuels and Lubricants, Powerplants, Transportation Meetings*, Pittsburgh, PA, USA, 30 October 1967; p. 670931. [\[CrossRef\]](#) [\[PubMed\]](#)
42. Lavoie, G.A.; Heywood, J.B.; Keck, J.C. Experimental and Theoretical Study of Nitric Oxide Formation in Internal Combustion Engines. *Combust. Sci. Technol.* **1970**, *1*, 313–326. [\[CrossRef\]](#)
43. Musculus, M.P.B.; Kattke, K. Entrainment Waves in Diesel Jets. *SAE Int. J. Engines* **2009**, *2*, 1170–1193. [\[CrossRef\]](#)
44. Abramovich, G.N.; Schindel, L. Jet of an Incompressible Fluid in a Coflowing External Stream. In *The Theory of Turbulent Jets*; The MIT Press: Cambridge, MA, USA, 2003. [\[CrossRef\]](#)
45. Naber, J.; Siebers, D.L. Effects of Gas Density and Vaporization on Penetration and Dispersion of Diesel Sprays. In *International Congress & Exposition*; SAE International: Warrendale, PA, USA, 1996; p. 960034. [\[CrossRef\]](#)
46. Livengood, J.C.; Wu, P.C. Correlation of autoignition phenomena in internal combustion engines and rapid compression machines. *Symp. (Int.) Combust.* **1955**, *5*, 347–356. [\[CrossRef\]](#)
47. Mancaruso, E.; Todino, M.; Vaglieco, B.M. Study on dual fuel combustion in an optical research engine by infrared diagnostics varying methane quantity and engine speed. *Appl. Therm. Eng.* **2020**, *178*, 115623. [\[CrossRef\]](#)
48. Azimov, U.; Tomita, E.; Kawahara, N. Combustion and Exhaust Emission Characteristics of Diesel Micro-Pilot Ignited Dual-Fuel Engine. In *Diesel Engine—Combustion, Emissions and Condition Monitoring*; Bari, S., Ed.; IntechOpen: London, UK, 2013; Section 2. [\[CrossRef\]](#) [\[PubMed\]](#)
49. Frerichs, J.; Eilts, P. A New Combustion Model for Medium Speed Dual-Fuel Engines in the Course of 0D/1D Simulation. *Methane* **2022**, *1*, 158–176. [\[CrossRef\]](#)
50. Yang, R.; Yan, Y.; Liu, Z.; Liu, J. Formation and Evolution of Thermal and Fuel Nitrogen Oxides in the Turbulent Combustion Field of Ammonia Internal Combustion Engines. In *WCX SAE World Congress Experience*; Technical Report; SAE International: Warrendale, PA, USA, 2023. [\[CrossRef\]](#)
51. Ma, T.; Feng, W.; Sun, X.; Chen, G.; Jing, G. Numerical study of NO_x formation mechanism in ammonia-hydrogen compound fuel marine engines under varying conditions. *Int. J. Hydrogen Energy* **2024**, *91*, 1422–1434. [\[CrossRef\]](#)
52. Goodwin, D.G.; Moffat, H.K.; Schoegl, I.; Speth, R.L.; Weber, B.W. *Cantera: An Object-Oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes*; Zenodo: Geneva, Switzerland, 2025. [\[CrossRef\]](#)
53. Stagni, A.; Arunthanayothin, S.; Dehue, M.; Herbinet, O.; Battin-Leclerc, F.; Bréquigny, P.; Mounaïm-Rousselle, C.; Faravelli, T. Low- and intermediate-temperature ammonia/hydrogen oxidation in a flow reactor: Experiments and a wide-range kinetic modeling. *Chem. Eng. J.* **2023**, *471*, 144577. [\[CrossRef\]](#)
54. Liu, J.; Ulishney, C.; Dumitrescu, C.E. On the Conversion of Diesel Engines to Dedicated Ammonia: Lean, Stoichiometric or Rich Operation. *Energy Proc.* **2022**, *26*. [\[CrossRef\]](#)
55. Morel, V.; Won, H.W.; Kumar, D.; Tarot, M.; Mounaïm-Rousselle, C.; Bréquigny, P.; Bouriot, J.; Houille, S. Towards the Optimization of the Piston Design for a Premixed Ammonia Combustion Engine with a CFD Modelling Approach. In *Internationaler Motorenkongress 2023*; Heintzel, A., Ed.; Series Title: Proceedings; Springer Fachmedien: Wiesbaden, Germany, 2024; pp. 257–272. [\[CrossRef\]](#)
56. Westlye, F.R.; Ivarsson, A.; Schramm, J. Experimental investigation of nitrogen based emissions from an ammonia fueled SI-engine. *Fuel* **2013**, *111*, 239–247. [\[CrossRef\]](#)
57. Feng, Y.; Zhu, J.; Mao, Y.; Raza, M.; Qian, Y.; Yu, L.; Lu, X. Low-temperature auto-ignition characteristics of NH₃/diesel binary fuel: Ignition delay time measurement and kinetic analysis. *Fuel* **2020**, *281*, 118761. [\[CrossRef\]](#)
58. Zhang, Y.; Zhou, W.; Liang, Y.; Yu, L.; Lu, X. An experimental and detailed kinetic modeling study of the auto-ignition of NH₃/diesel mixtures: Part 1—NH₃ substitution ratio from 20% to 90%. *Combust. Flame* **2023**, *251*, 112391. [\[CrossRef\]](#)
59. Zhang, Y.; Liang, Y.; Zhou, W.; Yu, L.; Lu, X. An experimental and detailed kinetic modeling study of the auto-ignition of NH₃/diesel mixtures: Part 2—Wide pressures up to 120bar. *Combust. Flame* **2024**, *259*, 113131. [\[CrossRef\]](#)

60. Qiao, L.; Wang, H.; Chen, P.; Gu, M.; Luo, K.; Hu, X. The influence mechanism of CO₂ on the transformation of nitrogen-containing components in ammonia-coal co-firing: An experimental and kinetic mechanism investigation. *Combust. Flame* **2026**, *283*, 114585. [[CrossRef](#)]
61. Frassoldati, A.; Faravelli, T.; Ranzi, E. Kinetic modeling of the interactions between NO and hydrocarbons at high temperature. *Combust. Flame* **2003**, *135*, 97–112. [[CrossRef](#)]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.