



Numerical Investigation of Combustion Mechanisms and Emission Trade-Offs in a Two-Stroke Direct- Injection Ammonia/Diesel Dual-Fuel Marine Engine

Thesis for the Degree of Master of Science

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Abstract

This study investigates the combustion and emission characteristics of a two-stroke, direct-injection ammonia/diesel dual-fuel compression-ignition engine under low-load conditions relevant to large marine engines. Although ammonia is carbon-free and can reduce direct CO₂ emissions, its low reactivity, strong evaporation cooling, and nitrogen chemistry may cause incomplete combustion, NH₃ slip, and N₂O formation. A closed-cycle CFD framework was therefore applied using an Eulerian–Lagrangian spray formulation, a modified gRNG k - ε turbulence model, detailed spray sub-models, and a 69-species/389-reaction ammonia/ n -heptane kinetic mechanism. One diesel-only case and three ammonia/diesel cases with ammonia injection durations of 3 ms, 4 ms, and 5 ms were simulated, corresponding to ammonia energy ratios up to 49.4%. The model was assessed against experimental data and reference simulations, followed by analyses of grid independence, engine performance, emissions, combustion processes, and swirl ratio sensitivity.

The simulations reproduce the main combustion and emission trends with acceptable accuracy. Increasing ammonia injection duration and ammonia energy ratio increases the second-stage heat release from ammonia oxidation and raises indicated mean effective pressure from 1.84 bar to 3.70 bar. Carbon-related emissions decrease per energy input, but incomplete ammonia oxidation increases NH₃ slip and N₂O emission, causing total greenhouse-gas-equivalent emissions to rise from 79.0 g/MJ to 192.9 g/MJ. In-cylinder analysis shows that ammonia combustion depends on its engulfment by the diesel flame, while colder or weakly connected hot regions promote unburned ammonia and N₂O. The swirl ratio analysis indicates that moderate swirl improves spray–flame interaction, whereas excessive swirl over-disperses the fuel, resulting in incomplete combustion. Among the tested cases, a swirl ratio of 15 gives the best overall emission balance. This study concludes that cleaner ammonia/diesel operation requires not only a higher ammonia energy ratio, but careful control of spray interaction, turbulent mixing, ignition structure, and nitrogen chemistry.

Keywords: Marine engine; Ammonia/diesel dual fuel; Direct dual-fuel stratification; Computational fluid dynamics; Greenhouse-gas emissions; Ammonia slip; Swirl ratio

Popular Science Summary

Large ships need powerful engines, but they also need cleaner fuels. Ammonia is considered promising because it contains no carbon and can reduce direct CO₂ emissions. However, ammonia is difficult to burn: it ignites poorly, burns slowly, cools the surrounding gas during evaporation, and may form harmful emissions if combustion is incomplete. This study looks into a two-stroke marine engine where diesel and liquid ammonia are directly injected into the cylinder, asking whether replacing part of the diesel with ammonia truly makes the engine cleaner.

The answer is not simply yes. Adding ammonia increases engine load and reduces carbon-based emissions such as CO and CO₂ for a fixed engine power output. However, more ammonia also makes complete combustion harder. Some ammonia remains unburned as ammonia slip, and some forms nitrous oxide, i.e., N₂O, a much stronger greenhouse gas than CO₂. In the ammonia/diesel cases, total greenhouse-gas-equivalent emissions increase even though direct carbon emissions decrease. This means that a carbon-free fuel does not automatically lead to a climate-friendly engine.

The simulations show that diesel works as the ignition source for ammonia. Ammonia burns effectively only when its spray meets the hot diesel flame in the right region and at the right time. If ammonia enters colder parts of the cylinder or misses the most reactive flame zone, it burns incompletely, producing ammonia slip and N₂O. This study also shows that air swirl inside the cylinder must be carefully controlled. Moderate swirl improves mixing and helps ammonia burn, while excessive swirl spreads the fuel into colder regions and worsens combustion. Among the tested cases, a swirl ratio of 15 gives the best balance.

Overall, ammonia can help decarbonize marine engines, but the path forward is not simply to inject more ammonia, while it is to make engine design ensure more complete ammonia combustion so that the whole system will become cleaner in reality, not just on paper.

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Last but not least, Chairman Mao once wrote in his poetry: "To count the truly great figures, one must look to the present age." I would like to dedicate these words to myself and to all the readers who have reached this point. May we all find meaning, achieve something worthwhile, and strive forward with courage and determination amid the profound changes of our time, unseen in a century.

Zichen Qiu
Lund, June 2026

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Nomenclature

Abbreviations

Acronym	Description
ADDF	Ammonia/Diesel Dual-Fuel
AER	Ammonia Energy Ratio
AHRR	Apparent Heat Release Rate
ALE	Arbitrary Lagrangian–Eulerian
ATDC	After Top Dead Centre
CA	Crank Angle
CCM	Chemistry Coordinate Mapping
CFD	Computational Fluid Dynamics
CI	Compression Ignition
DDFS	Direct Dual-Fuel Stratification
DICI	Direct-Injection Compression-Ignition
DI	Direct Injection
DME	DiMethyl Ether
DNS	Direct Numerical Simulation
EL	Eulerian–Lagrangian
GHG	GreenHouse Gas
GWP	Global Warming Potential
gRNG	generalized ReNormalization Group
HC	HydroCarbon
ICE	Internal Combustion Engine
ID	Injection Duration
IMEP	Indicated Mean Effective Pressure
KH	Kelvin–Helmholtz
LES	Large Eddy Simulation
LHV	Lower Heating Value
PPC	Partially Premixed Combustion
PPm	Parts Per million
RANS	Reynolds-Averaged Navier–Stokes
RCCI	Reactivity-Controlled Compression Ignition
RNG	ReNormalization Group
RT	Rayleigh–Taylor
SOI	Start Of Injection
SR	Swirl Ratio
TDC	Top Dead Centre
WSR	Well-Stirred Reactor

Symbols

Symbol	Description
CH_4	Methane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
H	Hydrogen Radical
H_2	Hydrogen
HNO	Nitroxyl
H_2O	Water
N_2	Nitrogen
NH	Imidogen Radical
NH_2	Amidogen Radical
NH_3	Ammonia
NO	Nitric Oxide
NO_2	Nitrogen Dioxide
NO_x	Nitrogen Oxides
N_2O	Nitrous Oxide
O_2	Oxygen
I	Identity Tensor
t	Time
k - ε model	Two-equation turbulence model based on turbulent kinetic energy k and turbulent dissipation rate ε

1 Introduction

1.1 Background

The continuous increase in anthropogenic greenhouse gas (GHG) emissions has created an urgent call for a switch to low-carbon energy [1]. Internal combustion engines (ICEs) remain indispensable in sectors like heavy-duty transport and marine propulsion, since they can provide high power density, robust operation, and compatibility with existing infrastructure [2, 3]. However, their dependence on fossil fuels results in direct emissions of carbon oxides, nitrogen oxides, and some other pollutants. Compared with light-duty road transport, maritime transport is more difficult to electrify due to its long operating range, huge carrying capacity, and high installed power. Therefore, the development of low-carbon fuels for marine engines is a key pathway toward reducing GHG emissions from the maritime sector [4].

Large two-stroke low-speed compression-ignition (CI) engines are of particular interest because they are widely used in ocean-going vessels, and exhibit high efficiency, economy, and reliability [5]. Their slow speed, large cylinder volume, and direct-injection (DI) architecture make them attractive platforms for alternative liquid fuels. At the same time, the scale of these engines means that even a partial replacement of conventional marine fuels can have a significant environmental impact. For such reasons, two-stroke ammonia/diesel dual-fuel (ADDF) combustion has become a technically important research direction for future marine propulsion [5].

Ammonia, NH_3 , is considered a promising carbon-free fuel and hydrogen carrier [6]. Unlike hydrocarbon fuels, ammonia contains no carbon atom in its molecular structure, so complete oxidation does not directly form CO_2 . What's more, ammonia is synthesized from hydrogen and nitrogen, where the hydrogen can be produced by various renewable routes, thus achieving decarbonization of the overall ammonia production [7, 8, 9, 10]. Compared with hydrogen, ammonia is easier to liquefy, has a higher volumetric energy density under practical storage conditions, and benefits from a mature global production, storage, and transportation infrastructure [6, 10]. These characteristics make ammonia not only a fuel but also a chemical energy carrier suitable for long-distance transport and large-scale energy storage.

Nevertheless, as discussed in Table 1.1, ammonia is a challenging fuel for CI engines. It has a low lower heating value (LHV) on a mass basis, low chemical reactivity, high autoignition temperature, low laminar flame speed, narrow flammability range, and large latent heat of vaporization [5, 9, 11]. These properties hinder autoignition and flame propagation. In DI applications, liquid ammonia evaporation can also cause strong local cooling, which lowers the local gas temperature and delays chemical reactions [12]. As a result, pure ammonia operation in conventional CI engines is difficult, and a high-reactivity pilot fuel is usually required to initiate and stabilize combustion.

Table 1.1 Key fuel properties relevant to ammonia/diesel dual-fuel compression-ignition combustion [5]

Property	Ammonia	Hydrogen	Diesel	Comments
Density @ 1 bar, 25 °C (kg/m ³)	0.718	0.0837	849	Density will affect fuel delivery, jet penetration, and in-cylinder mixing characteristics.
Lower heating value (MJ/kg)	18.8	120	45	The low LHV of ammonia requires a larger fuel mass to achieve the same energy input.
Latent heat of vaporization (kJ/kg)	1370	455	232.4	High ammonia latent heat can cause strong charge cooling and influence ignition delay.
Boiling point (°C)	−33.34	−252.7	282–338	The low boiling point of ammonia promotes evaporation but may also induce flash-boiling effects.
Autoignition temperature (K)	930	773–850	527–558	The high autoignition temperature of ammonia makes diesel pilot ignition necessary.
Laminar flame speed @ $\varphi = 1.0$ (cm/s)	7	351	86	The very low ammonia flame speed may slow flame propagation and reduce combustion completeness.
Flammability limit φ	0.63–1.4	0.1–7.1	0.8–6.5	The relatively narrow ammonia flammability range limits stable combustion under lean conditions.
Stoichiometric air–fuel ratio by mass	6.05	34.6	14.5	The low stoichiometric air–fuel ratio of ammonia changes air demand and mixture equivalence ratio.
Adiabatic flame temperature (°C)	1800	2110	2300	Lower ammonia flame temperature can reduce thermal NO _x formation but may weaken combustion intensity.

Ammonia combustion also introduces a specific emission problem. Some recent research [3, 13] shows that increasing the ammonia energy ratio (AER) reduces conventional emissions such as CO_2 , but it substantially increases N_2O and unburned ammonia. In particular, N_2O has a very high global warming potential (GWP) and may offset the climate benefit of replacing carbonaceous fuel if its formation is not controlled [1, 14]. It reveals a fundamental trade-off: ammonia adoption and carbon reduction do not automatically imply an improvement in the greenhouse effect. This study is thereby motivated by this trade-off. ADDF combustion offers a realistic pathway for decarbonizing large marine engines, but its success depends on whether ammonia can be burned efficiently without excessive N_2O , ammonia slip, or combustion instability. Therefore, the core scientific issue is the coupling among liquid-ammonia injection, spray interaction, turbulent mixing, and emission control in a two-stroke direct-injection compression-ignition (DICI) engine.

1.2 Literature Review

Since ammonia is difficult to auto-ignite, most practical CI concepts use a reactive pilot fuel such as diesel, dimethyl ether (DME), or hydrogen [15]. The pilot fuel supplies high-temperature combustion products and active radicals that promote ammonia oxidation [16]. Nowadays, two major strategies are commonly investigated.

1.2.1 Premixed Ammonia Port Injection

One widely investigated approach is reactivity-controlled compression ignition (RCCI), in which ammonia is premixed with the intake air, and a small amount of high-reactivity fuel is injected directly to initiate ignition [17]. The high-reactivity pilot fuel forms locally reactive zones that trigger the oxidation of the lower-reactivity ammonia/air mixture.

The advantage of RCCI is that a large fraction of the total fuel energy can be supplied by ammonia while retaining a reliable ignition source. However, ammonia RCCI combustion is constrained by incomplete ammonia oxidation and near-wall flame quenching [14]. Xu et al. [18] investigated an ADDF marine engine using the RCCI concept and showed that directly replacing premixed natural gas with ammonia at the same low diesel energy share caused poor combustion efficiency. Increasing the diesel fraction improved combustion stability, but also increased carbon-containing emissions. This indicates that ammonia fraction alone is not an adequate optimization target, while the amount and timing of pilot fuel must be sufficient to support complete ammonia oxidation [19].

Numerical investigations [14, 20] have further shown that the combustion structure of ammonia RCCI differs from conventional hydrocarbon dual-fuel systems. They showed that unburned ammonia tends to originate from near-wall regions, the cylinder centre and crevice zones, whereas N_2O is closely associated with the quenched ammonia flame front. This highlights the importance of low-temperature zones in nitrogen-containing GHG

formation. Xu and Bai [20] also demonstrated that ammonia/hydrogen/n-heptane RCCI operation can tolerate a significant AER, but excessive ammonia substitution deteriorates combustion efficiency unless reactivity is enhanced by hydrogen addition.

High-fidelity numerical simulations have provided additional insight into the fundamental flame structures of ammonia/diesel combustion. Direct numerical simulation (DNS) studies [21, 22] identified multiple reaction layers, including lean premixed flames, rich premixed flames, diffusion flames, and rich ammonia oxidation layers. These layers have different roles in fuel conversion and emission formation. Lean premixed ammonia oxidation can be an important source of NO, while diffusion-flame and rich-ammonia regions may either consume or produce nitrogen-containing intermediates depending on local temperature, equivalence ratio, and radical availability. Therefore, ammonia dual-fuel combustion cannot be understood only through global equivalence ratio or total fuel energy; instead, it requires local analysis of reaction-zone interaction.

1.2.2 Liquid Ammonia Direct Injection

Another important strategy is direct liquid ammonia injection combined with diesel pilot ignition [3, 11, 12, 13, 23]. In this method, ammonia and diesel are injected directly into the cylinder, and the combustion process is governed by spray penetration, evaporation, turbulent mixing, and the spatial overlap between the ammonia spray and diesel flame. It is attractive for marine two-stroke engines because it preserves the DI architecture of large CI engines while allowing fuel stratification to be controlled by injection timing and injector geometry [12]. This strategy is also known as direct dual-fuel stratification (DDFS). Through improving the fuel injection scheme, DDFS can combine the benefits of RCCI and partially premixed combustion (PPC) [24]. Besides, proper coordination between diesel and ammonia injection can shorten ammonia combustion duration, improve thermal efficiency, and mitigate excessive NO_x formation [25].

Zhang et al. [26] experimentally investigated a two-stroke low-speed engine using an ammonia/diesel dual DI strategy. Their results showed that diesel injection timing can effectively control the phasing of ammonia combustion because the diesel flame provides the heat and radicals required to ignite ammonia. This work also demonstrates that, in DI ammonia engines, combustion is not dominated by homogeneous ammonia autoignition but by jet-controlled pilot ignition and subsequent flame development. The studies [3, 26] further showed that increasing AER at low load can reduce conventional pollutants such as CO, CO₂, and soot, while dramatically increasing N₂O emissions and total GHG-equivalent emissions. The interpretation is that ammonia ignition depends on its engulfment by the diesel flame [27]. When ammonia and diesel sprays interact favorably, ammonia can burn during the mixing-controlled combustion stage. However, if part of the ammonia spray escapes the high-temperature diesel-flame region or is cooled near the wall, slow oxidation and incomplete combustion promote ammonia slip and N₂O formation.

Xu et al. [27] studied ammonia/diesel spray interaction in a constant-volume vessel under engine-relevant conditions and proposed further insight for DDFS. In early interaction cases, the diesel flame encounters a relatively fuel-rich ammonia/air mixture and can ignite it directly. This leads to self-sustained ammonia flame propagation and substantial heat release. In late interaction cases, ammonia has more time to evaporate and mix with air, producing a leaner and less reactive mixture that may fail to ignite or may extinguish after partial oxidation. Such quenching promotes N_2O formation near the flame front.

Recent developments [13, 27, 28] have emphasized that the relative timing and spatial arrangement of ammonia and diesel sprays are decisive for combustion completeness, which is supported by full-engine computational fluid dynamics (CFD) studies. Lewandowski et al. [12] simulated direct liquid-ammonia injection in a CI engine and showed that injection timing strongly influences evaporation, cooling, mixture formation, combustion efficiency, and exhaust emissions. Very early injection may increase the risk of over-dilution, wall interaction, and low-temperature ammonia zones, whereas appropriately timed late injection can improve interaction with the pilot flame. Pedersen et al. [29] further showed that N_2O accumulation is associated with incomplete combustion, wall cooling, ammonia-rich low-temperature pockets, and slow oxidation during the expansion stroke. These studies indicate that DI ammonia/diesel operation should be optimized as a controlled stratification problem rather than as a simple fuel-substitution problem.

Overall, the literature shows that ammonia dual-fuel combustion is feasible but highly sensitive to the interaction between fuel properties, injection strategy, turbulent mixing, wall cooling, and chemical kinetics. A successful engine strategy must ensure that ammonia-rich regions encounter sufficiently hot and reactive diesel-flame environments before the expansion stroke reduces temperature and suppresses oxidation.

1.3 Knowledge Gap and Research Goals

Although recent studies have advanced the understanding of ammonia dual-fuel combustion, several knowledge gaps remain. First, much of the available literature focuses on RCCI concepts, constant-volume vessels, or four-stroke engines, while fewer studies address two-stroke low-speed DICI configurations representative of marine propulsion. Second, direct liquid ammonia injection presents strong coupling among spray interaction, turbulent mixing, and chemical kinetics. These coupled processes are difficult to interpret using experimental measurements alone. Third, ammonia substitution introduces a new emission trade-off. Increasing AER and reducing CO_2 emission do not necessarily lead to a lower total climate impact. Thus, a rigorous evaluation of ammonia/diesel marine engines must include both combustion efficiency and GHG-equivalent emissions.

To address these gaps, this study investigates combustion and emission characteristics in a two-stroke direct-injection compression-ignition ammonia/diesel dual-fuel engine. It follows a low-load operating range relevant to large marine engines, with diesel direct

injection used as the ignition source and liquid ammonia direct injection used as the carbon-free main energy carrier. The main research goals are as follows:

- To establish a physically consistent framework for analysing ADDF combustion in a two-stroke DICI engine.
- To examine how increasing AER affects engine performance and emission characteristics under fixed diesel-pilot support.
- To evaluate the emission trends of NO_x , N_2O , unburned NH_3 , CO , and CO_2 , with special attention to the trade-off between carbon-emission reduction and nitrogen-related GHG penalties.
- To interpret physical mechanisms responsible for incomplete in-cylinder combustion, ammonia slip, and N_2O formation.
- To give instructive engineering implications for future ammonia-fuelled marine engines.

The central objective of this study is therefore not simply whether ammonia can replace part of diesel fuel, but under what in-cylinder conditions ammonia substitution can provide a meaningful carbon benefit without causing unacceptable losses in combustion efficiency or excessive N_2O -dominated GHG emissions. The following sections develop the methodology, operating cases, numerical framework, and analysis procedure used to address this question.

2 Methodology

2.1 Governing Equations

The numerical model adopted in this study is formulated for a compressible, turbulent, multicomponent, two-phase reacting flow in a moving-piston engine cylinder. The in-cylinder gas phase is treated as an Eulerian continuum, whereas liquid ammonia and diesel sprays are represented by Lagrangian computational parcels. The two phases are coupled through interphase exchange terms of mass, momentum, species, and energy. This Eulerian–Lagrangian (EL) formulation is widely used in two-phase combustion [30], because it provides a practical compromise between physical fidelity and computational cost for high-pressure fuel injection, evaporation, turbulent mixing, and combustion simulations.

Since the piston motion continuously changes the cylinder volume, the governing equations are written in an arbitrary Lagrangian–Eulerian (ALE) form [31]. In this formulation, the convective transport is expressed with the relative velocity between the gas phase and the moving mesh. This treatment is essential for closed-cycle engine simulations because compression and expansion alter both the computational domain and the thermodynamic state of the trapped charge. In the present ammonia/diesel dual-fuel engine, the ALE description also allows the direct coupling of spray injection, evaporation, ignition, and pollutant formation with the piston-induced volume change.

2.1.1 Gas-Phase Conservation Equations

The gas phase is governed by the conservation equations of mass, momentum, chemical species, and sensible enthalpy. The source terms in these equations account for the exchange between the evaporating liquid spray and the surrounding gas. For ammonia/diesel DI combustion, such coupling is particularly important because liquid ammonia has strong evaporation cooling effects and can significantly alter local temperature, mixture composition, ignition delay, and nitrogen-containing emission formation.

The gas-phase continuity equation is written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho(\mathbf{u} - \mathbf{u}_g)] = S_m \quad (2.1)$$

where ρ is the gas density, $\mathbf{u}$ is the gas velocity, $\mathbf{u}_g$ is the mesh velocity, and S_m is the mass source term caused by fuel evaporation.

Equation (2.1) expresses the conservation of gas-phase mass in a moving control volume. The velocity appearing in the convective flux is $\mathbf{u} - \mathbf{u}_g$, indicating that mass transport is evaluated relative to the moving mesh. The source term S_m is positive when liquid

droplets evaporate and add vapour to the gas phase. In the present dual-fuel configuration, S_m includes both diesel-vapour and ammonia-vapour contributions, and therefore directly controls the formation of local fuel-rich or fuel-lean regions.

The gas-phase momentum equation is:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot [\rho \mathbf{u}(\mathbf{u} - \mathbf{u}_g)] = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{S}_u \quad (2.2)$$

where p is the thermodynamic pressure, $\boldsymbol{\tau}$ is the effective viscous stress tensor, and $\mathbf{S}_u$ denotes the interphase momentum source term due to the liquid spray.

Equation (2.2) describes the transport of momentum under the combined effects of pressure force, viscous, turbulent stress, and spray–gas momentum exchange. The source term $\mathbf{S}_u$ is generated mainly by droplet drag. During high-pressure diesel and ammonia injection, droplets transfer momentum to the gas, inducing local jet motion, entrainment, and turbulence. These effects influence the spatial overlap between the diesel flame and ammonia-rich mixtures, which is one of the key factors controlling ammonia ignition and subsequent combustion completeness.

For a Newtonian fluid with a turbulent eddy-viscosity closure, the effective stress tensor is expressed as:

$$\boldsymbol{\tau} = \mu_{\text{eff}} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3}(\nabla \cdot \mathbf{u})\mathbf{I} \right] \quad (2.3)$$

where

$$\mu_{\text{eff}} = \mu + \mu_t \quad (2.4)$$

Here, μ is the molecular dynamic viscosity, and μ_t is the turbulent eddy viscosity.

Equation (2.3) gives the deviatoric stress tensor used in the momentum equation. The effective viscosity includes both molecular transport and turbulence-enhanced momentum transport. In engine flows, molecular viscosity alone is insufficient to describe mixing because the flow is dominated by swirl, squish, jet entrainment, and compression-induced turbulence. Therefore, the turbulent viscosity μ_t plays a vital role in representing unresolved turbulent transport in the Reynolds-averaged Navier-Stokes (RANS) framework.

The transport equation for the mass fraction of species i is:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot [\rho Y_i(\mathbf{u} - \mathbf{u}_g)] = -\nabla \cdot \mathbf{J}_i + \dot{\omega}_i + S_{Y_i} \quad (i = 1, \dots, N_s) \quad (2.5)$$

where Y_i is the mass fraction of species i , $\mathbf{J}_i$ is the diffusive flux, $\dot{\omega}_i$ is the chemical source

term, S_{Y_i} is the species source term associated with spray evaporation, and N_s is the total number of species.

Equation (2.5) is essential for predicting both fuel conversion and pollutant formation. For ammonia/diesel combustion, the species set must include major reactants and products, such as NH_3 , O_2 , N_2 , H_2O , CO and CO_2 , as well as nitrogen-containing intermediates and pollutants such as NH_2 , NH , HNO , NO , NO_2 and N_2O . The term S_{Y_i} introduces ammonia-vapour and diesel-vapour species into the gas phase, while $\dot{\omega}_i$ determines their chemical production and consumption. Therefore, accurate prediction of N_2O and ammonia slip requires both a proper spray model and a sufficiently detailed nitrogen chemistry mechanism.

The diffusive flux can be approximated using a gradient-diffusion formulation:

$$\mathbf{J}_i = -\rho D_{i,\text{eff}} \nabla Y_i \quad (2.6)$$

where $D_{i,\text{eff}}$ is the effective diffusivity, including molecular and turbulent contributions.

Equation (2.6) represents the transport of species due to concentration gradients. In RANS engine simulations, unresolved turbulent mixing is usually included through an effective diffusivity. This approximation is particularly relevant in the present engine because the local ammonia concentration depends strongly on turbulent entrainment and mixing with hot diesel-combustion products.

The sensible enthalpy equation is written as:

$$\frac{\partial(\rho h_s)}{\partial t} + \nabla \cdot [\rho h_s (\mathbf{u} - \mathbf{u}_g)] = \frac{Dp}{Dt} + \nabla \cdot (\lambda_{\text{eff}} \nabla T) - \nabla \cdot \left(\sum_i h_i \mathbf{J}_i \right) + \dot{Q}_{\text{chem}} + S_h \quad (2.7)$$

where h_s is the sensible enthalpy, T is the gas temperature, λ_{eff} is the effective thermal conductivity, h_i is the specific enthalpy of species i , $\dot{Q}_{\text{chem}}$ is the chemical heat-release term, and S_h is the energy source term associated with spray evaporation and interphase heat transfer.

Equation (2.7) describes the thermal evolution of the gas mixture. The pressure-work term Dp/Dt accounts for compression and expansion effects, which are dominant in reciprocating engines. The conduction term represents molecular and turbulent heat diffusion, whereas the enthalpy-diffusion term accounts for heat carried by species diffusion. The chemical heat-release term raises the local temperature during diesel and ammonia oxidation. The spray energy source S_h is especially important for liquid ammonia because its evaporation can remove a large amount of heat from the surrounding gas. This local cooling may delay ignition, weaken ammonia flame propagation, and promote the survival

of intermediate species such as N_2O in low-temperature regions.

The thermodynamic state of the multicomponent gas is closed by the ideal-gas equation of state:

$$p = \rho R_u T \sum_i \frac{Y_i}{W_i} \quad (2.8)$$

where R_u is the universal gas constant, and W_i is the molecular weight of species i .

Equation (2.8) relates pressure, density, temperature, and composition. Since the molecular weights of ammonia, oxygen, nitrogen, water vapour, carbon dioxide, and intermediate species differ, the mixture gas constant changes during combustion. This equation is therefore required to couple chemical conversion, heat release, pressure rise, and density variation in the cylinder.

2.1.2 Turbulence Model

The in-cylinder flow of a two-stroke DI engine is highly turbulent due to swirl motion, piston-induced compression, spray entrainment, and rapid heat release. Resolving all turbulent scales in a full engine simulation is computationally prohibitive for multi-case parametric studies. Therefore, this study adopts a RANS approach, and a modified generalized renormalization group (gRNG) k - ε model is used as the turbulence closure [32]. Compared with standard k - ε models, the gRNG formulation is more suitable for compressing and expanding engine flows because it introduces additional corrections for strong strain and variable-density effects.

The transport equation for turbulent kinetic energy k is:

$$\frac{\partial(\rho k)}{\partial t} + \nabla \cdot [\rho k(\mathbf{u} - \mathbf{u}_g)] = P_k - \rho \varepsilon + \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] \quad (2.9)$$

where k is the turbulent kinetic energy, P_k is the production term of turbulent kinetic energy that is proportional to the mean flow strain rate, ε is the turbulent dissipation rate, and σ_k is the turbulent Prandtl number for k .

Equation (2.9) states that turbulent kinetic energy is generated by mean velocity gradients, dissipated into internal energy at small scales, and transported by molecular and turbulent diffusion. In the ammonia/diesel engine, P_k is strongly affected by spray-induced shear, swirl, and squish flow. A higher k generally enhances fuel–air mixing and can improve the probability that ammonia-rich regions interact with the diesel flame. However, excessive mixing may also produce overly lean ammonia mixtures that are difficult to ignite.

The transport equation for turbulent dissipation rate ε is:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \cdot [\rho\varepsilon(\mathbf{u} - \mathbf{u}_g)] = C_{\varepsilon 1} \frac{\varepsilon}{k} P_k - C_{\varepsilon 2} \rho \frac{\varepsilon^2}{k} + \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + R_{\text{RNG}} \quad (2.10)$$

where $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, σ_ε are model constants, and R_{RNG} is the RNG correction term.

Equation (2.10) determines the rate at which turbulent kinetic energy is dissipated. The first source term represents the generation of dissipation associated with turbulence production, the second term represents dissipation destruction, and the third term accounts for diffusive transport. The RNG correction term improves model behaviour under rapidly strained flows, which are common during engine compression, injection, and combustion.

The turbulent viscosity is calculated as:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (2.11)$$

where C_μ is a model coefficient.

Equation (2.11) provides the Boussinesq eddy-viscosity closure. It connects unresolved turbulent momentum transport to the resolved mean velocity field. A larger k or smaller ε leads to a larger turbulent viscosity and stronger turbulent transport. The same turbulent scale information is also used to estimate turbulent diffusion of heat and species.

2.1.3 Engine Performance and Emissions

The computed flow and combustion fields are further post-processed to obtain engine performance and emission indicators. These quantities allow direct comparison between different AERs and provide a compact description of how fuel substitution affects combustion phasing, work output and GHG-equivalent emissions.

The apparent heat release rate (AHRR) is obtained from the in-cylinder pressure trace by using a single-zone thermodynamic approximation:

$$\frac{dQ_{\text{app}}}{d\theta} = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} \quad (2.12)$$

where Q_{app} is the apparent heat release, θ is the crank angle, V is the instantaneous cylinder volume, and γ is the ratio of specific heats.

Equation (2.12) is derived from the first law of thermodynamics for a closed engine cylinder. The first term represents the contribution associated with piston work, while the second term represents the internal-energy change inferred from the pressure rise. Although heat transfer and crevice losses are not explicitly separated in this apparent formulation, it

remains a standard and useful metric for identifying ignition timing, combustion duration, and the relative contributions of diesel and ammonia combustion.

The indicated mean effective pressure (IMEP) is calculated as:

$$\text{IMEP} = \frac{1}{V_d} \oint p \, dV \quad (2.13)$$

where V_d is the engine displacement volume.

Equation (2.13) represents the indicated work per cycle normalized by displacement volume. It is a load-related parameter that allows different cases to be compared independently of engine size. In ADDF operation, IMEP reflects the combined effect of diesel pilot combustion, ammonia energy addition, combustion efficiency, and heat-release phasing.

The ammonia energy ratio (AER) is defined as:

$$\text{AER} = \frac{m_{\text{NH}_3} \text{LHV}_{\text{NH}_3}}{m_{\text{NH}_3} \text{LHV}_{\text{NH}_3} + m_d \text{LHV}_d} \quad (2.14)$$

where m_{NH_3} and m_d are the injected ammonia and diesel masses per cycle, and LHV_{NH_3} and LHV_d are their corresponding LHVs.

Equation (2.14) quantifies the fraction of total fuel energy supplied by ammonia. A higher AER indicates greater replacement of carbonaceous diesel fuel and therefore a stronger potential for direct CO_2 reduction. However, increasing AER also reduces the relative amount of high-reactivity pilot fuel and may worsen ammonia oxidation if diesel-flame support is insufficient. This trade-off is the key to evaluating ADDF engines.

The GHG-equivalent emission is evaluated as [1, 18]:

$$\text{GHG} = \text{CO}_2 + 28 \text{CH}_4 + 273 \text{N}_2\text{O} \quad (2.15)$$

Equation (2.15) converts the major GHG into a CO_2 -equivalent metric using weighting factors for methane and nitrous oxide. This metric is essential for ammonia combustion because CO_2 reduction alone does not guarantee a lower climate impact. In ammonia/diesel engines, N_2O can increase substantially in low-temperature or incompletely burned ammonia regions. Consequently, the total CO_2 -equivalent GHG emission may increase even when CO_2 decreases. This makes N_2O mitigation a primary objective in the design of ammonia-fuelled marine engines.

2.2 Computational Algorithm

2.2.1 CFD Solver

The CFD simulations were performed using an in-house solver named DDFSEngineFoam, which was developed based on the OpenFOAM v7 library. This solver is consistent with the code in the previous related work and was verified in prior cases [3]. In the standard release of OpenFOAM v7, piston motion is handled mainly through mesh deformation in the squish region. Under this strategy, the total number of computational cells remains unchanged, while the piston displacement is represented by compressing or stretching the existing mesh according to the piston moving direction. Although this approach is straightforward to implement, it can lead to considerable deterioration of mesh resolution and cell quality during compression and expansion. To avoid excessive cell distortion, preserve reasonable cell size and shape, and improve computational efficiency, an improved dynamic meshing procedure was introduced [3, 33]. In this method, mesh layers are added or removed according to the instantaneous piston position, rather than relying solely on continuous cell deformation.

2.2.2 Liquid-Phase Spray Model

As discussed in Section 2.1, diesel and ammonia sprays were modelled under the well-established EL approach. The gas phase was solved as a continuum in the Eulerian system, whereas the discrete liquid phase was tracked in the Lagrangian framework. From injection to complete vaporization, the spray droplets undergo a series of physical processes that are described by corresponding sub-models. These include Kelvin–Helmholtz (KH)/Rayleigh–Taylor (RT) breakup model, Ranz–Marshall correlation heat transfer model, Spalding evaporation model, a trajectory collision model, and a spray/wall interaction model. The hybrid KH/RT model was used to describe the disintegration of liquid parcels [34]. In this model, primary breakup is attributed to KH instability developing on the droplet or liquid-jet surface, while secondary breakup is predicted by combining the KH mechanism with RT instability induced by acceleration effects. Heat exchange between an individual droplet and the surrounding hot gas was calculated using the Ranz–Marshall correlation [35], and droplet evaporation was evaluated with the Spalding formulation [36]. Droplet–droplet collision was modelled using a trajectory-based approach [37], where the collision probability is determined from the position and velocity vectors of the droplets. The spray/wall interaction was simplified into stick and rebound behaviours [38]. Such a spray modelling framework has been demonstrated to capture diesel and ammonia spray characteristics under a range of operating conditions. More detailed descriptions of these sub-models can be found in previous studies [18, 18].

2.2.3 Chemical Kinetic Mechanism

A skeletal chemical kinetic mechanism containing 69 species and 389 reactions was employed to calculate the instantaneous reaction rates and to describe the formation and consumption of major emission species [39]. The mechanism was developed for ammonia/*n*-heptane blended fuels, where *n*-heptane is used as a surrogate fuel to represent the main combustion properties of diesel. This mechanism has been extensively validated against various experimental datasets, including species-concentration profiles, ignition delay times of diesel/ammonia mixtures, and laminar burning velocities of pure ammonia and ammonia/hydrogen mixtures. The interaction between turbulence and chemistry was treated using the well-stirred reactor (WSR) model. To accelerate the incorporation of chemical reaction rates into the species and energy transport equations, a speed-up algorithm known as the chemistry coordinate mapping (CCM) method was applied [40]. In the CCM approach, cells with similar thermochemical states are grouped in a six-dimensional chemistry phase space, and reaction rates are evaluated for these cell groups rather than independently for every computational cell. The phase-space coordinates consist of equivalence ratio, scalar dissipation rate, temperature, hydrogen-element mass fraction, ammonia mass fraction and *n*-heptane mass fraction. The hydrogen-element mass fraction was included as one coordinate because it reflects the effects of differential diffusion of hydrogen-containing species, especially H_2 and H radicals, which are important intermediates of ammonia and diesel combustion.

2.3 Boundary Conditions

Since this study focuses on in-cylinder combustion, ammonia/diesel spray interaction, and emission formation, the numerical calculation was performed as a closed-cycle simulation. The gas-exchange process was not explicitly resolved. Instead, the calculation started at -95° crank angle (CA) after top dead centre (ATDC) and ended at 100° CA ATDC, which covers the late compression, fuel injection, ignition, main combustion, and early expansion processes. Such closed-cycle treatment is consistent with the physical objective of this study. In a two-stroke engine, intake scavenging and exhaust gas discharge strongly affect the trapped charge state. However, the primary mechanisms investigated here, such as liquid ammonia evaporation, diesel pilot ignition, flame-assisted ammonia oxidation, NO_x formation and N_2O accumulation, mainly take place after port closure and before the late expansion stage. Accordingly, the computational domain was initialized at the beginning of the closed-cycle period using Zhang et al.'s experimental intake and boost conditions [26] as reference values.

The cylinder head, cylinder liner, and piston surfaces were treated as solid wall boundaries. A non-slip velocity condition was applied on all solid surfaces. The piston boundary moved according to the crank-slider kinematics of the engine, while the cylinder head and liner were fixed. Both the piston crown and cylinder head were geometrically simplified as flat

surfaces, which is able to reduce geometric complexity while preserving the dominant features of spray interaction and turbulent mixing in the central combustion chamber.

The initial flow field was assigned with a swirl motion to represent the in-cylinder air motion after scavenging. Xu et al. [3] showed that ammonia combustion in DDFS configuration is highly sensitive to swirl-enhanced mixing. When the swirl ratio is too low, the ammonia spray cannot interact sufficiently with the diesel flame, leading to poor ammonia oxidation. Once the swirl ratio exceeds approximately 10, ammonia combustion efficiency increases sharply and then approaches a plateau. Since the swirl number is not available in the experiments, an initial swirl ratio of 12 at -95°CA ATDC was adopted in most simulations of this study.

3 Experimental and Numerical Setup

3.1 Experimental Setup

The experiments were tested on a lab-scale, water-cooled, single-cylinder, two-stroke engine at Dalian University of Technology [26]. The engine was modified from a commercial engine to accommodate an ammonia/diesel dual direct-injection system. Major components, including the cylinder head, cylinder liner, and exhaust manifold, were redesigned to enable direct injection of liquid ammonia and diesel into the cylinder via two opposed injectors mounted on the cylinder head. The schematic layout of the engine test bench is shown in Figure 3.1, and the main engine parameters are listed in Table 3.1.

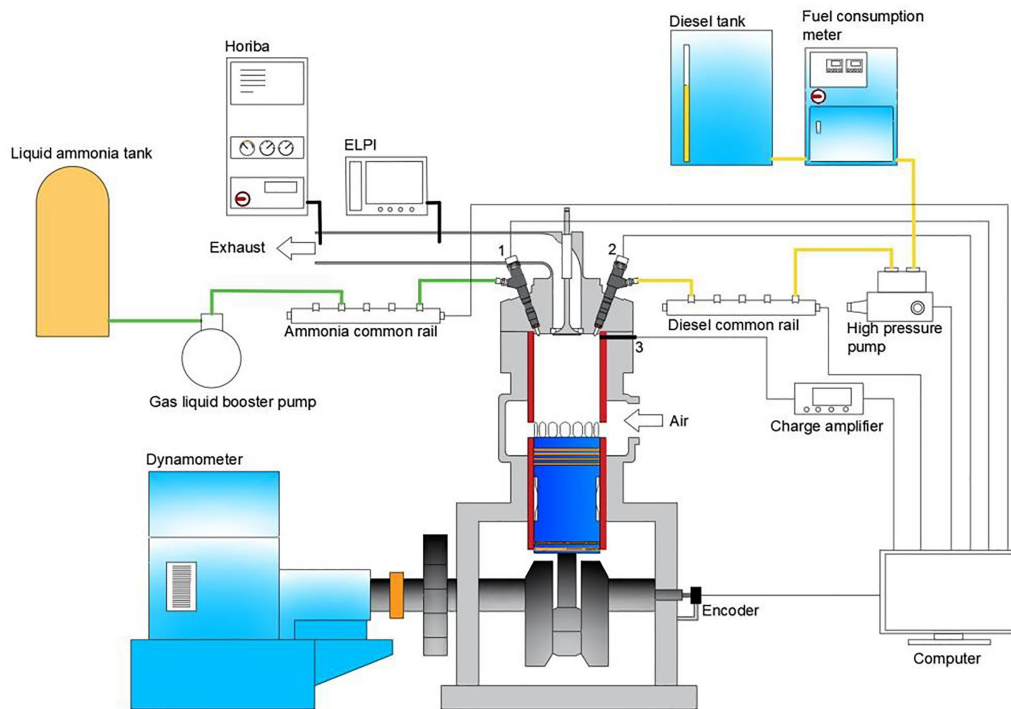


Figure 3.1 Schematic layout of engine test bench (1: liquid ammonia injector, 2: diesel injector, 3: Kistler pressure transducer) [26]

The engine was operated at a constant speed of 375 rpm, with a rated torque of 360 N·m and an effective compression ratio of 13.8:1. The exhaust port was open from approximately 110°CA ATDC to 265°CA ATDC, while the scavenging port was open from 130°CA ATDC to 230°CA ATDC. A simulated turbocharging system was used to control the intake air supply. The coolant and oil temperatures were maintained at approximately 80 °C by an external temperature-control system.

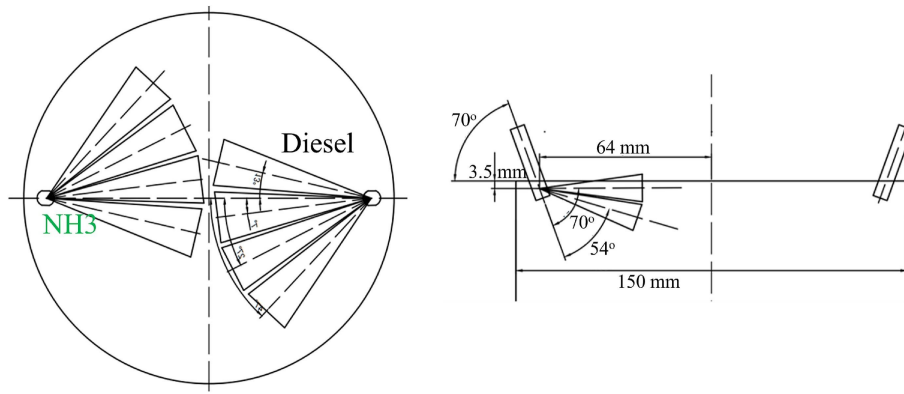
The in-cylinder pressure was measured using a Kistler pressure sensor mounted on the cylinder head, with a resolution of 0.5°CA. Exhaust species including CO, CO₂, O₂, unburned hydrocarbons (HCs) and NO_x were measured using a Horiba MEXA 7100D/EGR analyser. Following the manufacturer's standard procedures, the analyzer was calibrated

Table 3.1 Main engine parameters [3]

Parameters	Values
Injection pressure (MPa)	65 (ammonia)/100 (Diesel)
Bore and stroke (mm×mm)	150×225
Displacement (L)	3.97
Effective compression ratio	13.8
Engine speed (rpm)	375
Rated torque (N·m)	360
Simulated boost pressure (kPa)	135
Exhaust valve opening interval (°CA ATDC)	106–276
Coolant and oil temperature (°C)	80

before and after experiments, including both zero and span calibrations using certified calibration gases. The calibration deviation was within 2% of the calibration gas concentration, which confirmed the stability of this measurement system. For NO and CO, the measurement range was 0–1000 ppm, with an accuracy better than $\pm 2\%$ of the full-scale value. The exhaust sample was taken approximately 1 m downstream of the exhaust port, and a heated sampling line maintained at 191 °C was used to avoid condensation.

The dual-fuel supply system was designed for high-pressure direct injection of liquid-phase ammonia and diesel. The two injectors were symmetrically installed on the cylinder head, inclined by 30° relative to the cylinder axis and offset by 64 mm from the cylinder centre. The injector-hole plane was located 3.5 mm below the cylinder head. Each injector had four holes with a diameter of 0.17 mm. For each fuel, two sprays were arranged in the horizontal plane, while the other two were directed downward by 16°. Overall configuration of fuel injectors is illustrated in Figure 3.2.

**Figure 3.2** Layout of ammonia and diesel injectors and distribution patterns of both fuel sprays [3]

The injection pressure was 60 MPa for ammonia and 100 MPa for diesel. Four operating conditions were considered to investigate the effect of various ammonia/diesel fuel mass ratios under fixed injection timing. In all cases, diesel injection started at -8°CA ATDC , with an injection duration of 0.8 ms and an injected mass of 43.1 mg per cycle. For the ADDF cases, ammonia injection also started at -8°CA ATDC , while the ammonia

injection duration was varied from 3 ms to 5 ms. In the baseline Case 0, the ammonia injector was disabled and only diesel was injected. The detailed operating conditions are summarized in Table 3.2.

Table 3.2 Experimental and computational cases (SOI: start of injection, ID: injection duration, Φ_g : global equivalence ratio) [3]

Case	Diesel			Ammonia			AER	Φ_g	Engine IMEP (bar)
	SOI (°CA ATDC)	ID (ms)	Mass (mg/cyc)	SOI (°CA ATDC)	ID (ms)	Mass (mg/cyc)			
0	−8	0.8	43.1	−	0	0	0	0.215	1.84
1	−8	0.8	43.1	−8	3	62.3	37.5%	0.339	2.60
2	−8	0.8	43.1	−8	4	81.4	43.9%	0.378	3.19
3	−8	0.8	43.1	−8	5	103.7	49.4%	0.422	3.70

3.2 Numerical Setup

The interaction between ammonia and diesel sprays plays a significant role in determining the mixing, ignition, and emission characteristics. As introduced in Section 2.2.1, numerical simulations were carried out using a self-developed CFD solver to further investigate these interactions and their impact on engine performance and emissions. Since simulations are focused on the closed cycle spanning from -95°CA ATDC to 100°CA ATDC, the inlet and exhaust ports were not explicitly modelled during the CFD window, and both the intake and scavenging processes were neglected.

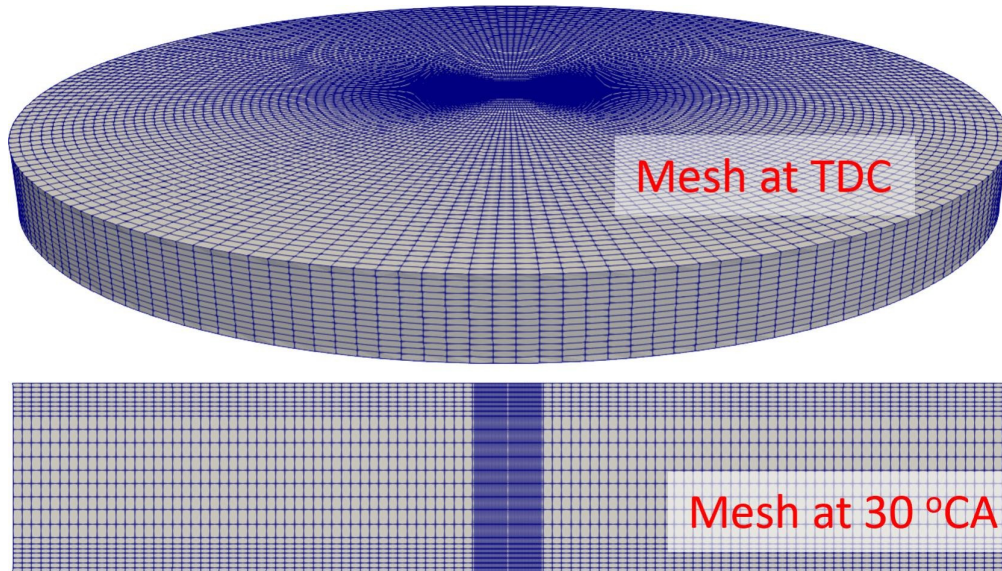


Figure 3.3 Piston geometry and computational meshes created for present simulations [3]

The computational mesh is shown in Figure 3.3. The mean grid size was around 1.25 mm, corresponding to approximately 168 thousand cells at TDC and nearly 1 million cells at -95°CA . This mesh resolution was selected based on previous engine CFD simulations [3, 18, 20], where a comparable grid size was found to offer a suitable balance between

grid independence and computational cost, while still providing reasonable predictions of in-cylinder pressure, heat release rate, and major emission trends. Nevertheless, in order to further ensure the reliability of the selected mesh resolution, a brief grid sensitivity analysis was performed in Section 4.1.

As discussed in Section 2.1.2, RANS model was used in this study because of its high computational efficiency, which is necessary for exploring a broader parameter space. Although alternative approaches such as large eddy simulation (LES) can provide higher accuracy, they generally require substantially greater computational resources, since multiple engine cycles are typically needed to obtain statistically averaged engine data.

Accurately modelling the spray and combustion behaviours of diesel remains challenging due to its complex chemical composition. Therefore, surrogate fuels such as *n*-heptane and *n*-dodecane are widely adopted in simulations to represent diesel combustion characteristics. However, the physical properties of *n*-heptane differ considerably from those of real diesel, which limits its capability to capture diesel spray behaviour. In the present simulations, *n*-heptane was used to represent the combustion characteristics of diesel, while the physical properties of *n*-hexadecane were employed to describe the spray process. Liquid ammonia properties are not included in the standard OpenFOAM v7 platform, so a customized thermophysical property library for ammonia fuel was developed to exactly model the evaporation process of liquid ammonia [27]. The relevant physical properties were obtained from the reference [41], and the modelling framework was validated against ammonia spray experiments in the previous work [27]. Additional details towards this numerical setup can be found in previous studies on ADDF engines [3, 18].

4 Results and Discussion

This section discusses numerical results of the two-stroke direct-injection ADDF engine. The analysis is organized in five parts. First, a grid independence test is conducted to ensure that numerical results are not significantly affected by mesh resolution. Second, the overall engine performance is evaluated by comparing the present simulations with both experimental measurements and reference simulations. Third, the emission characteristics are examined, with particular attention to the interaction among carbon-containing emissions, nitrogen oxides, nitrous oxide, and unburned ammonia. Fourth, the in-cylinder combustion process is illustrated from temperature and species distributions in order to clarify the physical mechanisms responsible for combustion development and emission formation. Finally, the sensitivity to swirl ratio is investigated to identify a more suitable flow condition for balancing ammonia conversion and emission reduction.

The four operating cases considered in this study have been mentioned in Table 3.2, including a pure-diesel baseline and three ADDF cases. In Case 0, only diesel is injected. In Cases 1–3, the diesel injection duration and timing are kept unchanged, while the ammonia injection duration is increased from 3 ms to 5 ms. This design allows the effect of increasing ammonia substitution to be isolated under fixed diesel-pilot support. Since ammonia has low chemical reactivity, high autoignition temperature, low flame speed, and strong evaporation cooling, its combustion in a CI engine depends strongly on whether the ammonia spray can interact effectively with the high-temperature diesel flame. Therefore, the following discussion links global indicators, such as pressure, heat release rate, and emissions, with the local in-cylinder mixing and reaction processes.

4.1 Grid Independence Test

Table 4.1 Mesh size information for the normal and fine grids

Mesh resolution	Min. cell volume (mm^3)	Cells at -95°CA ATDC	Cells at TDC
Normal grid	0.0335	936,390	168,070
Fine grid	0.0129	3,089,295	436,870

Before conducting the parametric analysis, it is necessary to verify that the numerical solution is sufficiently independent of the computational mesh. In this study, two sets of grids with different resolutions were used to verify grid independence, including one normal grid and one fine grid. Detailed grid size information can be found in Table 4.1. The two grids are compared using in-cylinder pressure and cylinder-mean temperature. These two variables were selected because they represent two essential aspects of the engine simulation. The pressure trace is a direct indicator of ignition timing, combustion phasing, total heat release, and indicated work output. It is also the basis for calculating the AHRR. The mean temperature is equally important because ammonia oxidation, NO

formation, and N_2O formation are all highly sensitive to the thermal history of the charge. If both pressure and temperature are insensitive to further grid refinement, the mesh can be considered adequate for the following performance and emission analysis.

As shown in Figure 4.1a, the pressure histories predicted by the normal and fine grids show very close agreement over the whole closed-cycle interval. The two curves nearly overlap during compression, around TDC, and throughout the expansion stroke. The peak pressure and its crank-angle location are almost unchanged after grid refinement, indicating that the main combustion phasing and the integrated heat release are already well captured by the normal grid. Since pressure is a global thermodynamic response of the whole cylinder, such agreement provides strong evidence that the normal grid has sufficient resolution for predicting engine load and combustion timing.

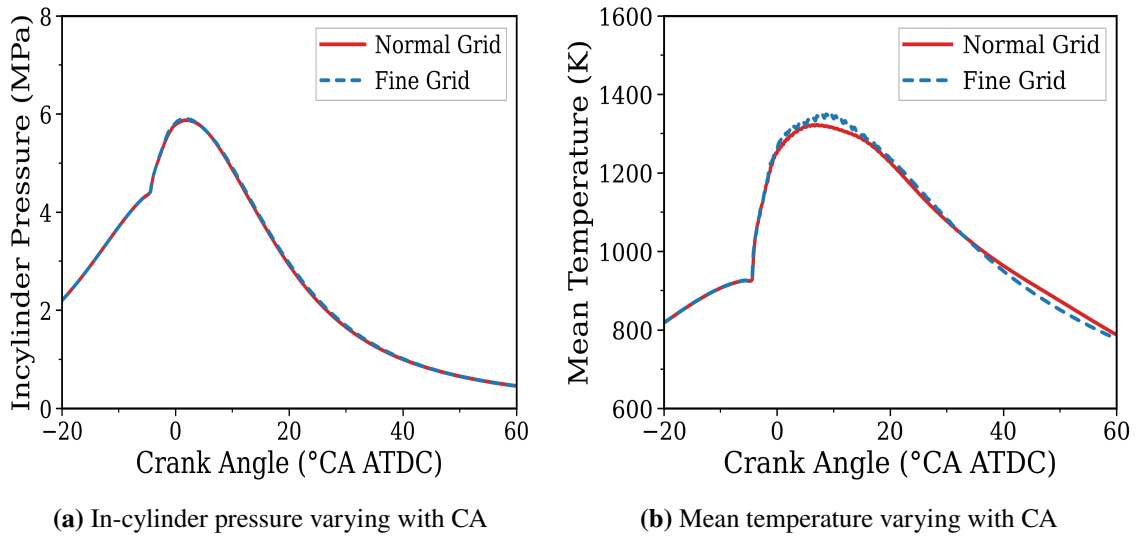


Figure 4.1 Grid independence measured by in-cylinder pressure and mean temperature

The mean-temperature comparison in Figure 4.1b shows slightly larger differences than the pressure comparison, but the overall agreement remains acceptable. Both grids predict the same thermal evolution, characterized by a gradual temperature increase during compression, a rapid temperature rise after ignition, a broad high-temperature region after TDC, and then a cooling during expansion. The fine grid produces a marginally higher peak mean temperature and a slightly faster temperature decrease in the late expansion stage. This difference is physically reasonable because temperature is more sensitive than pressure to local heat release distribution, turbulent mixing, wall heat transfer, and numerical diffusion. However, the difference is small compared with the overall temperature range, and it does not change the interpretation of the combustion process.

Therefore, the normal grid is adopted for all subsequent simulations. This selection is not only based on computational efficiency, but also on physical and methodological considerations. This study includes multiple operating cases and an additional swirl ratio sensitivity analysis; thus, using the fine grid for all cases would substantially increase the computational cost while providing only limited improvement in the key thermodynamic

indicators. Since the normal grid reproduces the pressure and temperature histories with sufficient accuracy, it offers a reasonable balance between numerical fidelity and computational affordability.

4.2 Overall Engine Performance

The overall engine performance is evaluated by comparing three datasets of experimental measurements from Zhang et al. [26], reference simulations from Xu et al. [3], and present simulations from this study. The experimental data provide the physical benchmark for the actual engine behaviour. The reference simulations provide an additional numerical baseline because they were performed for the same engine configuration and operating conditions. The present simulations are therefore assessed not only against experiments, but also against a previously validated numerical framework. This three-way comparison is useful because it helps determine whether the present model can reproduce both the measured trends and the level of predictive accuracy achieved in earlier work.

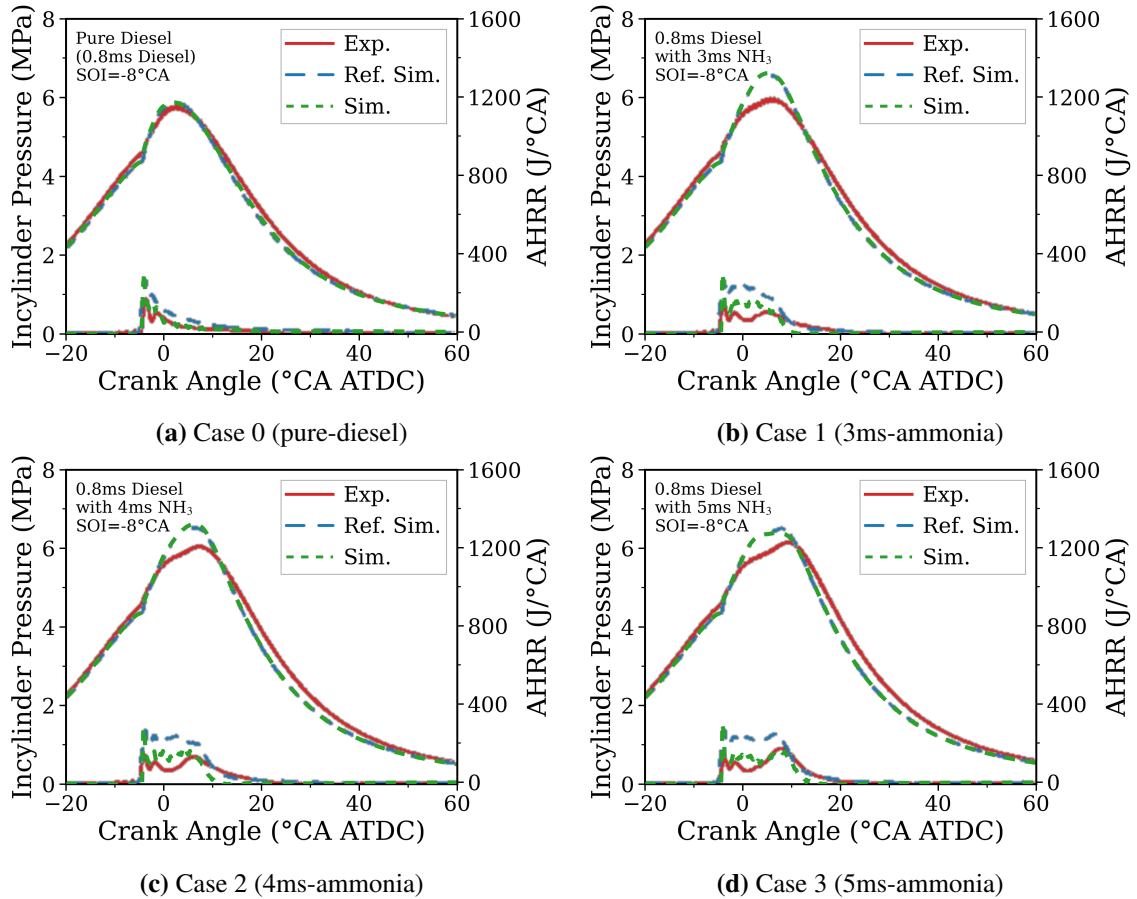


Figure 4.2 Three-way comparison (experiments, reference simulations, and current simulations) of in-cylinder pressure and AHRR varying with CA for Case 0–3

For the pure-diesel baseline case, i.e., Case 0 shown in Figure 4.2a, the agreement among the experiment, reference simulation, and present simulation is the best. The pressure traces are very close, and the main heat-release event occurs within a similar crank-angle

range, which indicates that the numerical model can reasonably reproduce the compression process, diesel spray ignition, and main diesel combustion behaviour. Since Case 0 does not involve ammonia evaporation, ammonia–diesel spray interaction, or nitrogen–fuel chemistry, it serves as a fundamental validation case for the thermodynamic and diesel-combustion framework.

When ammonia is introduced, the combustion process becomes more complex, and the discrepancies among the three datasets become more visible. In Cases 1–3 indicated separately in Figures 4.2b, 4.2c, and 4.2d, the present simulations still capture the general pressure level and combustion trend, but differences appear in AHRR. In particular, the simulated heat-release peaks are generally sharper than the experimental ones. This behaviour is reasonable for two main reasons. First, the experimental pressure curve is obtained from cycle-averaged measurements and is usually processed by filtering, which tends to smooth local fluctuations. In contrast, the simulation represents a deterministic numerical cycle, so localized heat-release features may remain more pronounced. Second, ammonia direct injection introduces additional uncertainties associated with liquid breakup, evaporation cooling, turbulent mixing, and the spatial overlap between ammonia vapour and diesel flame. These processes are represented through sub-models in the RANS framework and cannot be fully resolved at all relevant turbulent and chemical scales.

Despite these differences, the overall trends are physically consistent. Compared with Case 0, all ammonia/diesel cases exhibit a more evident two-stage heat-release structure. The first heat-release peak is mainly associated with diesel ignition. The second heat-release stage corresponds to ammonia combustion initiated by the high-temperature products and active radicals generated by diesel combustion. As the ammonia injection duration increases from Case 1 to Case 3, the second-stage heat release becomes stronger, and the in-cylinder pressure level increases accordingly. This shows that the injected ammonia is not simply diluted in the charge but increasingly participates in the energy release process.

The increase in engine load with ammonia injection can be explained by the larger total fuel energy input and the enhanced contribution of ammonia combustion. However, the contribution of ammonia is not automatic. Unlike diesel, ammonia does not readily auto-ignite under investigated conditions. Its oxidation depends on whether the ammonia-rich mixture can be entrained into sufficiently hot and reactive regions. Therefore, the pressure and heat release results suggest that the diesel flame plays a controlling role in determining ammonia ignition and combustion completeness.

The turbulent kinetic energy (k) distributions further support this interpretation. As demonstrated in Figure 4.3, compared with the pure-diesel case, the ammonia/diesel cases show more developed turbulent structures during the main combustion period. This is mainly caused by the additional momentum of the ammonia jet and its interaction with the diesel spray and surrounding gas. Higher turbulent kinetic energy can enhance entrainment and mixing, thereby increasing the probability that ammonia vapour encounters the diesel

flame. In Case 3, where the ammonia injection duration is the longest, the high-turbulence region is more extensive, which is consistent with the stronger second-stage heat release and higher engine load.

Nevertheless, stronger turbulence is not always beneficial for ammonia combustion. Moderate turbulence promotes ammonia–diesel interaction and accelerates fuel conversion. Excessive or poorly organized mixing may transport part of the ammonia into colder peripheral regions, where oxidation becomes slow or incomplete. This point becomes important when explaining emission characteristics and swirl ratio sensitivity. Overall, the engine performance results show that increasing ammonia injection duration improves engine output under fixed diesel-pilot support, but also makes the combustion process more dependent on the quality of spray interaction and turbulent mixing.

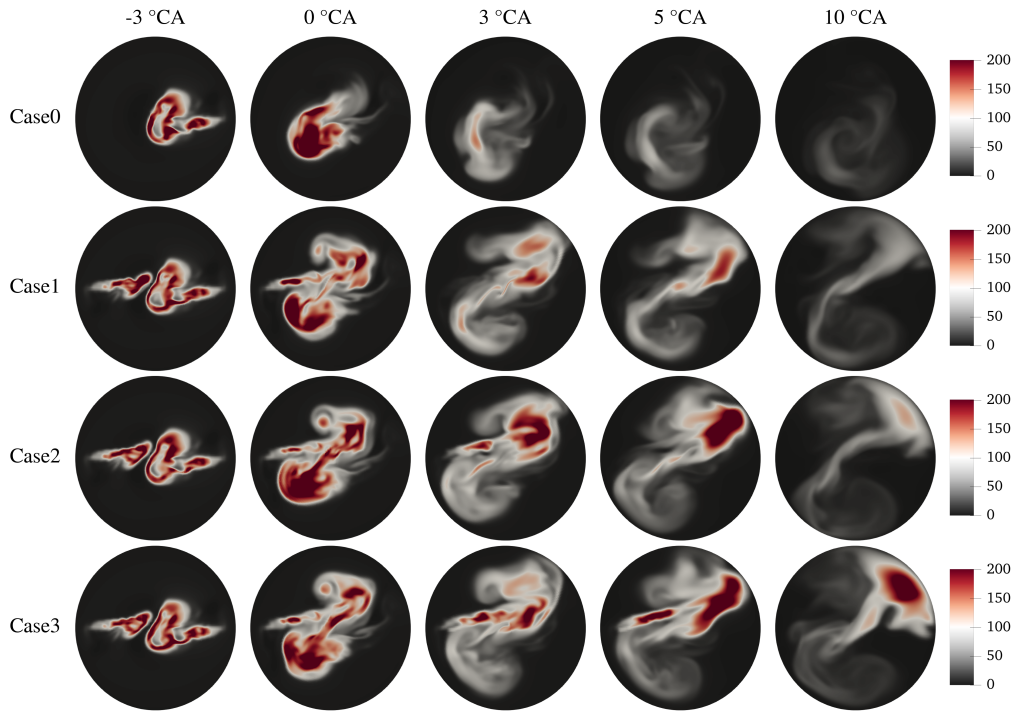


Figure 4.3 In-cylinder turbulence development for Case 0–3 at a plane 5 mm below the piston head

4.3 Emission Characteristics

The emission analysis begins with CO and NO, since these two species represent different aspects of combustion. CO is mainly related to incomplete oxidation of diesel fuel, whereas NO reflects high-temperature nitrogen chemistry and fuel-nitrogen conversion in ammonia combustion.

As shown in Figure 4.4a, CO emissions decrease significantly when ammonia is introduced. This trend is expected because, as ammonia injection duration increases, the total heat release and in-cylinder temperature can increase, which promotes the oxidation of CO to CO₂ in sufficiently hot and oxygen-rich regions.

Although CO emissions in the present simulations and the reference simulations generally agree with each other, they do not reproduce the exact experimental CO values in all cases. The simulations predict an increase in CO emissions as the injected amount of ammonia increases, whereas the experiments show the opposite. The discrepancy is acceptable because CO is highly sensitive to local late-cycle conditions. It can be produced in rich or low temperature regions and then oxidized only if the gas remains hot enough for a sufficient residence time. Small differences in predicted temperature, mixing, or expansion stage reaction rate can therefore cause noticeable differences in final CO emissions. In ammonia/diesel combustion, this sensitivity is further increased by the local cooling caused by ammonia evaporation and by the redistribution of diesel-derived intermediates through turbulent mixing.

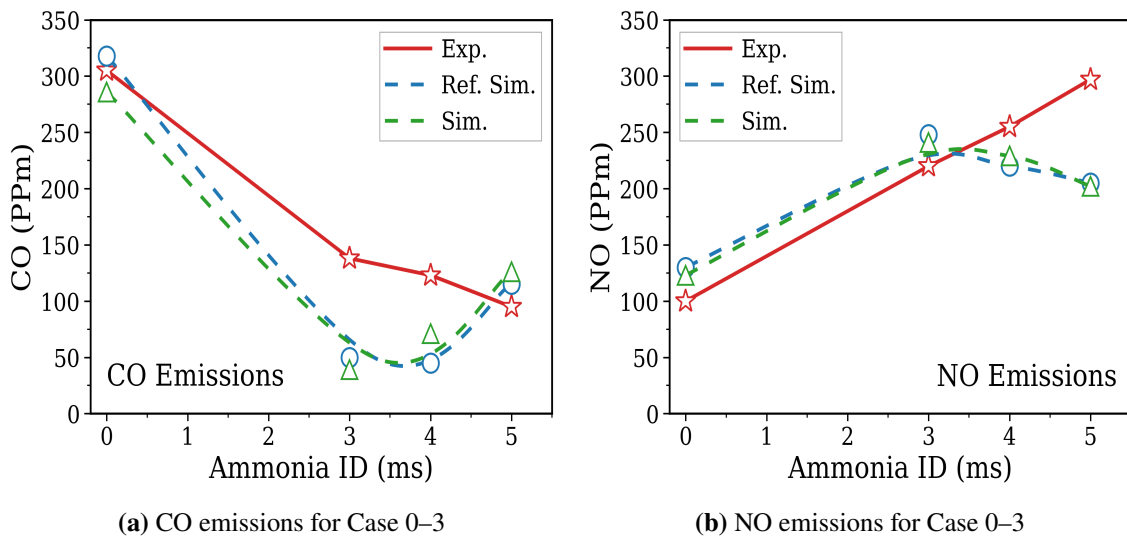


Figure 4.4 Three-way comparison (experiments, reference simulations, and current simulations) of CO and NO emissions for Case 0-3

The NO emissions in Figure 4.4b show a different trend, where NO increases with increasing ammonia injection duration. This increase is caused by two coupled mechanisms. First, higher heat release can increase the volume and duration of high-temperature regions, which favours thermal-NO formation. Second, ammonia itself contains nitrogen, so ammonia oxidation provides an additional fuel-NO pathway. As more ammonia is injected, more fuel-bound nitrogen becomes available for conversion into NO and other nitrogen-containing species.

The present simulations and the reference simulations capture the general increase from diesel baseline to ammonia-containing cases, but they do not perfectly reproduce the experimental magnitude at high ammonia injection duration. This difference can be attributed to the difficulty of predicting ammonia oxidation efficiency under strongly stratified conditions. If the simulation underestimates the amount of ammonia that burns in hot regions, it may also underpredict the associated NO formation. Furthermore, unburned ammonia can react with NO, converting it into species such as H_2O and N_2O through the de- NO_x pathway. Therefore, the observed differences are consistent with the known

modelling challenges of liquid-ammonia direct injection, turbulent spray interaction, and nitrogen chemistry.

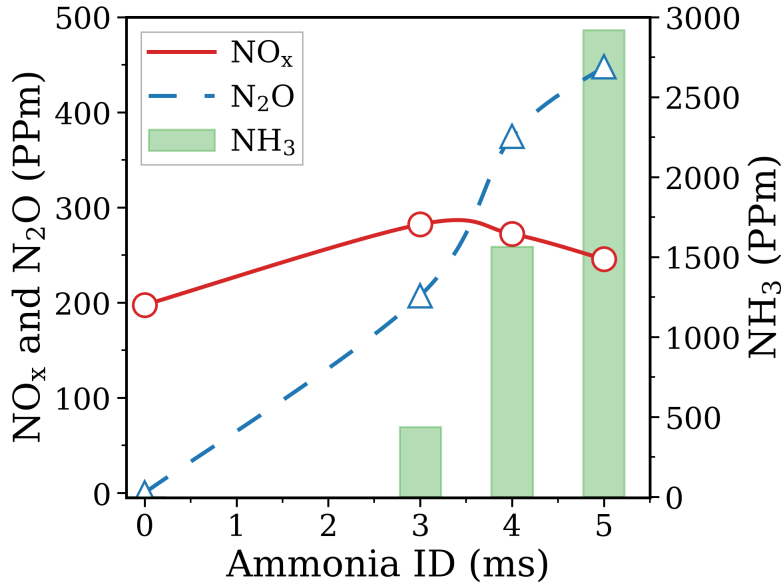


Figure 4.5 Combined trends of NO_x, N₂O and unburned NH₃ emissions for Case 0–3

The combined trends of NO_x, N₂O and NH₃ in Figure 4.5 reveal the central emission trade-off in ammonia/diesel combustion. With increasing ammonia injection duration, NH₃ slip increases strongly, indicating that a growing fraction of ammonia escapes complete oxidation. This occurs because the additional ammonia cannot always be fully engulfed by the diesel flame before the expansion stroke lowers the temperature and slows chemical reactions. Ammonia-rich regions that remain outside the main high-temperature zone are therefore prone to incomplete conversion.

At the same time, N₂O increases markedly with ammonia addition. N₂O is not a dominant product of pure diesel combustion, but it becomes important when partially oxidized ammonia exists in moderate or low temperature regions. These regions are sufficiently reactive to convert ammonia through intermediate nitrogen pathways, but not hot enough to completely decompose N₂O into N₂ or further oxidize it to NO. Therefore, N₂O formation is closely associated with incomplete ammonia oxidation and flame quenching.

The behaviour of NO_x is more complex. Increasing ammonia supply tends to promote NO_x formation through fuel-nitrogen chemistry, but unburned ammonia can also reduce NO through de-NO_x-type reactions during the expansion stroke. As a result, NO_x does not necessarily increase monotonically with ammonia injection in the simulations. Instead, part of the fuel nitrogen is redistributed among NO_x, N₂O and unburned NH₃. This redistribution is a key feature of ammonia combustion, showing that reducing one nitrogen-containing emission may increase another if the in-cylinder temperature and mixing conditions are not properly controlled.

Table 4.2 further quantifies the emission trade-off discussed above through listing sim-

Table 4.2 Emission data of key species from numerical simulations for Case 0–3 (the emission unit of various species is g/MJ_{total-fuel-energy}, the total GHG emissions are calculated as Equation (2.15))

Case	NO	NO ₂	NO _x	CO ₂	N ₂ O	CH ₄	GHG	CO	NH ₃	NH ₃ /NO _x
0	0.202	0.188	0.391	78.68	0.001	0.0026	78.97	0.439	0	0
1	0.257	0.068	0.326	44.81	0.325	0.0001	133.54	0.039	0.266	0.817
2	0.222	0.064	0.287	40.06	0.533	0.0004	185.63	0.065	0.861	3.006
3	0.178	0.058	0.236	35.54	0.576	0.0010	192.94	0.103	1.455	6.163

ulated emissions normalized by the total fuel energy input. With increasing ammonia injection duration, carbon-containing emissions are markedly reduced. The CO₂ emission decreases from 78.68 g/MJ in Case 0 to 35.54 g/MJ in Case 3, corresponding to a reduction of approximately 55%, which is mainly because the total energy input increases with increased ammonia injection while the amount of diesel injected remains constant. The CO emission also drops sharply from 0.439 g/MJ in Case 0 to 0.039 g/MJ in Case 1, indicating enhanced oxidation of carbonaceous intermediates under dual-fuel operation. However, CO rises slightly again to 0.103 g/MJ in Case 3, suggesting that local incomplete oxidation becomes more evident at higher ammonia injection duration due to stronger evaporation cooling, mixture stratification, and less favourable late-cycle reaction conditions.

The nitrogen-containing emissions show a more complex redistribution. The NO emission first increases from 0.202 g/MJ in Case 0 to 0.257 g/MJ in Case 1 because ammonia oxidation introduces an additional fuel-NO pathway, but then decreases to 0.178 g/MJ in Case 3. Meanwhile, NO₂ and total NO_x decrease from 0.188 g/MJ and 0.391 g/MJ to 0.058 g/MJ and 0.236 g/MJ respectively, implying stronger de-NO_x effects involving ammonia-derived radicals. In spite of that, this NO_x reduction is accompanied by pronounced increases in N₂O and unburned NH₃. From Case 0 to Case 3, N₂O rises from 0.001 g/MJ to 0.576 g/MJ, while NH₃ increases from zero to 1.455 g/MJ. The NH₃/NO_x ratio also increases from 0.817 in Case 1 to 6.163 in Case 3, showing a shift from a NO_x-dominated nitrogen-emission pattern toward one increasingly governed by ammonia slip. Thus, the decrease in NO_x should not be explained alone as an overall emission improvement. Instead, it reflects the redistribution of fuel-bound nitrogen among NO_x, N₂O and unburned NH₃ as incomplete ammonia oxidation becomes more significant.

The GHG-equivalent results further emphasize this point. As demonstrated in Figure 4.6, the total GHG-specific emissions increase from approximately 79.0 g/MJ in the pure-diesel baseline to about 133.5 g/MJ, 185.6 g/MJ and 192.9 g/MJ in Cases 1–3 respectively. Although ammonia addition reduces direct carbon-containing emissions per energy input, the increasing N₂O contribution dominates the total GHG-equivalent emission. The CH₄ contribution is negligible in comparison, while the CO₂-equivalent contribution decreases as more ammonia is injected to the engine. Therefore, the climate benefit of ammonia combustion is offset, or even reversed, by N₂O formation under the present

operating conditions.

This result has important implications. Ammonia cannot be evaluated as a carbon-free fuel only by considering CO₂ reduction. If ammonia oxidation is incomplete and substantial N₂O is produced, the total climate impact may increase despite lower carbon emissions. Therefore, the key challenge for ADDF engines is not simply to increase ammonia energy ratio, but to ensure that ammonia is consumed in sufficiently hot and reactive regions while suppressing N₂O and ammonia slip.

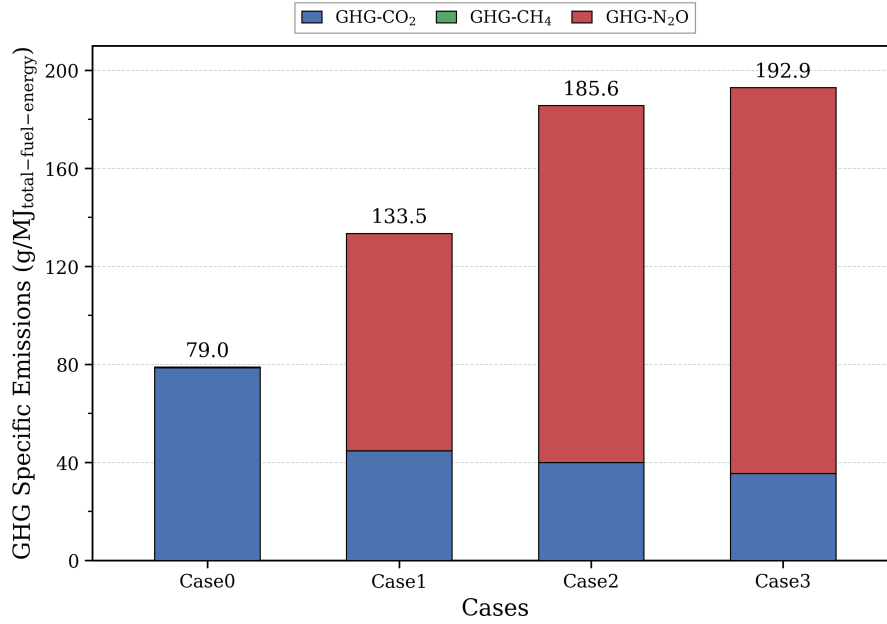


Figure 4.6 CO₂-equivalent GHG specific emissions based on Equation (2.15) for Case 0–3

4.4 Combustion Process Analysis

To understand the emission trends more deeply, the in-cylinder combustion process is analysed using the temperature and species distributions of Case 3, which is shown in Figure 4.7. Case 3 is selected because it has the longest ammonia injection duration and the highest ammonia energy contribution among the investigated cases. Therefore, it exhibits the most pronounced ammonia–diesel interaction, the strongest incomplete-ammonia-oxidation tendency, and the clearest formation of nitrogen-containing emissions.

At -3°CA ATDC, the temperature field already shows localized high-temperature regions generated by early diesel ignition. Meanwhile, the NH₃ distribution still retains a clear jet-like structure. This indicates that ammonia has not ignited independently at this stage. Instead, the combustion process is still governed by diesel pilot ignition. The NO field is limited to the hottest diesel-combustion regions, while N₂O is nearly absent. The CO distribution is also localized, reflecting early incomplete oxidation of diesel-derived carbonaceous intermediates.

From 0°CA to 3°CA ATDC, the main spray–flame interaction becomes more evident. The

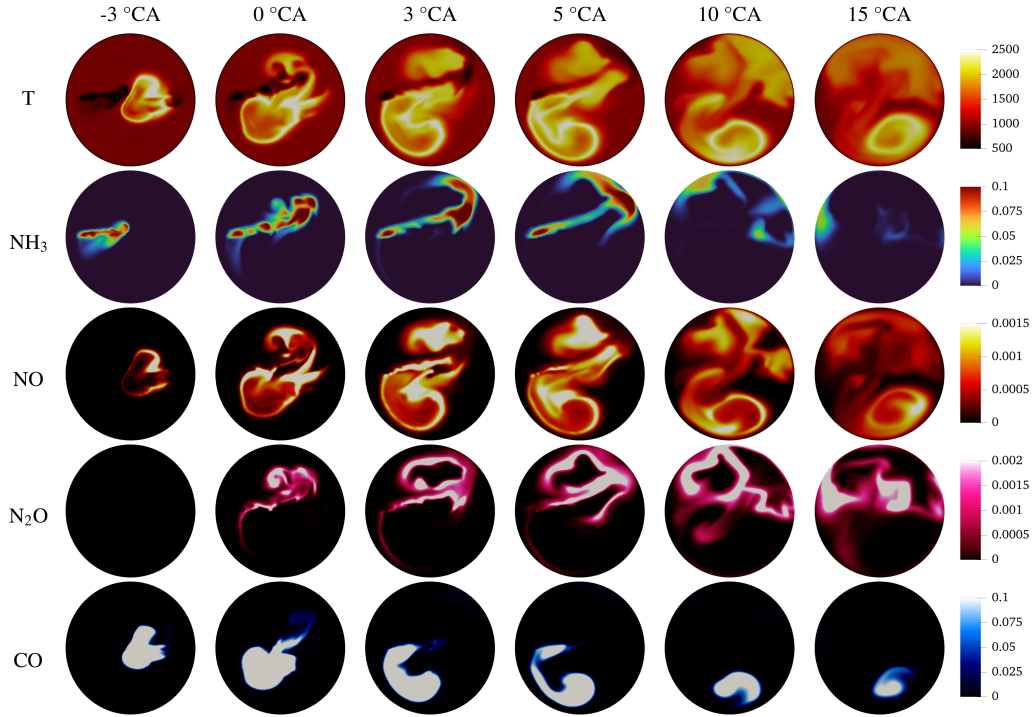


Figure 4.7 In-cylinder temperature and NH_3 , NO , N_2O , CO distributions for Case 3 at a plane 5 mm below the piston head

high-temperature region expands rapidly, and part of the ammonia-rich jet is entrained into the diesel-flame zone. This is the key stage for ammonia ignition. Where ammonia vapour is exposed to high temperature and active radicals from diesel combustion, its oxidation rate increases and contributes to the second-stage heat release observed in AHRR curves. However, the NH_3 field remains highly stratified, which means that not all ammonia experiences the same thermochemical environment. Some ammonia-rich pockets remain outside the most reactive region and are therefore more likely to survive into the later cycle.

At about 5°CA ATDC, the cylinder reaches the main dual-fuel combustion stage. The temperature field shows a broad high-temperature region, demonstrating that ammonia is now actively participating in heat release. The NO distribution becomes stronger in the hot reaction zones, where both thermal- NO and fuel- NO pathways are active. In contrast, N_2O appears preferentially around cooler, partially reacted regions rather than in the hottest core. This spatial separation is important. It shows that NO is mainly associated with high-temperature oxidation, whereas N_2O is associated with intermediate-temperature ammonia oxidation and flame-front regions.

During the later combustion stage, from approximately 10°CA to 15°CA ATDC, the expansion process reduces pressure and temperature. The reaction rates of ammonia oxidation decrease, and the opportunity for complete conversion becomes limited. The NH_3 field shows that residual ammonia remains in some regions, especially in zones that are relatively far from the strongest diesel-flame interaction. The N_2O field remains visible

because the lower temperature prevents its efficient destruction. In the meantime, the NO region becomes more diffuse, and part of the NO may be consumed by reactions with unburned ammonia. These processes explain why high-ammonia cases can simultaneously show ammonia slip, significant N_2O emissions and non-monotonic NO_x behaviour.

The combustion process analysis therefore provides a direct link between in-cylinder behaviour and exhaust emissions. Successful ammonia combustion requires the ammonia spray to be engulfed by the diesel flame before expansion-induced cooling freezes the chemistry. Regions that satisfy this condition contribute to engine load and NO formation. Regions that remain cold, fuel-rich or weakly connected to the diesel flame become sources of unburned NH_3 and N_2O . Thus, the emission problem is fundamentally controlled by local mixing and reaction-zone overlap rather than by the global ammonia energy ratio alone.

Although Case 3 is used as the representative case in this analysis, the overall combustion process behaves similarly in all four cases. Diesel ignites first, ammonia combustion develops after interaction with the diesel flame, and emission formation depends on the local coexistence of temperature, equivalence ratio, fuel vapour and radicals. The corresponding combustion process diagrams for remaining cases can be found in Appendix B.

4.5 Swirl Ratio Sensitivity Analysis

The swirl ratio (SR) sensitivity analysis is carried out to evaluate whether in-cylinder flow control can improve ammonia–diesel interaction and reduce emissions. Swirl affects the spatial distribution of fuel vapour, entrainment of surrounding air, interaction between ammonia jet and diesel flame and residence time of reacting mixtures in high-temperature zones. Since ammonia combustion is strongly mixing-controlled in the present DDFS configuration, swirl ratio is expected to play an important role in both engine performance and emission formation.

The turbulent kinetic energy (k) distributions in Figure 4.8 illustrate that increasing swirl ratio modifies the organization of the in-cylinder flow. At relatively low swirl ratio, the ammonia and diesel sprays are less strongly redistributed by the bulk rotational flow, which may limit the contact between ammonia vapour and diesel-flame products. As the swirl ratio increases to a moderate level, the flow enhances entrainment and promotes a wider interaction region. This can help ammonia vapour enter hot, radical-rich zones and improve its oxidation. However, when the swirl ratio becomes too high, the flow may over-disperse the fuel jets, stretch the reacting mixture, and transport ammonia toward colder peripheral or near-wall regions. Under such conditions, stronger flow motion does not necessarily improve combustion, instead, it can reduce the effective residence time of ammonia in the most favourable reaction zone.

The emission results displayed in Figure 4.9, confirm this non-monotonic behaviour. For $\text{SR} = 12$, three repeated simulations were performed. The plotted values correspond to

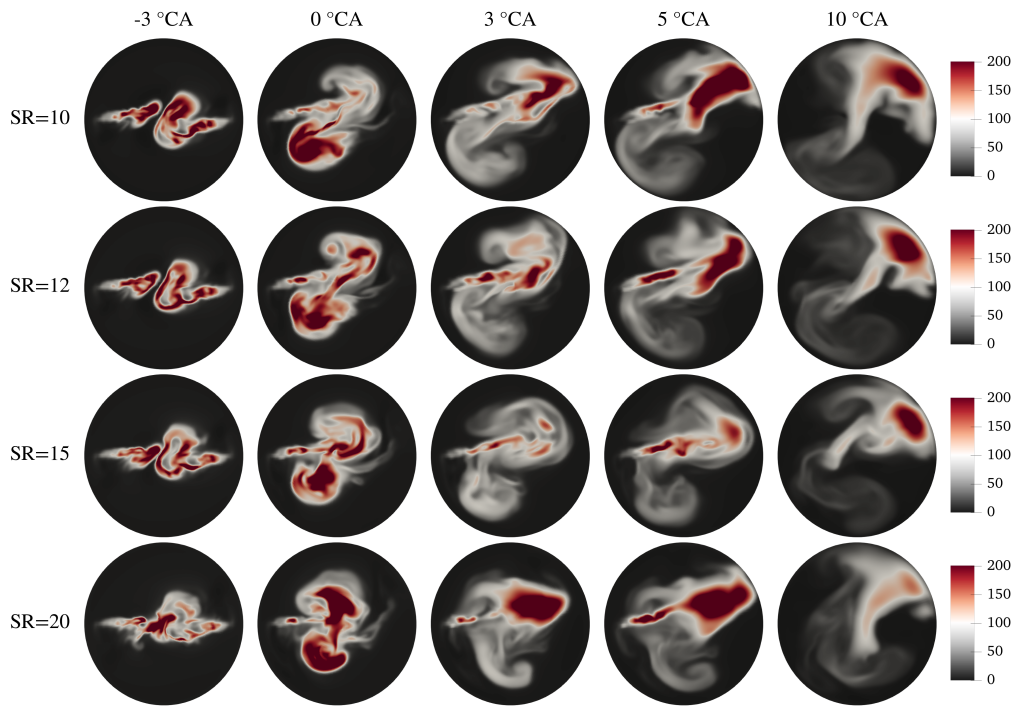


Figure 4.8 In-cylinder turbulence development for cases with various swirl ratios at a plane 5 mm below the piston head

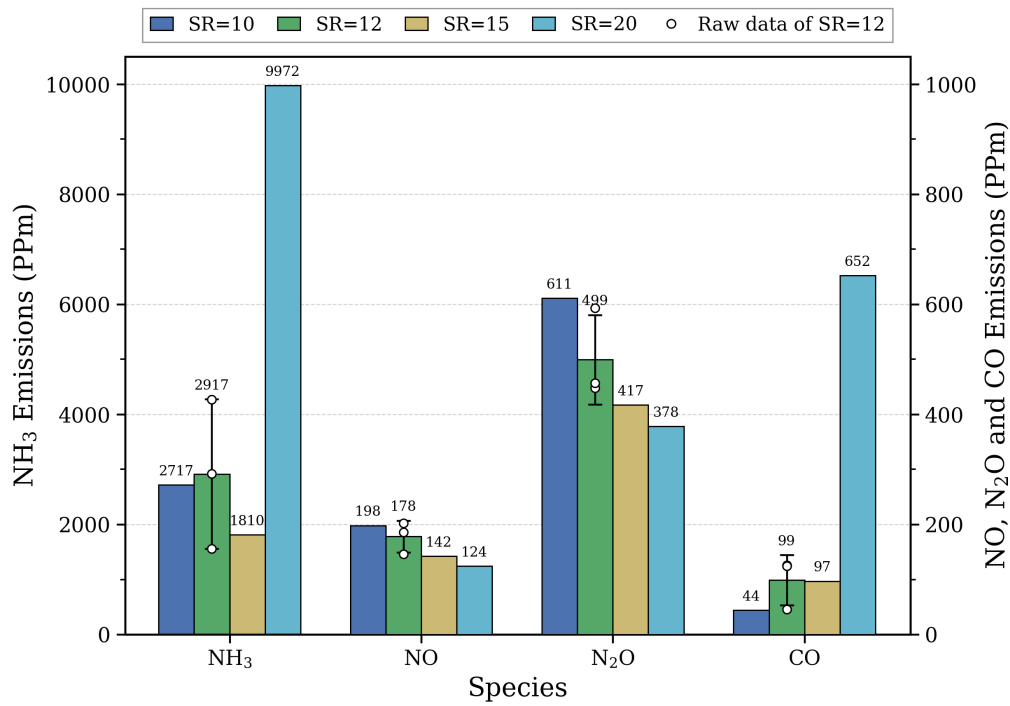


Figure 4.9 NH₃, NO, N₂O, CO emissions for cases with various swirl ratios (including three repeated simulations of SR = 12)

the mean of the three simulations, the small white circular markers represent the raw data, and the error bars denote the standard deviation. The existence of simulation-to-simulation scatter is reasonable because ammonia ignition and nitrogen chemistry are highly nonlinear. Small differences in Lagrangian parcel distribution, local spray evaporation, turbulence–chemistry interaction and moving-mesh flow development can be amplified into measurable differences in final emissions. Therefore, the error bars do not invalidate the results, they rather provide a useful indication of the expected numerical variability. It is also reasonable to infer that similar uncertainty would exist for the other swirl ratios if repeated simulations were run. Since the main trends among different swirl ratios are larger than the observed scatter at $SR = 12$, the conclusions remain robust.

The NH_3 emission is highly sensitive to swirl ratio. At $SR = 10$ and $SR = 12$, ammonia slip remains at a moderate level, with values of approximately 2717 PPm and 2917 PPm respectively. At $SR = 15$, NH_3 decreases to about 1810 PPm, indicating improved ammonia conversion. This suggests that a moderate increase in swirl enhances the contact between ammonia vapour and the diesel-flame region. However, at $SR = 20$, NH_3 increases dramatically to nearly 9972 PPm. Such a sharp increase indicates severe deterioration of ammonia oxidation. The most plausible explanation is that excessive swirl transports a large fraction of ammonia away from the high-temperature reaction zone and into colder regions, where it cannot be fully oxidized before expansion.

The NO emission decreases monotonically with increasing swirl ratio, from about 198 PPm at $SR = 10$ to 124 PPm at $SR = 20$. This trend may be caused by reduced local high-temperature residence time and more distributed combustion under stronger swirl. Better mixing can also weaken stoichiometric hot spots, thereby suppressing thermal-NO formation. However, the decrease in NO should not be interpreted as an unconditional improvement, because the very high NH_3 slip at $SR = 20$ indicates that the low NO value is partly associated with incomplete ammonia oxidation rather than truly cleaner combustion.

The N_2O emission also decreases as swirl ratio increases, from approximately 611 PPm at $SR = 10$ to 378 PPm at $SR = 20$. At low and moderate swirl ratios, this reduction may reflect improved ammonia conversion and reduced residence of partially reacted ammonia in quenching-prone zones. However, the lowest N_2O value at $SR = 20$ must be explained carefully. It occurs together with extremely high NH_3 slip, meaning that a large portion of ammonia escapes oxidation before it can even progress through the intermediate pathways that form N_2O . Thus, the apparent reduction in N_2O at excessive swirl is not necessarily a sign of better combustion, but rather a consequence of incomplete reaction.

The CO emission provides further evidence for this explanation. CO remains relatively low at $SR = 10$, $SR = 12$ and $SR = 15$, with values around 44–99 PPm. At $SR = 20$, however, CO increases sharply to about 652 PPm. Since CO is a typical product of incomplete carbon oxidation, this increase indicates that excessive swirl not only harms ammonia conversion but also disturbs the oxidation of diesel-derived intermediates. The

simultaneous rise of NH_3 and CO at $\text{SR} = 20$ clearly shows that combustion completeness deteriorates under overly strong swirl.

Considering all four emissions together, $\text{SR} = 15$ is recommended as the most suitable emission-oriented swirl ratio in this study. Compared with $\text{SR} = 10$ and $\text{SR} = 12$, $\text{SR} = 15$ reduces NO, N_2O and NH_3 while keeping CO at a low level. Although $\text{SR} = 20$ further reduces NO and N_2O , it causes unacceptable increases in both NH_3 slip and CO. Therefore, the optimal strategy is not to maximize swirl intensity, but to tune the swirl ratio to a moderate level that strengthens ammonia–diesel interaction without over-dispersing the fuel into cold or weakly reactive regions. Under the present operating conditions, $\text{SR} = 15$ provides the best overall balance between ammonia conversion, combustion completeness and pollutant control.

It should be noted that the present simulations do not account for the intake flow; therefore, the in-cylinder swirl is not physically generated by the intake air motion. As a result, the prescribed swirl number is not directly representative of physical reality. Nevertheless, the trends observed in the present simulations with respect to variations in swirl number remain valuable for understanding the interactions among in-cylinder flow, turbulence, and chemical processes in the ADDF combustion.

5 Conclusions and Future Outlook

5.1 Conclusions

This study numerically investigated the combustion and emission characteristics of a two-stroke direct-injection ammonia/diesel dual-fuel (ADDF) engine. Diesel was used as the pilot fuel to initiate combustion, while liquid ammonia was directly injected as the main carbon-free energy carrier. By comparing different ammonia injection durations under fixed diesel-pilot conditions, this study examined how increasing ammonia energy share affects combustion development, engine performance, emission formation and the role of in-cylinder swirl.

The results show that the ADDF combustion process exhibits a typical two-stage heat-release behaviour. The first stage is governed by diesel ignition, while the second stage is associated with ammonia oxidation promoted by the high-temperature products and active radicals from diesel combustion. This confirms that ammonia can contribute substantially to heat release, but its conversion is highly dependent on local spray interaction, turbulent mixing, and the spatial overlap between ammonia-rich mixtures and reactive diesel-flame regions.

The emission analysis reveals the main limitation of ammonia combustion. Although increasing the ammonia energy share reduces carbon-containing emissions such as CO and CO₂ per energy input, it also promotes NH₃ slip and N₂O formation when ammonia is not completely oxidized. Since N₂O has a much stronger greenhouse effect than CO₂, the total greenhouse-gas-equivalent emission can increase despite the reduction in direct carbon emissions. Therefore, the climate benefit of ammonia-fuelled engines cannot be assessed only from the perspective of CO₂ reduction. Complete ammonia oxidation and effective suppression of N₂O are essential for achieving a meaningful reduction in overall greenhouse impact.

The in-cylinder analysis indicates that incomplete ammonia oxidation is mainly associated with low-temperature, fuel-rich, near-wall or weakly reactive regions where ammonia fails to be fully engulfed by the diesel flame. In contrast, ammonia located in hot and radical-rich regions can be consumed more effectively and contributes to the main heat release. The swirl ratio study further shows that moderate swirl can improve ammonia–diesel interaction and reduce incomplete-combustion emissions, whereas excessive swirl may over-disperse the fuel into colder regions and deteriorate combustion completeness. Under the present conditions, a swirl ratio of 15 provides the most favourable balance between ammonia conversion and emission control. The essence of the swirl effect lies in promoting favourable interactions between the ammonia and diesel flames, whereby the ammonia–air mixture is effectively entrained and engulfed by the hot diesel flame.

Overall, this study confirms the feasibility of direct-injection ammonia/diesel combustion

for reducing carbon-containing emissions in two-stroke marine engines. However, it also demonstrates that ammonia substitution alone does not guarantee a lower total climate impact. The key to future ammonia engine development is not simply to maximize the ammonia energy ratio, but to control the coupled processes of spray evolution, turbulent mixing, ignition, heat release, and nitrogen chemistry so that ammonia can burn completely while N_2O and NH_3 emissions remain sufficiently low.

5.2 Future Outlook

Future work should focus on integrated optimization of injection strategy, in-cylinder flow, and combustion-chamber design. The relative timing, duration, and pressure of ammonia and diesel injection should be further investigated over a wider range of loads and engine speeds, since these parameters directly determine the interaction between ammonia-rich mixtures and diesel flame. At the same time, injector orientation, spray targeting, swirl intensity, and piston geometry should be optimized together to promote ammonia oxidation in high-temperature reaction zones while avoiding wall impingement, over-dilution, and low-temperature ammonia pockets.

Further experimental and numerical efforts are also required to improve the reliability of emission prediction. Accurate measurements of N_2O , NH_3 , NO , and NO_2 , together with optical diagnostics of spray and flame development, would provide valuable data for validating chemical mechanisms and combustion models. On the numerical side, higher-fidelity approaches such as LES or hybrid RANS–LES, combined with uncertainty analysis, could help clarify the effects of turbulent mixing, evaporation cooling, wall heat transfer, and nitrogen chemistry on ammonia conversion.

For practical marine applications, engine optimization should eventually be combined with aftertreatment and life-cycle assessment. Even with improved in-cylinder combustion, NH_3 slip and N_2O formation may remain difficult to eliminate under all operating conditions. Therefore, aftertreatment technologies and system-level evaluation of ammonia production, storage, safety, efficiency, and total greenhouse-gas impact are necessary to determine the real decarbonization potential of ammonia/diesel dual-fuel engines.

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Appendix

A Supplementary Diagrams for Emission Trends Varying with Crank Angles

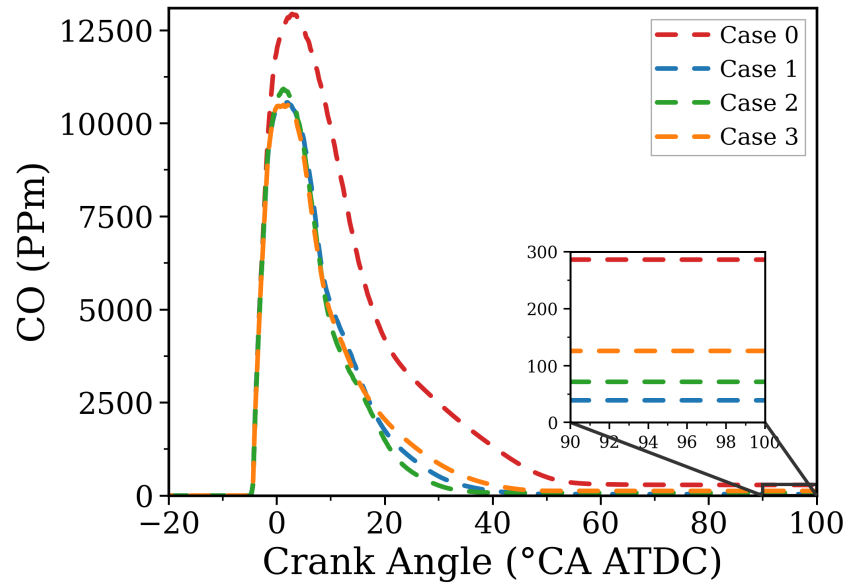


Figure A.1 CO emission trends varying with CA for Case 0–3

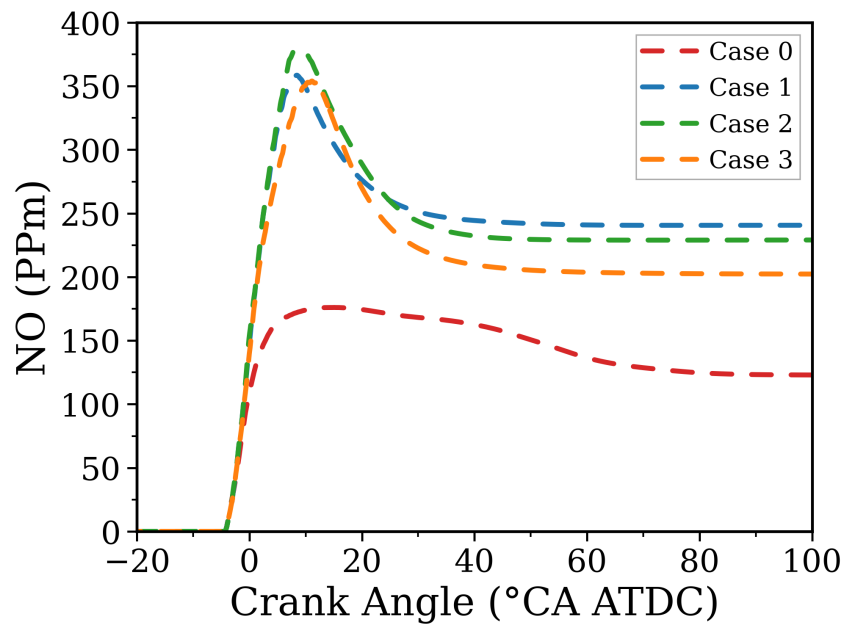


Figure A.2 NO emission trends varying with CA for Case 0–3

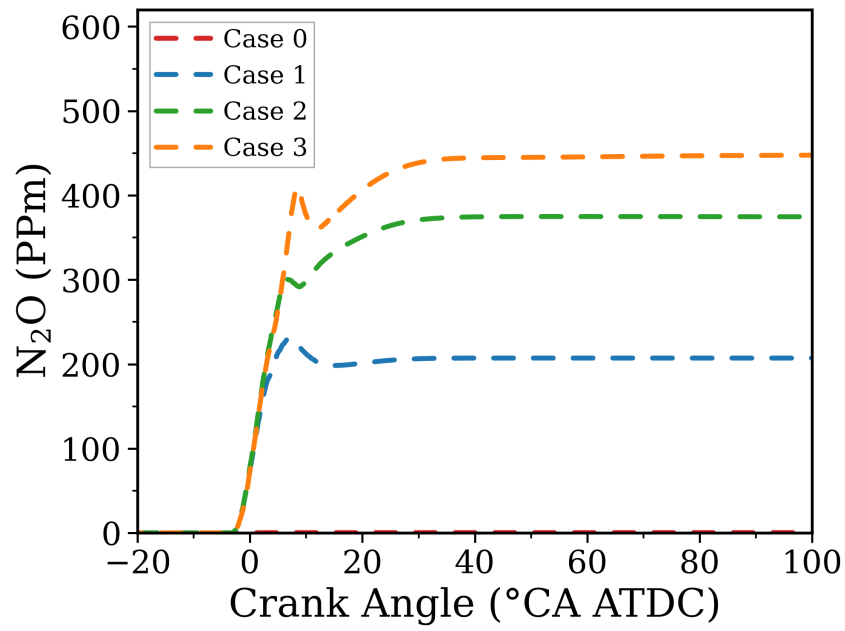


Figure A.3 N_2O emission trends varying with CA for Case 0–3

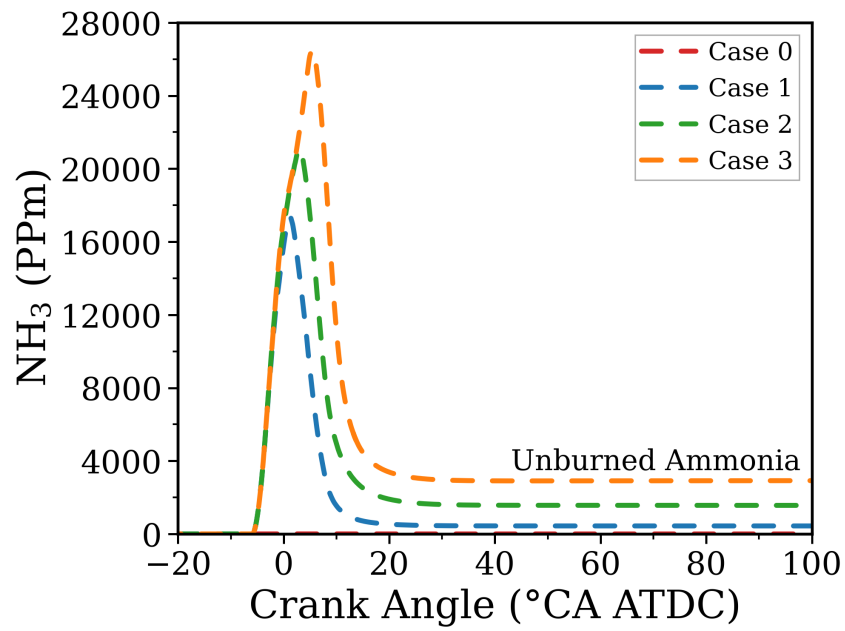


Figure A.4 NH_3 emission trends varying with CA for Case 0–3

B Supplementary Diagrams for Combustion Processes

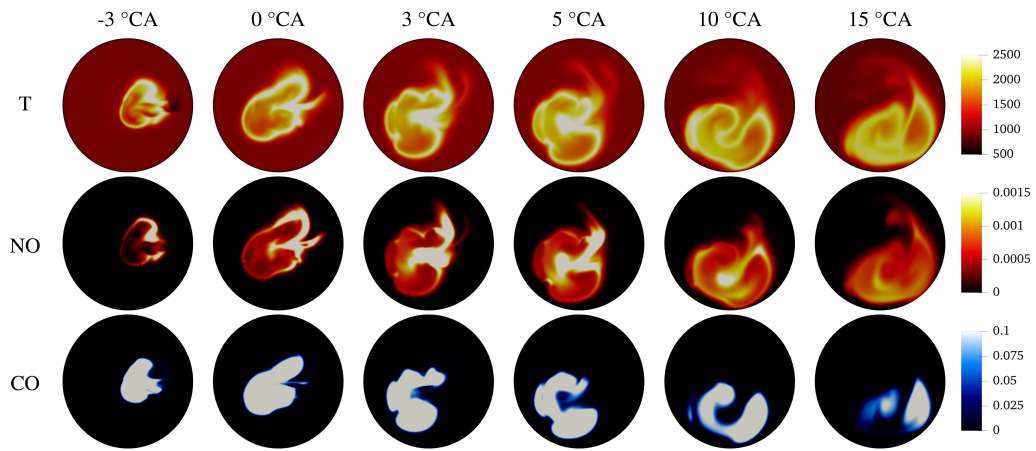


Figure B.1 In-cylinder temperature and NH_3 , NO, N_2O , CO distributions for Case 0 at a plane 5 mm below the piston head

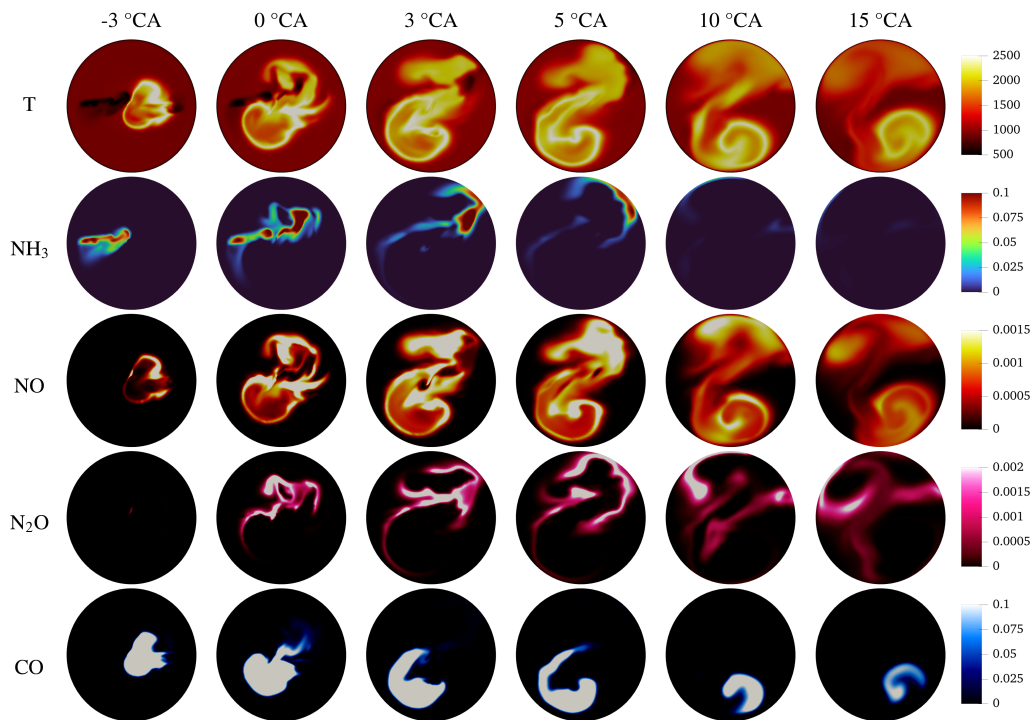


Figure B.2 In-cylinder temperature and NH_3 , NO, N_2O , CO distributions for Case 1 at a plane 5 mm below the piston head

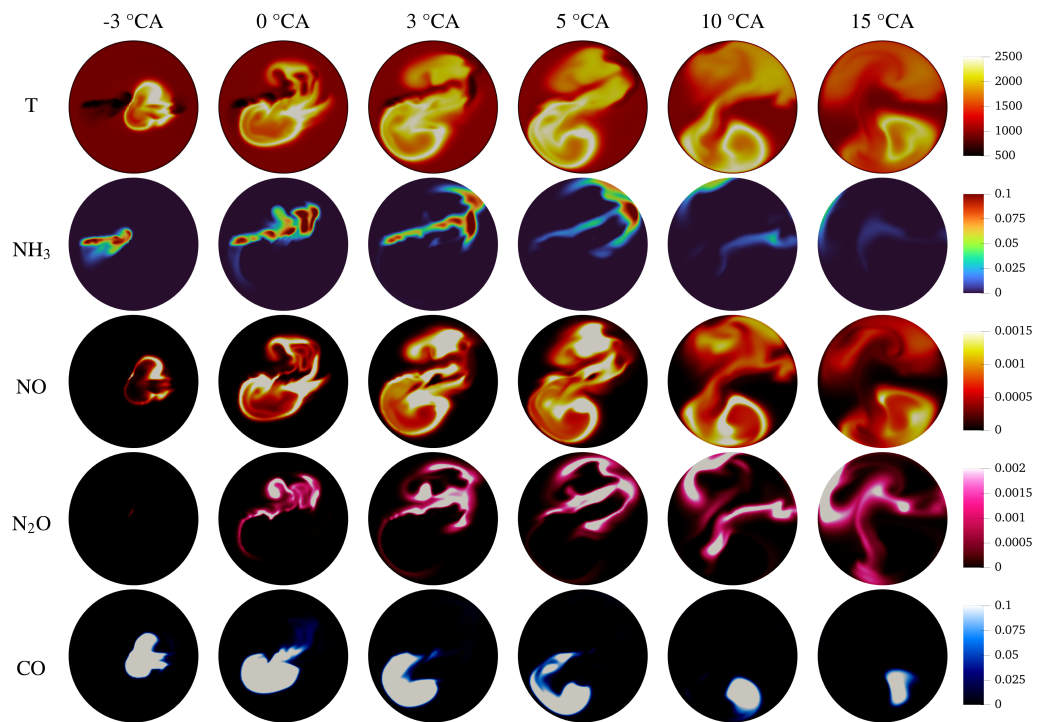


Figure B.3 In-cylinder temperature and NH₃, NO, N₂O, CO distributions for Case 2 at a plane 5 mm below the piston head

C Supplementary Diagrams for Swirl Ratio Sensitivity Analysis

Overall Engine Performance

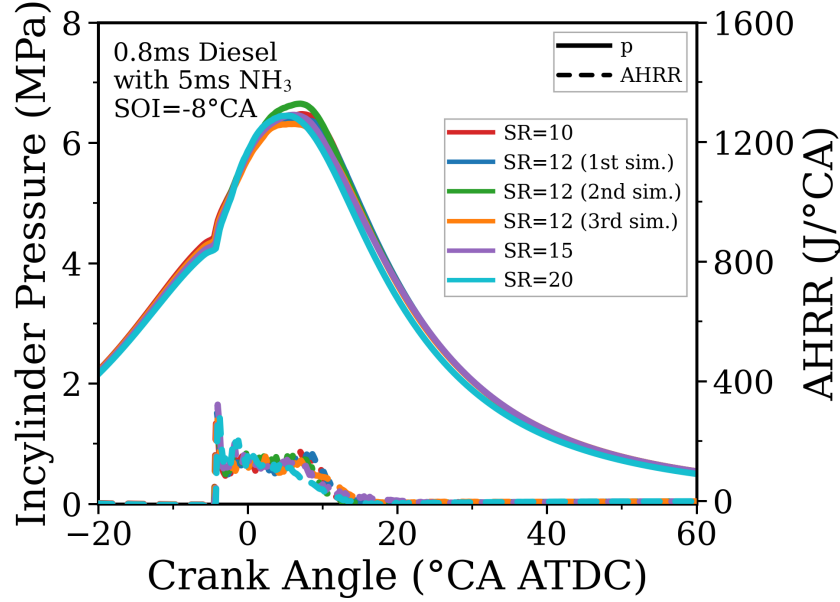


Figure C.1 In-cylinder pressure and AHRR varying with CA for all swirl ratio simulations

Emission Trends Varying with Crank Angles

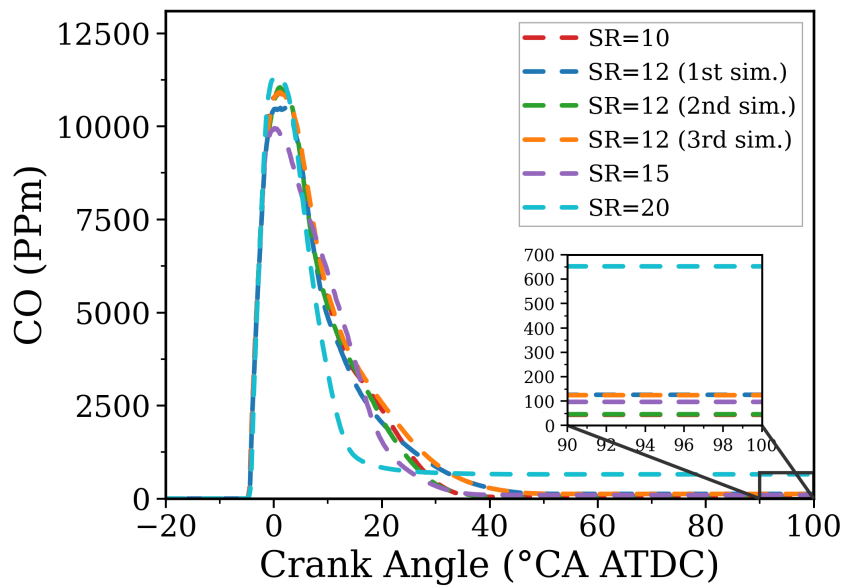


Figure C.2 CO emission trends varying with CA for all swirl ratio simulations

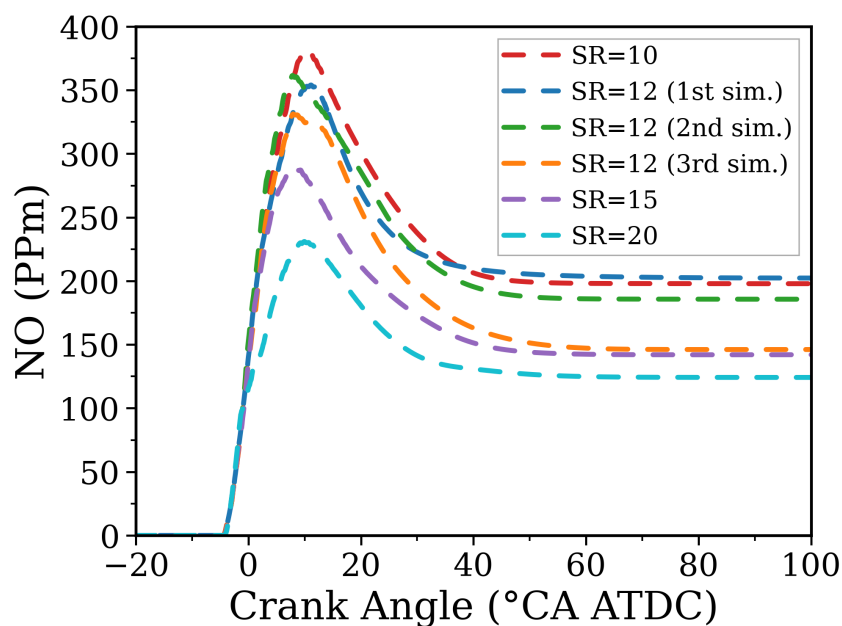


Figure C.3 NO emission trends varying with CA for all swirl ratio simulations

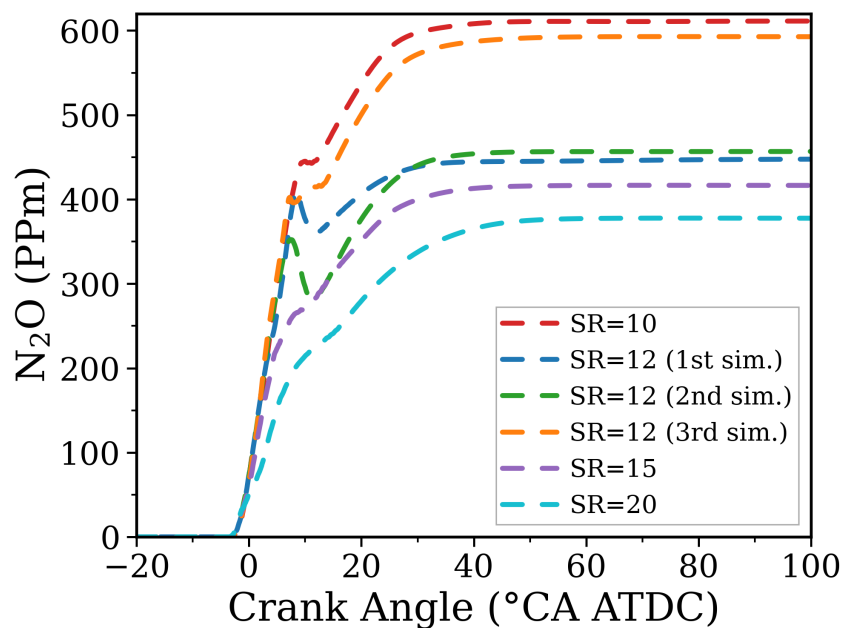


Figure C.4 N₂O emission trends varying with CA for all swirl ratio simulations

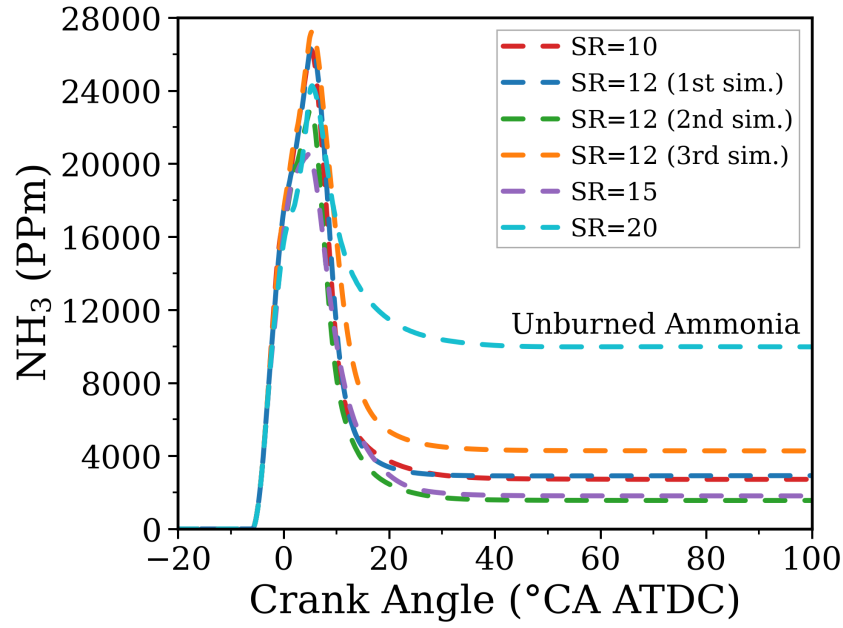


Figure C.5 NH_3 emission trends varying with CA for all swirl ratio simulations

Combustion Processes

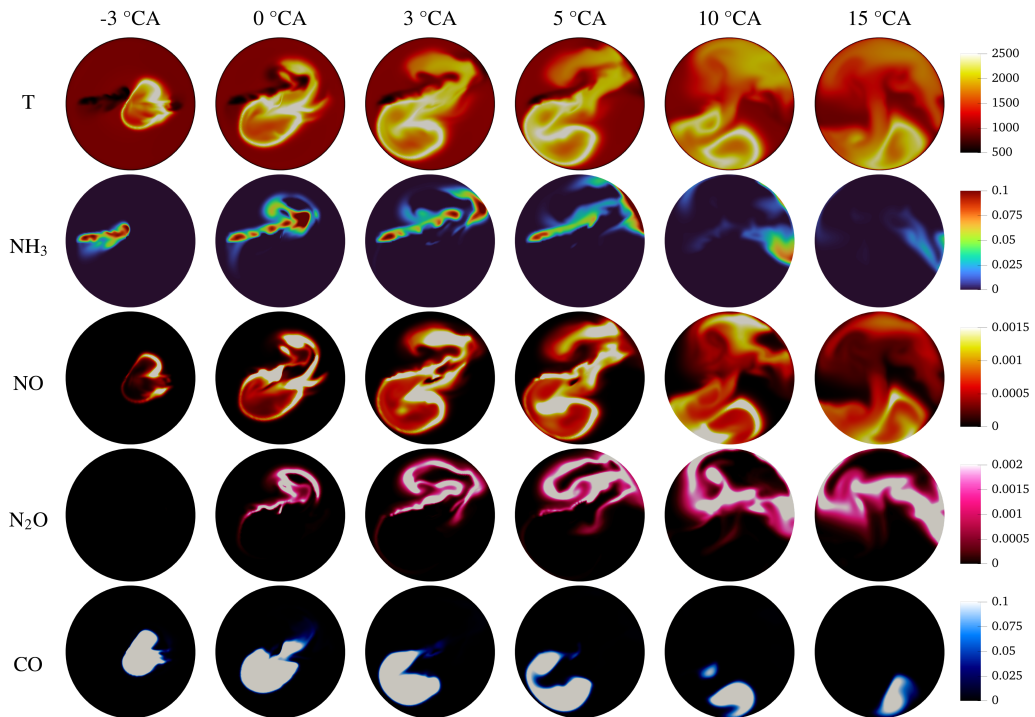


Figure C.6 In-cylinder temperature and NH_3 , NO, N_2O , CO distributions for SR = 10 at a plane 5 mm below the piston head

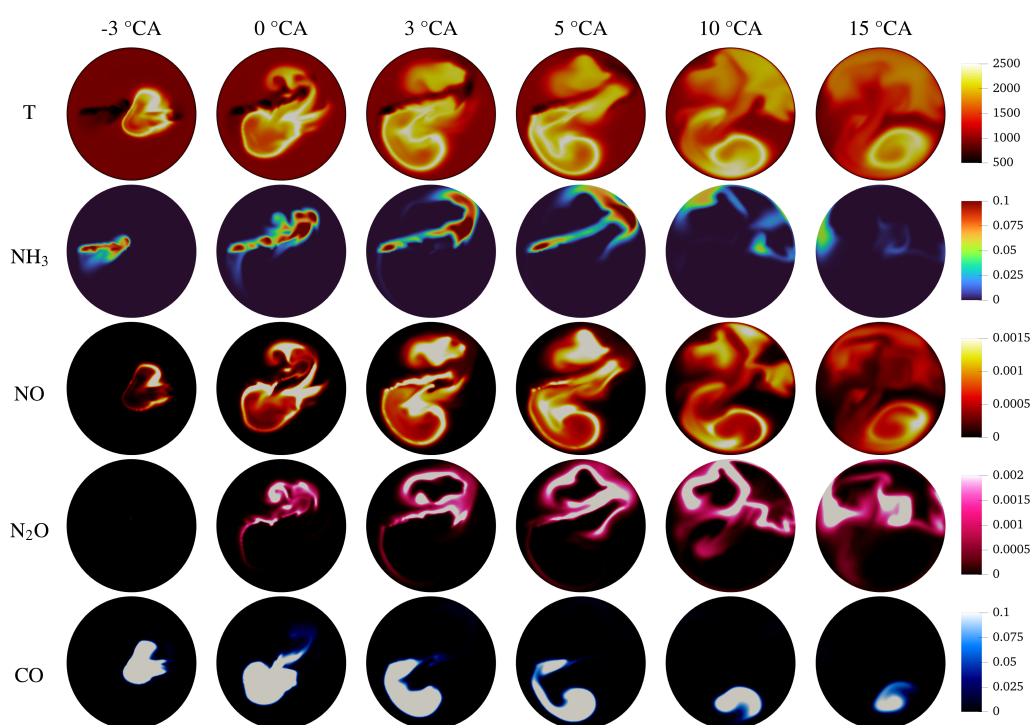


Figure C.7 In-cylinder temperature and NH_3 , NO , N_2O , CO distributions for the first simulation of $\text{SR} = 12$ at a plane 5 mm below the piston head

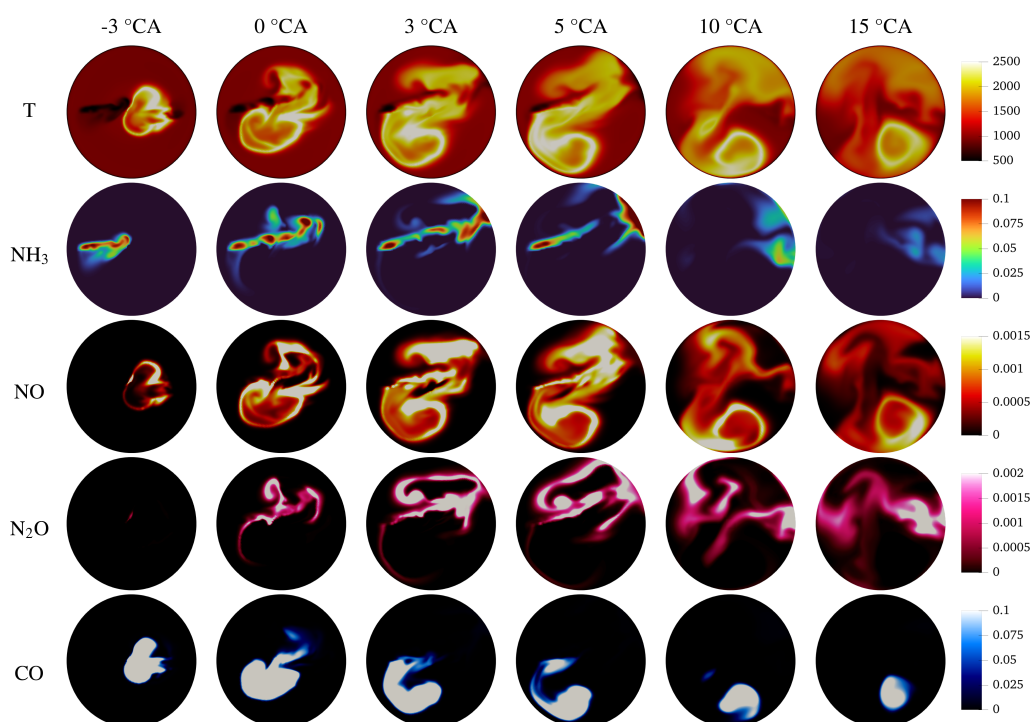


Figure C.8 In-cylinder temperature and NH_3 , NO , N_2O , CO distributions for the second simulation of $\text{SR} = 12$ at a plane 5 mm below the piston head

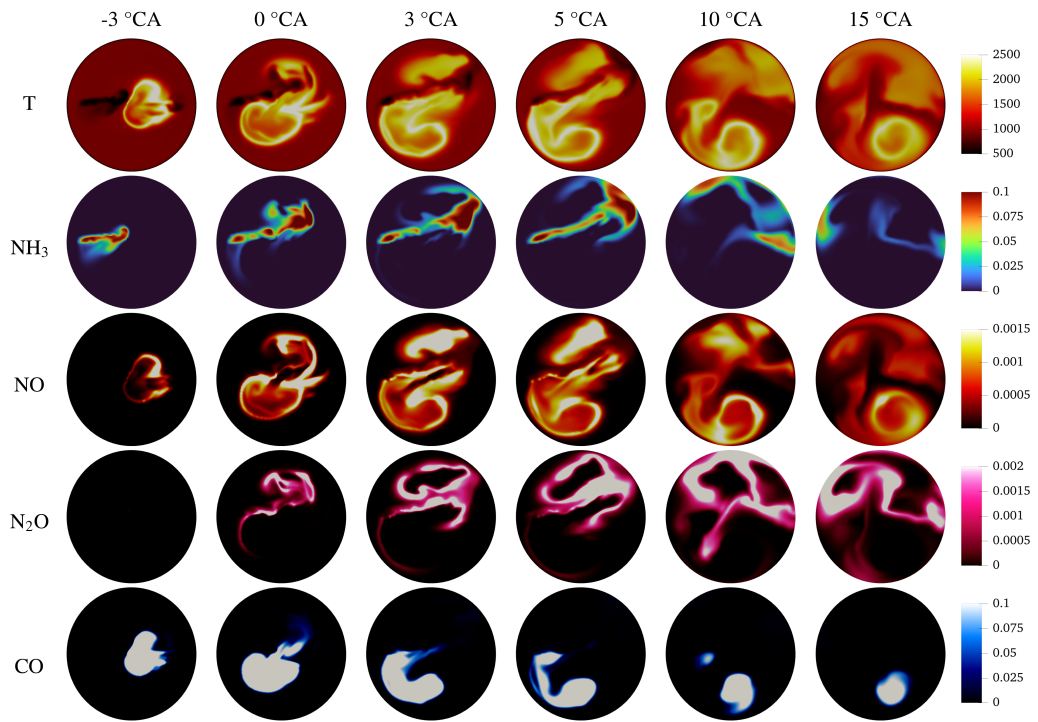


Figure C.9 In-cylinder temperature and NH_3 , NO , N_2O , CO distributions for the third simulation of $\text{SR} = 12$ at a plane 5 mm below the piston head

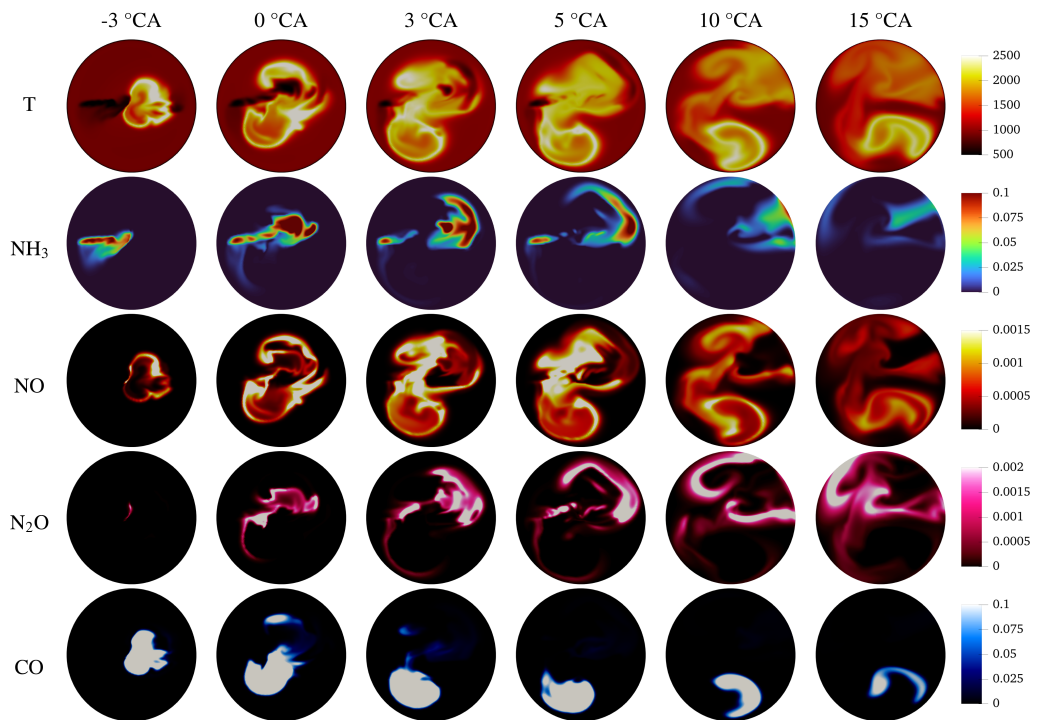


Figure C.10 In-cylinder temperature and NH_3 , NO , N_2O , CO distributions for $\text{SR} = 15$ at a plane 5 mm below the piston head

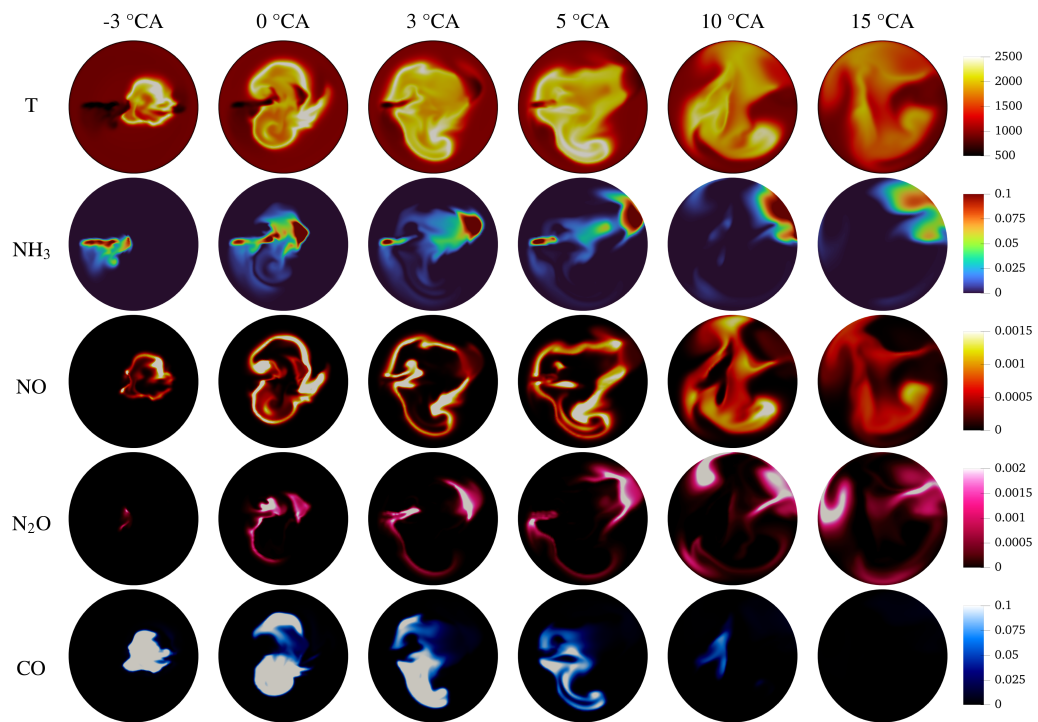


Figure C.11 In-cylinder temperature and NH₃, NO, N₂O, CO distributions for SR = 20 at a plane 5 mm below the piston head