

Ammonia for power – heating and powergen systems through a computational fluid dynamics review

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ABSTRACT

Ammonia has gained considerable interest from the combustion community as an alternative fuel. The chemical promises to remove carbon entirely from heating, power and propulsion processes without incurring extensive infrastructure developments. As such, the work on ammonia combustion expands from fundamental analyses to giga-Watt practical applications in power generation. However, experimental research usually lacks further information about radical interactions, blends' reactivity, emissions abatement, flame stability, and scalability parameters. Therefore, numerical modelling via Computational Fluid Dynamics (CFD) not only offers detailed insights into these combustion challenges using ammonia but also ensures that by applying novel methodologies ammonia resolution is accurate, relevant and affordable for a topic with such a large potential impact. Therefore, this review addresses a large literature survey from across the globe currently assessing ammonia as an energy vector in large power and heating systems. Finally, major challenges and future developments are presented, with conclusions that address the versatility of studies and most interesting areas of research relevant to the use of CFD ammonia modelling.

1. Introduction

1.1. Looking at the future

It is highly recognised that climate change will have considerable implications in the following decades, particularly if little-to-no-action is implemented to reduce impact towards the environment and the reduction of greenhouse gas emissions. Current estimates predict global temperature increments of ~ 2.0 °C [1], presenting a gloomy scenario that requires fast and decisive actions to mitigate the rise in global temperature.

Important bodies, such as the Hydrogen Council, currently evaluate the hydrogen case, which as the name implies, assesses the full hydrogen chain, overseeing not only past tendencies, but also predicting future scenarios for the production, storage, distribution and utilization of such a molecule. Hydrogen's vision is to enable power, heat and propulsion

fuelling by using a molecule that can reduce carbon emissions, hence producing water in the combustion process and abating the increase of carbon molecules in the atmosphere. By tapping into renewable sources, the hydrogen can be obtained through electrolysis, avoiding the reliance and emissions of carbon (product of steam methane reforming usually employed to produce the molecule). However, the lack of infrastructure, final investment decisions bound to uncertain scenarios, and macro-economic challenges, have made the progress on the topic slower than anticipated [2]. Therefore, estimates predict that out of the total amount of required hydrogen, a large portion will still depend on the production from fossil fuel sources (namely, grey hydrogen). As the transition towards net zero economy based on green sources moves on, the grey hydrogen share will decline, giving way to green hydrogen sources that will be employed in industry, mobility, heating and even power, Fig. 1. The growing market and the greater interconnection between regions will ensure that by 2050 most countries are part of the global network of

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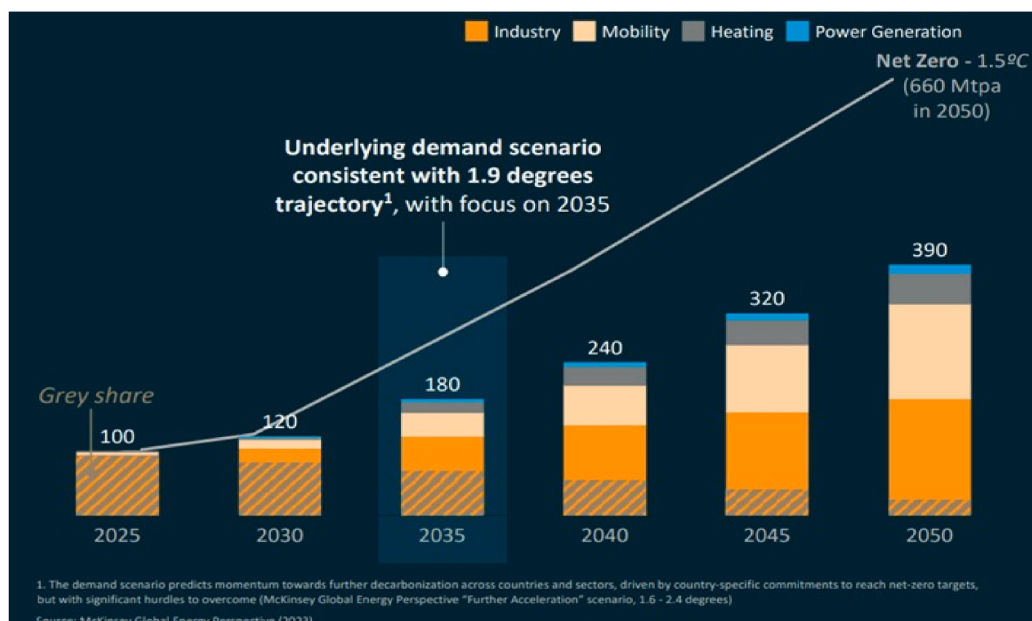


Fig. 1. Required global demand for H₂ and derivatives (in Mton per year) of grey and green hydrogen equivalent (Reprint from Ref. [3] with permission).

hydrogen and its derivatives around the planet. The concept becomes particularly interesting if other factors such as nuclear power and varied penetration of renewables in low-to-high GDP countries are considered, hence creating a complex scenario where the deployment of hydrogen vectors will have a crucial role towards energy independency, resilience and security [3].

However, infrastructural problems and risks make hydrogen still challenging, hence opening the door to other molecules that not only contain hydrogen in large quantities, but also possess greater versatility and a mature market. Ammonia, one of these solutions, being the second most commercialized chemical in the world and with a trading history of more than 150 years, will continue growing its share amongst hydrogen-deploying sectors. The largest share of large distance transported hydrogen is based on fertilizers (mainly ammonia), thus showing how economies with limited energy resources but fertilizing infrastructure will highly benefit from the utilization of such a molecule not only in farming but also other sectors, including power and heating.

Currently, the use of ammonia for energy has been mainly focused on its use for cracking purposes. Ammonia, with three hydrogen atoms, has more hydrogen than hydrogen itself, hence being a great candidate for its transportation and storage, which are achieved at relatively low pressures (~ 8 bar at 15°C) or high temperatures (-33°C compared to -253°C of hydrogen under atmospheric pressure). These characteristics enable ammonia to be moved globally relatively easily, with infrastructure that has served the fertilizing industry for decades. Hence, ammonia can be decomposed to obtain its hydrogen atoms, thus serving as hydrogen enabler. However, the decomposition or “cracking” process requires energy, which can account for up to 13% of the total energy content of the ammonia molecule [4]. Therefore, some applications will find the use of direct ammonia simpler and more economical, thus positioning ammonia as a fuelling net-zero vector. One interesting case is the one relevant to fuelling rural applications. Recent works performed by FloGas, Cardiff University and ERM [5] have demonstrated the potential of ammonia against hydrogen energy delivery for powering steam boilers currently running with LPG fuel. The concept, explained in more detail below, seeks to replace the fossil vector by green ammonia produced from clean sources. The replacement will not only reduce up to 98% carbon emissions, but would also be more competitive with hydrogen delivery. Estimated costs range from 142 to 247 £/MWh using either liquid or compressed hydrogen, whilst

ammonia ranges from 59 to 91 £/MWh. The main reason for the difference is the energy density of ammonia (~ 3.5 kWh/l), compared to hydrogen (~ 2.7 kWh/l). Concurrently, delivery of the latter would require more nursing tanks than those needed for ammonia. These types of scenarios show that there is an economic scope for ammonia in some niche applications.

This was also evidenced by works performed by Boero et al. [6,7] who demonstrated via numerical modelling that the techno-economics of using ammonia can be competitive to fossil fuels. Additionally, a cradle-to-gate assessment showed that electrolysis-based ammonia from renewable and nuclear energy for its use in power generation have a better profile in terms of global warming potential (0.09 – 0.70 t CO₂-eq/t NH₃), fossil depletion potential (3.62 – 213.56 kg oil-eq/t NH₃), and ozone potential (0.001 – 0.082 g CFC-11-eq/t NH₃) than when using fossils. In addition, surplus heat for district or industrial applications offsets some of the environmental burden, such as a more than 29% reduction in carbon footprint. In general, ammonia-based combined heat and power production presents a favourable environmental profile. Similarly, using ammonia in engines delivered significant reductions, above 70%, for GWP100, FDP, and ODP compared with the same vehicle fuelled on gasoline. The concept, requiring multi-variable analyses to expand on the impact of ammonia not only environmentally but also socially and economically [8], has recently been approached by Anwar et al. using machine learning strategies [9] that promise to reveal complex interactions between electricity costs, environmental restrictions, and operability constraints, all in line with additional requirements for the profitable, environmental operation of future systems operating with ammonia. However, more is still needed to address all the challenges that ammonia energy would bring. For example, and similar to the work done by Devianto et al. [8], an analysis of nitrogen-based molecules and their impact on GDP is still nonexistent -to the knowledge of the authors-, although NO_x are now at the core of regulatory bodies and industries for environmental improvement.

Similarly, other challenges critical to fundamental physics require further research. Ammonia combustion features relevant to ignition energy, flame stability, and NO_x emissions at various power loads are within the most critical aspects inspected by researchers and companies. Interestingly, NO_x and N₂O are also within the scope of government bodies, as these emissions have damaging effects on the environment, components and population [10]. However, works on the use of

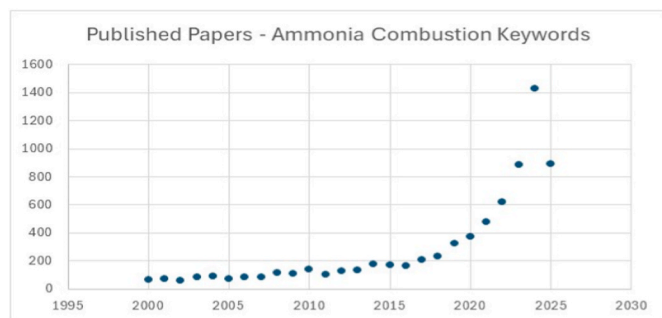


Fig. 2. Publications containing the keywords “Ammonia Combustion”, July 2025, Scopus Search.



Fig. 3. Chifeng green hydrogen and ammonia complex (Reprint from Ref. [12] with permission).

stratified injection, staged fuel/air combustion, residence time increase at post-combustion zones, afterburning selective catalytic reduction, and non-selective recombinations at high power, amongst others, are promising technologies that have demonstrated the abatement of these emissions below current legal limits. However, additional work is still needed for the more stringent regulations foreseen to be imposed by the next decade. This is where the work on innovative concepts, with support from computational fluid dynamics, could be the difference between having ammonia as a real fuel or just an unrealistic “low hanging fruit”.

Therefore, this review aims to cover the issues mentioned above by exploring the combustion of ammonia as a power and heating fuel, raising current challenges that the Computational Dynamics field faces. The manuscript will delve into crucial parameters currently evaluated via advanced modelling techniques that can provide valuable insights for improving our understanding of ammonia as a fuel at medium and large scales.

1.2. Current scenario

As previously raised, ammonia fuelling has received considerable attention due to its potential role in removing fossil fuels from the current energy mix. Reviews on the topic approach some of the history behind ammonia's role in the alternative fuel arena [11]. Furthermore, it has been obvious that the number of groups and researchers working in the area has considerably increased over the years, Fig. 2, leading to a variety of publications that have exponentially grown after 2020.

The trend is not different at the industrial level, where ammonia has picked up the news across novel fuelling applications for decarbonisation purposes. From the large investments conducted in Japan, China and South Korea [4], to bespoke innovations, ammonia seems to have captured interest in areas such as marine and hydrogen delivery at national levels. The commissioning of large green ammonia-producing

facilities has reached new heights during the last 5 years. Without more detail, as this review is not intended to address the producing side of the ammonia chain, it is enough to emphasize that companies such as Envision Energy, in Inner Mongolia, China, have officially commissioned facilities capable of producing >320,000 tonnes of green ammonia annually with energy requirements exceeding 500 MW with intentions of extending such capacity to 2.5 GW in following up phases, all with the intention of exporting the chemical worldwide by the end of 2025, Fig. 3 [12].

Envision Energy's vision, similar to many other producers, will seek to sell some of this green ammonia for fuelling applications as a decarbonisation strategy of several industries and countries. Similarly, large consortia led by major ports have already engaged in multimillion contracts for the delivery and bunkering of ammonia, with clear examples such as the one signed between Pilbara Port, Oceania Marine Energy, and NH3 Clean Energy Limited to distribute ammonia from the Port of Dampier [13]. The use of this ammonia in marine ecosystems goes from propulsion to its consumption in boilers as a method of consumption of residual ammonia traces, as documented through the joint agreement between Alfa Laval, WinGD and HD Hyundai Mipo [14].

It was announced by the end of 2025 that Ulsan Metropolitan City and Hyundai Oil Terminal have signed an MoU for the investment of the second phase of the City's new Namsin Port development, becoming the first commercial ammonia storage facility in Korea, capable of handling 1.25 million tons of ammonia every year. In the words of the CEO of Hyundai Oil Terminal, Shin Dong-Hwa, “This investment will be a key driving force to make Ulsan Port a global clean energy and logistics center. We will play a role as a leading eco-friendly fuel supply base (infrastructure) and win-win with the region” [15].

Other large technologies capable of consuming ammonia as a fuel are also under development at the time of writing this review. Of particular interest is the use of gas turbines and their decarbonisation potential through the use of ammonia. Although vast literature exists on efforts conducted by Japanese consortia [16], recent news from GE Vernova (in collaboration with IHI at Hyogo, Japan) [17], Baker Hughes (in collaboration with Hanwha in South Korea) [18] and Marvel (China) [19], amongst others, have released statements of their current works towards the development of gas turbines to burn pure or blended ammonia, hence making an important contribution towards the use of the chemical for propulsion or power applications using this molecule.

These announcements only strengthen the global interest on ammonia as a fuelling vector to support decarbonisation transitions in the power, heating, and propulsion sectors. However, using ammonia is not as simple as it was initially conceived. At a time where large demonstrators are expensive and difficult to operate due to stricter health and safety regulations, advanced modelling techniques such as Computational Fluid Dynamics (CFD) appear to support a faster, cleaner and efficient transition towards large power systems. Hence, this review addresses recent advancements in the field to enable numerical demonstration of medium to large power systems intended to transition and run using ammonia fuelling.

1.3. The critical role of CFD modelling in ammonia combustion

In an era where computational capabilities expand exponentially, CFD modelling plays a critical role to quickly progress from fundamental understanding to industrial applications. The increased interest in modelling tools, machine learning integration, and the progression of quantum computing as a more tangible resolution scheme, are all parameters that raise the crucial need to improve and maximise the use of CFD in areas such as ammonia energy, hence giving pace to a revolution of high-efficient components capable of using such a fuel by delivering stable, low polluting and cost-effective alternatives to fossil heat and power generation.

CFD modelling will preclude some of the most interesting advancements that the community will see in the foreseeable future. Ongoing

algorithmic and hardware progresses necessary to further facilitate high-fidelity methodologies for daily engineering designs will benefit from schemes assessed via CFD methods. This includes leveraging emerging platforms like open-sources that will expand global contributions on net zero fuels' subject. By tackling current challenges (some of them described in the following sections), the CFD community can fully unlock its potential to accelerate the development of sustainable energies within a continuously growing demand in an international scenario.

The stringent need to improve and advance the subject needs a critical assessment of current efforts seeking to unlock these capabilities at academic and industrial levels. Therefore, the scope of this review is focused on addressing a critical approach of works conducted on the field, focusing on CFD-based studies of ammonia combustion for fuel utilization, making emphasis on the use of the molecule in the heating and power generation sectors, a novel approach to other available literature. The manuscript first discusses the most common CFD turbulence methods, as the latter provide the physical basis for model assessment. Then, boilers and furnaces from small to large, industrial scales are considered, moving on to the assessment of micro and large gas turbines fuelled with ammonia. Through detailed discussions, complementary tables and several interconnections, the subjects are presented within a critical review that sets the foundations for further assessments. Future works and conclusions wrap up the document, hence providing both the combustion and CFD communities with information that expands on the comparison between models, approaches, strengths and weaknesses of the CFD methodologies used to address the utilization of ammonia in these critical energy sectors.

2. CFD modelling

2.1. Turbulence models

The substantial increase in computing power of the last twenty years has made Computational Fluid Dynamics an invaluable design and research tool to better understand the intricacy of turbulent reacting flames. Although very complementary to experiments, such tools still have limitations, the main one being the need for turbulent combustion closures which heavily rely on hypotheses and potential limits on the chemistry side. As of today, different modelling frameworks coexist. They all have advantages and drawbacks, one of which is clearly the computing effort inferred by a given framework which tries to compromise and leverage computing power versus accuracy and generality. In this context, three main approaches are available to the CFD community: Direct Numerical Simulation (DNS), Large-Eddy Simulation (LES) and Reynolds-averaged Navier-Stokes (RANS), all approaches that have been used to simulate ammonia flames, hence providing a priori validation and adjustments of the modelling specific to this new fuel.

2.1.1. Reynolds-averaged Navier-Stokes (RANS)

RANS equations are time-averaged equations of motion for fluid flows where an instantaneous quantity is decomposed into its time-averaged and fluctuating quantities. RANS is applicable to statistically stationary flow problems (or independent of time). Indeed, the approach provides closure for the problem to be solved numerically, reproducing the effect of the entire spectrum of scales present in the problem and which are known to significantly impact the mean flow physics coming either from turbulence or the flame. Alternatively, the framework remains computationally efficient since limited computational power is needed once the adequate model is derived and implemented. Therefore, many predictions can be obtained in a short time as usually needed in a design process, although the accuracy of these stationary predictions may be limited and often questionable.

2.1.2. Large-Eddy Simulation (LES)

With this approach, the flow is no longer ensemble- or time-averaged

but spatially filtered, removing parts of the small-scale turbulent structures which are costly to represent numerically and easier to model than the full turbulent spectrum as inferred in RANS. However, and due to this new mathematical context, the flow needs to be simulated in time and space thereby requiring a more important computational effort compared to RANS although modelling is still present. The essential difference is that now small-scales are more universal and easier to model provided access to the proper large flow scales which are of importance to the dynamics of the problem. Although not obvious, especially in the context of complex industrial applications, such requirements appear to be manageable and very interesting and reliable results have appeared recently around the combustion of ammonia flames.

Large Eddy Simulation is an emerging approach for ammonia research that offers significant advantages over RANS. Unlike RANS, which uses averaged turbulence models, LES directly simulates large-scale turbulent structures and their interactions with flames. This allows LES to capture cycle-to-cycle combustion variations and turbulent flame behaviour that RANS cannot predict. LES applications to ammonia systems are currently limited, but they show promise for understanding combustion instabilities, knock onset, and transient phenomena.

2.1.3. Direct Numerical Simulation (DNS)

Direct Numerical Simulation resolves all turbulent scales from the smallest (Kolmogorov) to the largest, providing fundamental understanding of turbulence-chemistry interactions. DNS relies solely on computing power and discretization capabilities. Although very accurate since the method relies only on a pure discretization of all the scales in time and space at play in the problem at hand, this approach remains very limited in terms of capabilities due to its inferred CPU costs. Therefore, DNS remains a fundamental academic tool to understand the interactions between the flow turbulent scales and all chemical steps of a reacting front. This method is not discussed in this review.

2.1.4. Hybrids

Although less rigorous in terms of framework and validation, all of the above-described methods can be mixed and interacted within a CFD tool, thus opening the door to the so-called hybrid models. The main idea behind such an approach is essentially to take advantage of each framework within a single simulation provided the proper introduction of switches or user defined transition regions while optimizing the overall CPU cost of the simulation.

2.2. Chemistry resolution

The treatment of chemical kinetics is perhaps the most decisive factor in ammonia combustion CFD modelling. Finite-rate approaches, such as the Eddy Dissipation Concept (EDC) and Partially Stirred Reactor (PaSR) models directly integrate chemical kinetics into the simulations. This approach is more accurate but vastly more expensive. Therefore, the choice of chemical mechanism becomes critical. A recurring theme across all studies is the uncertainty and trade-offs associated with chemical kinetics. Reduced mechanisms are computationally tractable but often lack fidelity. For instance, Taneja et al. [20] have reported that the nanosecond PPS can effectively decrease both ignition delay and post-ignition NO_x through directly reforming NH₃ to N₂ with 0D finite-rate chemistry. Wiseman et al. [21] employed DNS with finite-rate chemistry to show that the higher stability of NH₃/H₂ over methane is caused by a preferential diffusion in hydrogen, which locally enhances the burning rate within strained flame regions.

However, as mentioned, detailed mechanisms are very expensive to compute in 3D form. Therefore, tabulated chemistry methods such as Flamelet-Generated Manifold (FGM) have become popular. Mazzotta et al. [22], Davies et al. [23], and Lu et al. [24] applied FGM in both RANS and LES contexts and obtained comparable results for flame shapes and radical formation. Unfortunately, an important restriction to

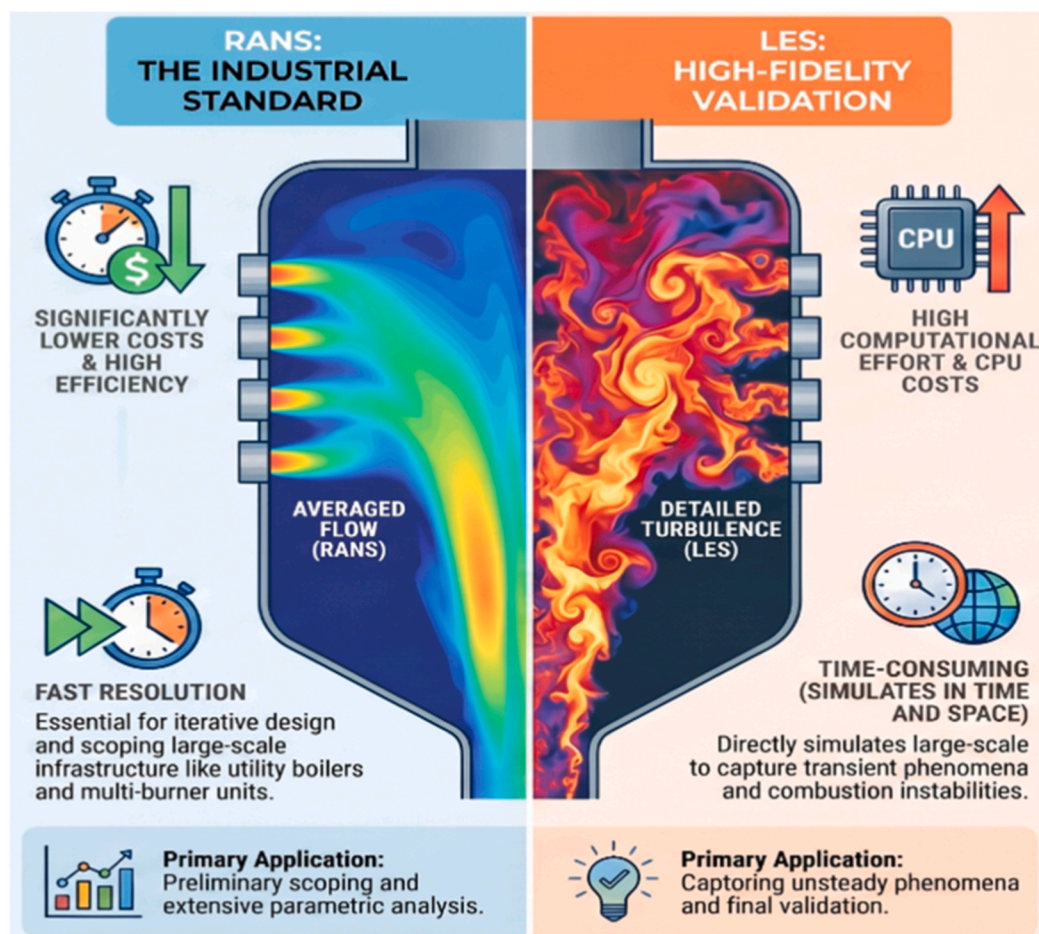


Fig. 4. Summary of advantages/disadvantages of using RANS and LES, main turbulence models for boilers, furnaces and gas turbines operating with ammonia. These implications will be critical for their use in either small or large systems.

the method was pointed out by Honzawa et al. [25] who found that the standard adiabatic FGM fails to predict emissions, hence a non-adiabatic FGM (NA-FGM) approach was needed to include heat loss effects on NO and CO – an important component in the use of ammonia firing. Due to ammonia's high Karlovitz number (Ka), the applicability of reduced-order models like FGM becomes limited, particularly in lean or highly strained conditions. Studies by Deng et al. [26] and Füzesi et al. [27] demonstrated that while FGM reduces computational cost, it underpredicts NO emissions—especially when paired with reduced mechanisms. Similar findings were reported by Zhang et al. [28], confirming that FGM performs poorly under stratified conditions. DNS results for a single-stage combustor revealed a marked disparity between the distribution of heat release rate (HRR) versus the reaction progress variable in turbulent ammonia flames and the corresponding laminar flame structure, a contrast not seen in methane combustion. Meloni et al. [29] approached the development of a User Defined Function (UDF), a “free-of-tuning” LES/FGM-based methodology for the assessment of the fuel bound NO_x emission relying on the distinction between an “in-flame” and “post-flame” contributions by using a combustion progress variable (set at $c = 0.99$), with the former being defined through FGM tabulations and the latter with Zeldovich's theory and 3-steps chemistry. Although the results were encouraging and showed good validation with experimental conditions, it was also evident that the approach only worked on specific cases. Thus, the challenges for FGM become more pronounced as the complexity of the system increases where transitions between multiple combustion modes render low-dimensional manifolds increasingly inadequate.

To bridge this gap, hybrid models are often used. For example, EDC

and PaSR models, employed by Somaratne et al. [30,31] and Zhang et al. [32], assume that reactions occur in fine turbulent structures where finite-rate chemistry is solved. The Dynamic Thickened Flame (DTF) model, used by Wang et al. [33–35] artificially thickens the flame to be resolvable on the computational grid while retaining finite-rate chemistry, making LES of complex configurations feasible. Work from statistical analyses (~72 publications) reveal that the distribution of computational methods and combustion model combinations is highly concentrated. The four primary combinations are: LES-DTF, LES-PaSR, RANS-EDC, and RANS-SAGE models, accounting for 75% of the literature. The DTF, PaSR, EDC, and SAGE models all compute chemical source terms via Arrhenius kinetics but diverge fundamentally in handling turbulence-chemistry interactions (TCI). Similarly, DTF artificially thickens flame fronts to resolve flame structures on computational grids, whilst PaSR treats each computational cell as an imperfectly mixed reactor where reaction rates are throttled by the ratio of chemical to turbulent mixing timescales. EDC confines reactions to fine turbulent structures, modelled as perfectly stirred reactors, but its performance shows extreme sensitivity to calibration constants. Finally, SAGE directly computes reaction rates using a presumed PDF method that needs to be properly resolved. In practical applications, Wei et al. [36] demonstrated strong agreement between LES-DTF simulations and OH-PLIF/PIV data, validating flame propagation and local extinction prediction. However, these models may over-thicken flames, limiting accuracy in lean or extinction-prone regimes.

2.3. Summary

Despite advancements in the various CFD methodologies and pros/cons in their utilization, Fig. 4, several interconnected challenges persistently limit the predictive accuracy of ammonia combustion CFD for practical applications. In the following paragraphs, the authors have found a great variety of works attempting to resolve several issues by using a great variety of approaches. Each would have its merits whilst also denoting challenges still to be resolved.

3. Industrial combustion systems

3.1. Boilers and furnaces

On a similar trend to small laboratory systems that have been studied for many topics on ammonia combustion, the use of the chemical for boilers and furnaces has also gained considerable interest. The main reason for this phenomenon is the lack of alternatives to provide sufficient energy-intensive substitutes to the use of natural gas or fossil-based fuels. Although many furnaces are migrating to electricity whilst boilers are considering bio-based resources for fuel switching, the reality is that ammonia remains as one of the best solutions to solve the problems of carbon intensity in these systems.

The potential of furnaces to serve as effective solutions for ammonia utilization as a primary fuel can be attributed to their inherent characteristics, including their geometrical scale, residence time, and the capacity for multi-stage fuel and oxidiser injection. A substantial amount of numerical research has been conducted on the characteristics and emissions of flammable mixtures for furnace-related applications, although primarily in the context of chemical reactors, reactor networks, and 1D flames. Conversely, factors that are promising in terms of stable and low-emission NH_3 combustion work adversely in terms of efficient modelling of the turbulent reacting flow, resulting in lengthy and detailed calculations for large-scale domains.

As a precedent, the work performed by Zhao et al. and their team evaluated the impact of ammonia in micro-planar combustors, which are systems developed to deliver high specific energy for systems similar to micro-thermo-photo-voltaic units. By designing a simple geometry, the team initially assessed the impacts of equivalence ratios, ammonia content and inlet flow rates, thus delivering emission trends [37]. Using OpenFOAM and integrating in the analyses the impact of solid boundary conditions (a Robin type condition that takes into account a natural convection heat transfer coefficient and a wall emissivity with values of $20 \text{ W m}^{-2} \text{ K}^{-1}$ and 0.85 for stainless steel 316), the group found that the small addition of ammonia to methane has large impacts on nitrogen oxides formation, particularly N_2O at the outlet region due to low gas temperatures and high NH concentrations (a problem raised in other research where the H^+ radical also contributes to the formation of the pollutant). In addition, and as expected, the inlet flow rate also has an impact on thermal performance, with CO being mitigated with the increase in NH_3 , impacting on components like radiation. Further analyses evaluated the same unit using ammonia, hydrogen and oxygen blends [38]. At low Re numbers, the variation of hydrogen content in the blend (from 0 to 50%) denoted in most cases a reduction in the outer wall temperature, a consequence of the reduction of the flame length due to the higher reactivity of hydrogen. Similarly, radiation efficiency is also affected at higher hydrogen content when the flowrates are low, a variation that decreases with higher flowrates as the flame power increases and its impact to the walls is of greater magnitude. Further analyses include perforated plates [39], previously described (as the study falls within the laminar velocity realm), where differential diffusion is intensified as a consequence of the change in flow profiles, further enhancing NOx abatement by the increased recirculation of species [40].

Other interesting analyses contemplate the use of other combustion methods. A considerable amount of effort has been dedicated to the

development of moderate or intense low-oxygen dilution (MILD) combustion furnaces. Operation within a favourable temperature range facilitates ammonia reduction pathways and achieves notably low NO emissions. However, a substantial increase in N_2O levels in lean conditions and combustion instabilities can markedly reduce MILD's applicability. The concept, experimentally validated, has attracted the attention of several groups worldwide. For example, Wang et al. [41] present an example of traditional and MILD ammonia combustion modelling in a reversed flow lab-scale furnace. The fuel composition comprised ammonia up to 4% in methane, and the results were validated using methane. The models employed in this study included EDC in Fluent formulation with Okafor mechanism, discrete ordinates (DO, method that discretizes the spatial domain and angular directions) for radiation, and k- ϵ standard for the turbulence RANS modelling. It is important to note that EDC application in MILD modelling can lead to overpredictions in NO emissions, with levels reaching 1400 ppm for 4% of NH_3 co-combustion. The combination of superfine pulverized coal combustion in a MILD regime has been demonstrated to exhibit potential for stable combustion and low NOx emission characteristics. In their study, Zha et al. [42] conducted numerical tests on a pilot-scale experimental 580 kW furnace. The aim of the study was to investigate the combustion mechanisms of traditional combustion (TC), unstable/-transition combustion, and MILD combustion. Their model was developed on the basis of RANS realizable k- ϵ , DO for radiation, and EDC in conjunction with DPM. The NOx calculations were decoupled using a β -temperature variable. Results showed that by controlling temperature and mass fraction recombinations, NOx could be considerably decreased compared to conventional combustion.

In a recent study, Ariemma et al. [43] presented preliminary results of ammonia/hydrogen and ammonia cracked combustion modelling in MILD combustor. The complementary simulation concentrated on hot spots in a Laboratory Unit CYclonic (LUCY) burner, a system extensively characterised experimentally to deliver good numerical validation. Turbulence modelling was conducted using the RSM model, while the radiation was represented by the DO model. The PaSR model was employed to simulate species transport, with a mixing constant of 0.5. The Shrestha et al. [44] mechanism was utilised. The experimental findings indicated the distributed nature of the reactive region for the cyclonic burner, while the PaSR model enabled the effective analysis of the MILD regime's specific aspects. In addition, a number of works were based on Rebola's et al. [45] methane-fuelled MILD furnace, with a capacity of 10 kW. Subsequent studies involved the extrapolation of results to ammonia combustion [46]. The objective of these works was to validate their axisymmetric numerical model. The dynamic PaSR model, incorporating the Mendiara and Glarborg mechanism, was implemented to model combustion-turbulence interaction. The reaction zone was identified based on NNH mole fraction. Numerical predictions showed rates exceeding 200 ppm of N_2O at 15% O_2 , a result that shows that careful tuning of the burner unit needs to be achieved even under MILD combustion.

Rashed et al. [47] modelled reduced 3D domain calculations for NH_3/H_2 mixtures with RNG k- ϵ and DO for radiation, using the CEU- NH_3 mechanism and dynamic mechanism reduction. For a 50% H_2 share in the fuel, NO emissions up to 9000 ppm were observed, and for H_2 levels exceeding 20%, a substantial increase in both temperature and NO emissions was present. This may be indicative of a transition to a classical flame structure. The numerical prediction of NO and N_2O was found to be consistently high in all cases. Furthermore, the numerical outcomes presented for Rebola's MILD configuration appeared to underestimate values along the axis, a phenomenon that extends even to the CH_4 validation. This outcome can be attributed to the implementation of the standard k- ϵ turbulence model, particularly in conjunction with axially centred two-dimensional round jets. This analysis is of importance, as it shows how the selection of the correct turbulence model would have different impacts on performance and emissions.

Ammonia in furnaces has also been mixed with other fuels. A

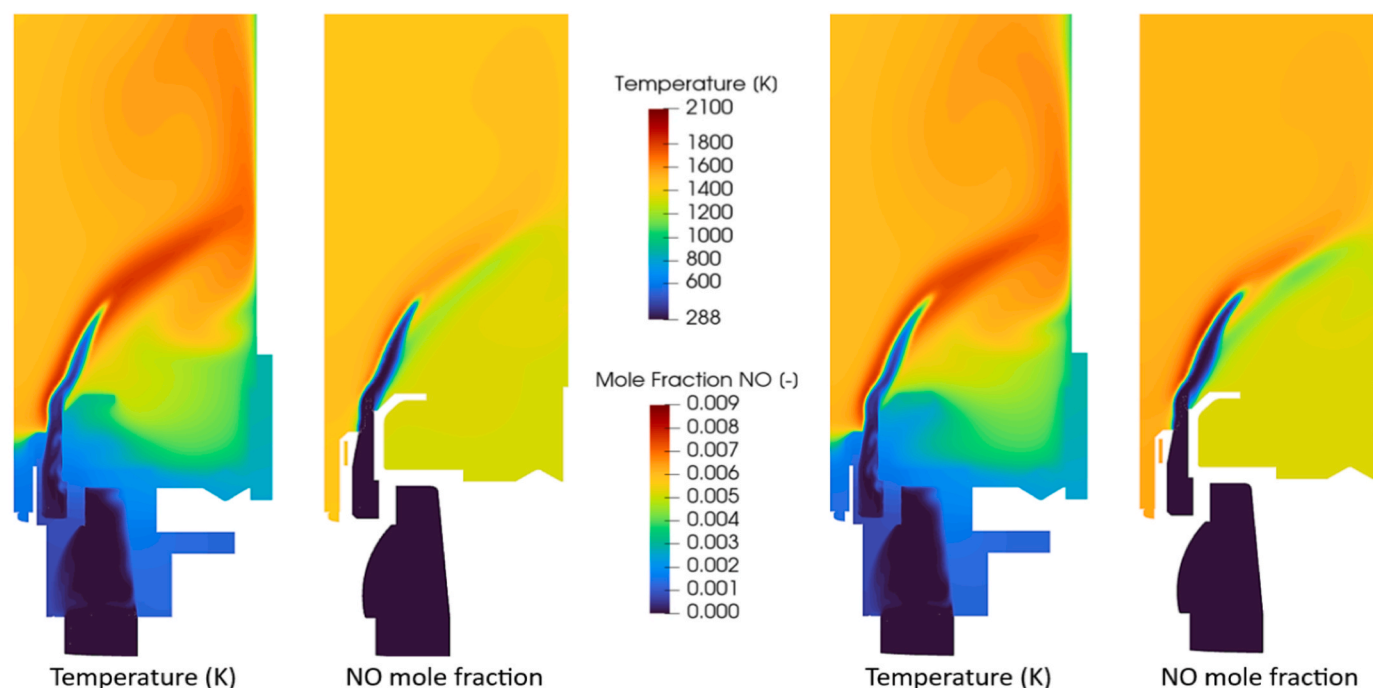
Nakamura 2019, 2734 ppmv NO (15 vol% O₂ dry)**Present work, 2853 ppmv NO (15 vol% O₂ dry)**

Fig. 5. Validates simulations show high reliability of burner units operating with ammonia blends. The work from Alnasif et al. delivered results 2.14 faster than other mechanisms (Reprint from Ref. [54] with permission).

numerical study of peroxide-enriched air for ammonia combustion operating in non-premixed mode was conducted by Gahdi and Lim for exploratory purposes [48]. The research demonstrated that the emission of NO increased with rising inlet and wall temperatures, as well as the percentage of H₂O₂ in the oxidiser mixture. As NO₂ denotes an opposite trend to NO, the effect emphasises the necessity to identify issue is raised by the unavailability of comprehensive experimental ammonia validation data for these types of furnaces.

Yang et al. [49] employed numerical simulations to assess the impact of an air-staged strategy and varying ammonia co-firing ratios on NO emissions. The study assessed a 10-kW ammonia co-firing furnace fuelled with city gas (methane (CH₄) at 88.9%, ethane (C₂H₆) at 6.8%, propane (C₃H₈) at 3.1%, and butane (C₄H₁₀) at 1.2% by volume fraction. It is important to note the high temperature dependence of the results, therefore great care should be taken when defining the conditions of heat transfer [49,50]. Conjugate heat transfer (CHT, directly coupling energy equations at the fluid-solid interfaces) was incorporated into the model. Research indicates that co-firing ratios exceeding 40% result in the production of N₂O, reaching up to 24 ppm in the context of pure ammonia staged combustion. The emission results were found to be consistent with the experimental campaign, showing that radiation tuning is also an important parameter when furnaces and boilers are numerically evaluated using the chemical.

Geometrical changes and their impacts have also been assessed. Methane-ammonia lean swirl flames were investigated by Jójka et al. [51] in a ceramic furnace chamber with optical access up to 25% of NH₃ in the fuel. The same furnace was tested utilising both jet [52] and swirl burners [53] during previous investigations. The modelling results were found to be in agreement with the emission and temperature measurements, with NO exceeding 2000 ppm for the maximal investigated NH₃ share. It was hypothesised that, due to the aerodynamically narrowed flow channels in the burner, small-scale combustion could be present through stirred premixed lean flames.

In a recent experimental and numerical campaign conducted under the AMBURN project, a combination of the previously mentioned thermo-flow models was utilised to extrapolate the power of the novel

Cardiff University ammonia burner applied to a 1 MW furnace chamber [5]. Laboratory-scale 10 kW burner validation tests with the Alnasif and Nagy mechanism [54] provided encouraging results, indicating the potential for low emissions across a diverse range of applications. Ambitious experimental campaigns supported the progression of the analyses at larger power rates. Specifically in the context of furnaces, the CFD results yielded valuable guidance for the scaling and modification of the burner, Fig. 5. By delivering a novel reaction mechanism and comparing it with highly influential mechanisms [55], the work showed the relevance of having a reliable, reduced mechanism for optimization exercises, a component that is critical to easily determine the reactivity of species interacting with structural components, flame profiles and heat transfer regimes. The findings were ultimately validated through experimental results and extrapolated for a 500 kW burner fuelled by 20% cracked ammonia. It seems possible to control the emissions of ammonia during combustion by carefully shaping local conditions, thereby achieving stable, industrial-scale flames. The findings of the study demonstrated that a collaborative effort between experimental and numerical investigators is vital for achieving low emissions and effective development of ammonia-related applications.

Zheng et al. [56] also evaluated the potential of using biomass co-firing with ammonia in a 15 kW power, non-swirling, non-premixed unit. Devolatilization and char combustion models were combined within the reaction domain. Although no further details are provided for the resolution of ammonia combustion (apart from some species formation), the results are of interest for progressing on the co-firing of these two fuels. Overall, the work shows the mitigation of CO₂ emissions, as anticipated, with the change in flame shape at various biomass/ammonia rates. Further work is recommended, particularly due to the awareness from industrial companies interested in using biomass/ammonia co-firing for processes relevant to farming, countryside locations and waste wood streams.

3.2. Ammonia-coal co-firing

In contrast to gas-fed boilers, there is another interesting application

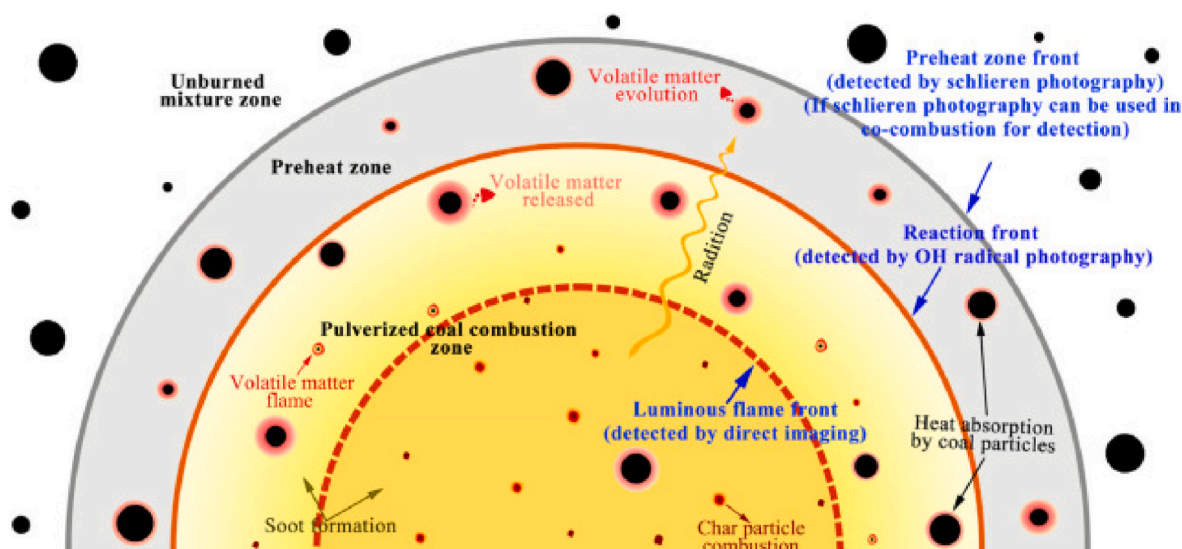


Fig. 6. One dimensional assumption of co-combustion flame structures (Reprint from Ref. [65] with permission).

for ammonia in boiler units of large capacity: co-firing with coal. The increase in power requirements in countries like China, and the use of coal in economies like Japan and South Korea, are taking vital roles in the use of ammonia replacement for these power applications. Several companies currently pursue the use of ammonia-coal co-firing as the process appears to be much more benign to the environment whilst also serving to improve some combustion features. For example, the company JERA (Japan) has reached agreements to procure up to 500,000 tonnes/year of ammonia for their plant in Hekinan, substituting up to 50% coal by 2030 [57]. Mitsubishi Power has also announced their intention to develop 100% ammonia-fed boilers for heating [58], whilst IHI has been promoting their combustor technology to approach countries like India, Malaysia, Vietnam and Indonesia to start considering ammonia replacement [59]. South Korea's national program for the use of hydrogen and ammonia as decarbonisation fuel by 2030 seeks to deliver electricity in up to 2.1% by 2030, scaling up to 7.1% by the mid-2030s [60]. The Korea Electric Power Corporation (KEPCO), one of the largest of its kind in Asia, just announced the completion of the country's largest ammonia combustion testing facility in May 2025. Located at KEPCO's Power Research Institute, the new 1 MW test bed is designed to verify high-efficiency, low-emission combustion of ammonia. As part of this transition, KEPCO aims to replace 32 coal plant start-up burners with ammonia-only models by 2027 and initiate a full-scale demonstration of 20% ammonia co-firing at a 1000-MW-class power station. The initiative is expected to cut carbon dioxide emissions by approximately 1 million tons annually [61]. With a similar vision, China jumped on the train of ammonia energy in 2022. The Chinese government took a significant step towards promoting the development of new energy storage, releasing the "14th Five-Year Plan for New Energy Storage Development Implementation Plan" jointly with the National Development and Reform Commission (NDRC) and National Energy Administration (NEA). Notably, ammonia was included as an energy storage medium for the first time [62]. In July 2024, an official ammonia co-firing strategy was released as part of the country's economic action plan. The strategy calls for the transition of China's existing coal-fired power plants. By 2027, retrofits must have achieved at least 10% co-firing ability with either biomass or green ammonia [63]. Finally, although the next Five-year plan will not be ready until 2026, energy experts believe that for China's energy independence a policy umbrella around the use of green ammonia is critical [64].

Therefore, the proper analysis of ammonia/coal co-firing is critical in this area. With the complexity of having solid particles in combination with gaseous ammonia, the problem becomes extremely challenging for experimentalists.

A very revealing, interesting study conducted by Xia et al. [65] reports the flame propagation mechanism for pulverized coal co-fired with ammonia. The research team observed that ammonia/coal co-firing produced higher flame propagation velocities than pure coal, whilst the use of pure ammonia would be dependent on the equivalence ratio employed. The study expanded on the explanation of the losses/gains during the combustion process of these blends through three zones (coal combustion zone, preheat zone, unburned mixture), Fig. 6. Coal particle devolatilization is within the reactions taking place in the process, whilst the formation of soot is also enhanced at the reaction front. The coal particle follows a sequence of heating up (by the reaction zone and radiation), the release of volatile matter and its combustion, and char combustion, all occurring simultaneously. Soot particles form as part of a secondary pyrolysis process that comprises the consumption of volatile matter. It was observed that using ammonia under lean conditions leads to some positive effects (i.e. radiation and volatile matter production) that are greater than the heat absorption of the coal particles. However, the increase of volatile matter, which increases the local equivalence ratio, is detrimental under rich conditions. Similarly, Zhu et al. [66] observed that ammonia ignites earlier than coal, which in turn accelerates the release of coal's volatiles, concurrently shortening the ignition time whilst increasing flame's temperature and length.

Interestingly, recent works have found that by co-firing in ratios of up to 30% increase NO_x, whilst above this point nitrogen oxides are reduced due to the post-combustion reactions and flame processes occurring with this ammonia addition [67]. It has also been observed that the carbon content in the unburned gas and fly ash increased, a process that is directly linked to the competition for the oxygen content in the field [68]. As for NO production, the high peak of HCN levels precludes the formation of the pollutant up to 30%, whilst higher ammonia concentrations generate unreacted, hot ammonia streams that DeNO_x the product gases [69]. Other important species such as HNO, NNH, ONNH, NH₂, H, etc. play an important role depending on the injection method and location of the air/fuel streams along the boilers/furnaces. More information can be found in the work by Wu et al. [68].

It is important to emphasize some recent reviews such as the one from Wu et al. [68] who clearly approach some of the current works dedicated to ammonia/coal co-firing. Apart from the description of the several methods used to resolve CFD modelling, their work presents an interesting aspect of the current research on the subject – the importance of ammonia in the radiation produced during coal combustion, which they argue is the focus of recent research. Models such as the Discrete Transfer Radiation Model (DTRM), the Rosseland model, the Discrete

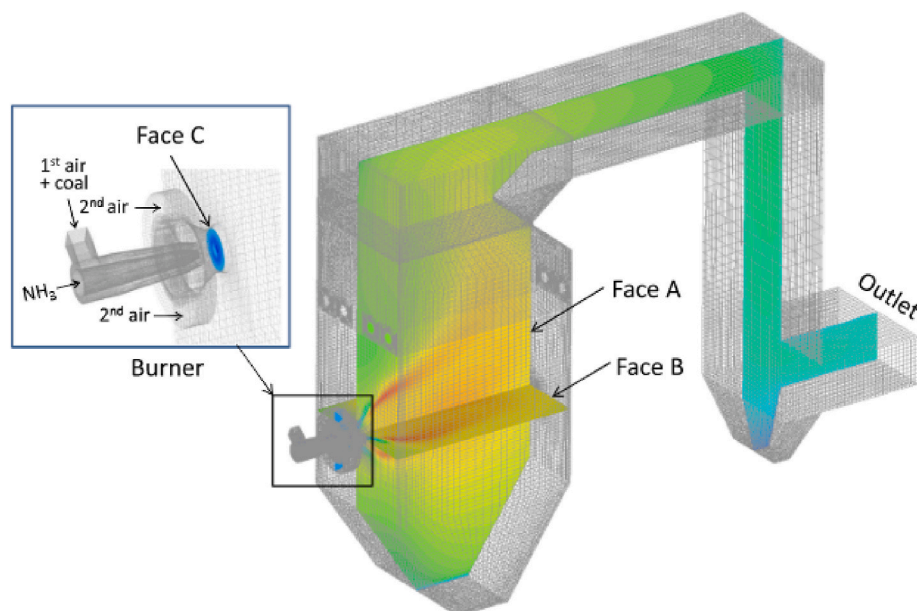


Fig. 7. Ammonia-coal co-firing numerical analyses in an industrial boiler (Reprint from Ref. [75] with permission).

Ordinates Model (DOM) and the P1 Model are described as the ones mainly used for the task. With variations that go from optical thickness, radiation exchange between gas and particulates, radiation fluxes validation, non-grey effects, and memory/computational requirements, each model has something to offer. Devolatilization, combustion models, volatiles, char oxidation, and the great variety of potential reaction mechanisms, make this concept an interesting, complex one for computational resolution.

Ma et al. [70] conducted some fundamental analyses to determine the pyrolysis and combustion behaviour of ammonia-coal blends. Apart from a new mechanism born from these studies, it was found that co-firing coal with ammonia accelerates the coal heating rate and pyrolysis process due to the heat released by the ammonia reaction. However, the consumption of oxygen by ammonia and its low reactivity delay the homogeneous ignition of the blends, particularly during high-temperature and low-oxygen atmospheres. Further, ammonia pyrolysis is slower than coal pyrolysis, an important parameter for the interaction of ammonia with downstream reaction pathways.

Having these points in consideration, the work of Zhang et al. [71] evaluated the potential of using MILD combustion for ammonia/coal co-firing. By studying the heat transfer characteristics of the system of interest, they found that as the ammonia ratio increased, the gas absorption coefficient increased, and as the radiation heat transfer was enhanced, the convective heat transfer also increased. Ammonia addition improved flame stability, and the strong flue gas recirculation of MILD combustion appeared to decrease NO_x emissions.

By evaluating a drop tube furnace, Wang et al. [72] evaluated the impact of coal on ammonia conversion using experimental and numerical methods. ANSYS FLUENT 18.0, the Realizable $k-\epsilon$ turbulence model, the finite-rate/eddy-dissipation model and the discrete ordinate (DO) model for radiation were used. Chemical reaction rates were adjusted based on experimental findings, and a ~ 3.7 million mesh was used for the geometry of interest. After experimental validation, the numerical study revealed different trends for the nitrogen bound to ammonia ($\text{NH}_3\text{-N}$) when interacting with either volatiles or char. It was found that the interaction of both pulverized coal and ammonia led to higher NO_x emissions than the pure coal case, with fuel-N showing three times greater the conversion towards the formation of NO_x. Interestingly, ammonia reaction with coal produced different NO reactions to those with char, a process that appears to be caused by the presence of ammonia and volatile species that compete for O and OH radicals, being

the latter more reactive initially, thus leaving char after their consumption. Char, less reactive than ammonia-based species (e.g. NH_x , NNH , etc.), would give pace to ammonia oxidation with the remaining oxygen-based radicals, accelerating the production of HNO and other NO formation species, increasing in this way the formation of NO_x compared to pure fuels.

Zhang et al. [73] numerically evaluated a novel design conceived to improve NO emissions when firing and co-firing coal and/or ammonia in a 50 kW power unit. The unit works using pulverized coal which is entrained by premixing with the primary air, and the use of secondary air that helps the pulverized coal to burn out. Both experimental and numerical analyses have demonstrated the versatility of the concept. At the bottom end of the primary air tube, there are several flame stabilizing teeth to enhance flame anchorage and improve flame stability. As the secondary air passes through a swirler, the resulting flow will create the average swirling flow field (i.e. with recirculation zones), which in turn helps the ignition and combustion of pulverized coal. When co-firing ammonia in this prototype burner as benchmark, ammonia is injected via the central tube of its array. By using 20% ammonia co-firing, the team found a drastic reduction in NO emissions ($\sim 52\%$) by the use of tertiary jets through their named concept "HAJA". This was particularly observed when the tertiary air jet was increased as a consequence of the lagging of the combustion region, which led to the increase of the ammonia pyrolysis region, although the effect also deepened the air-staging effect, thus leading to lower temperatures. Finally, it is suggested that the lowest NO emission is achieved with an air distribution ratio of 25:50:25 (between the three air injection modes) and a tertiary air injector diameter of 2.0 mm.

Work by Yadav et al. [74] performed analyses in a 760 kWth semi-industrial furnace using a non-adiabatic multi-stream flamelet/progress variable (FPV) approach with 20% ammonia in a coal co-firing configuration. Two ammonia injection cases were evaluated using either ammonia injection from the burner or from a further downstream injection port (at 1.0m away from the burner base) into the combustion chamber. A new approach was introduced by considering the oxidizer temperature as an additional lookup parameter through different streams (primary, secondary and tertiary). Large Eddy Simulation (LES) ammonia/coal flames were conducted using an unstructured Finite Volume Method (FVM) code, the NuFD/FrontFlowRed package. Using a 7-dimensional non-adiabatic chemtable model (7D NA-FPV-LES), oxygen and NO were properly captured and validated

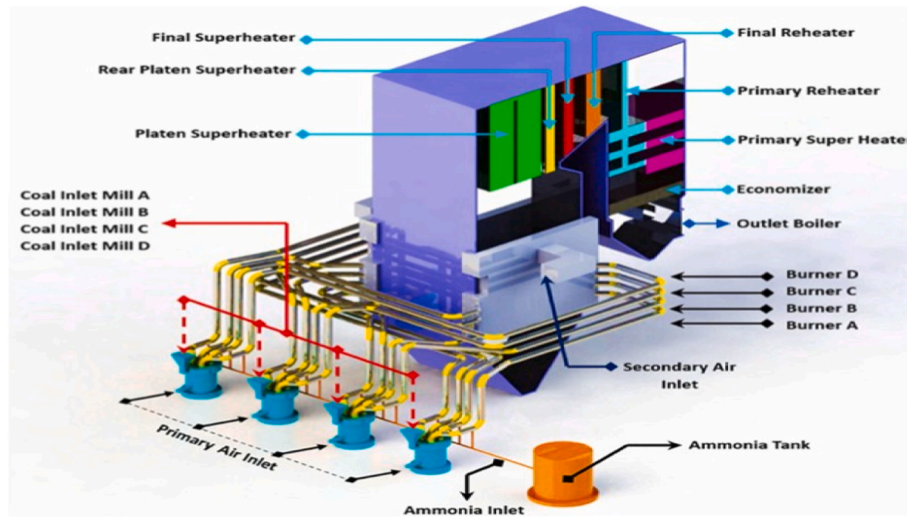


Fig. 8. Boiler simulation domain of Pangkalan Susu (Reprint from Ref. [76] with permission).

from experimental findings. Results showed that downstream ammonia injection leads to higher peak temperatures, whilst its injection under reducing conditions brings down NO concentrations, phenomena associated to the reduced dissociation of ammonia close to the burner head. Additionally, it was observed that a higher H_2O mole fraction was produced due to this dissociation under the studied conditions, leading to a water gas shift reaction that resulted in a decreased concentration of CO. The concept, exploratory at the time, opens several opportunities for implementation at larger scales.

On a more industrial scale, research has been conducted to evaluate the potential of coal power units being fed with ammonia. Zhang et al. [75] evaluated the use of ammonia (ranging from 0 to 80 vol%) in a 8.5 MW_{th} burner, Fig. 7. Excess air ratio and staging air ratio were kept constant at 1.18 and 30%, respectively, over 7 different cases. Results showed that the increase in ammonia content drastically shifts the flame shape with a central recirculation zone that is penetrated by the ammonia jet at values > 40%. The effect alters the swirl strength with a drastic change in heat flux distribution on the walls, leading to a secondary effect of improper ammonia combustion. While the proportion of radiative heat decreases with ammonia, the proportion of convective heat increases due to the amount and velocity of the gas. Conclusions are drawn on the high potential of ammonia-coal co-firing when ammonia content is below 40%.

Adi Saputra et al. [76] numerically evaluated the co-firing of

ammonia and coal in the Pangkalan Susu Power Station, Indonesia. The units of interest (3 and 4) have a capacity of 210 MW. The model, Fig. 8, denotes the strategy to use various burner injection ports for ammonia use. Ammonia concentrations varied from 5 to 15% using a reduced mechanism for ammonia in a 1.6 million elements mesh. The results show a decrease in temperature with the increase of ammonia, an effect believed to be caused by water increase due to ammonia reactions.

At higher powers (600 MW), Lyu et al. [77] conducted a very thorough analysis of the previously mentioned supercritical coal-fired utility boiler with air staging combustion. A RANS κ - ϵ model analysis was employed using a ~ 1.7 million cells mesh. Ammonia was varied from 0 to 50% in the blending ratio, whilst oxygen at 21, 30 and 40% was attempted with injection at various locations across the burner layout. Different to the lower power case, ammonia showed excellent burnout characteristics, whilst NO_x emissions were drastically reduced using air staging. However, the addition of ammonia also impacted on the flue gas temperature, an effect linked to the reduced radiation caused by the reduction in pulverized coal. The temperature decay was recovered by adding oxygen, although NO_x are also increased due to this increase in O₂ content. Finally, the overall exergy efficiency increases with the use of oxygenated combustion.

Works on a larger system operating at 660 MW were performed by Wei et al. [78] who studied the use of coal or sludge with ammonia for power generation. Using a complex, industrially relevant configuration

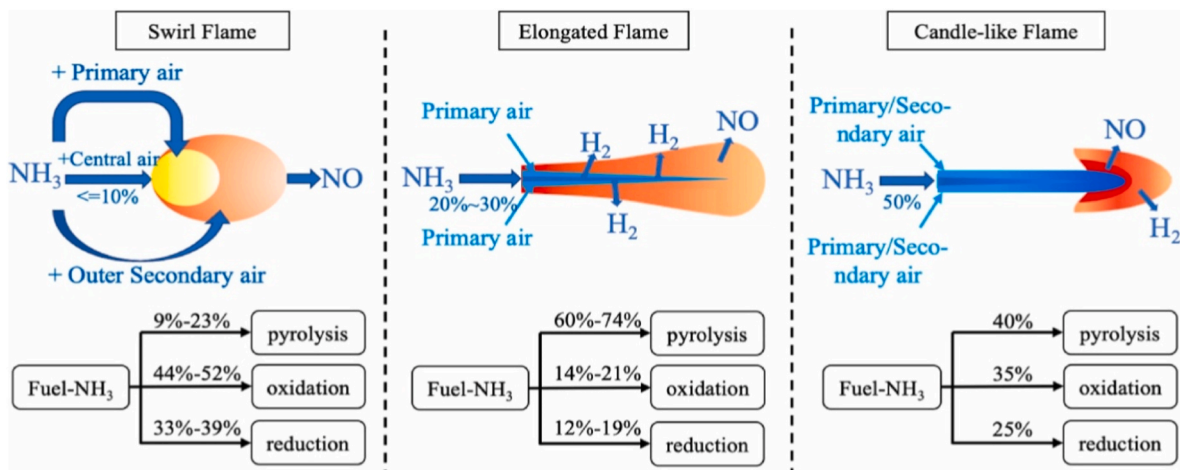


Fig. 9. Schematics of coal/NH₃ co-firing in a swirl burner with three different flame structures (Reprint from Ref. [79] with permission).

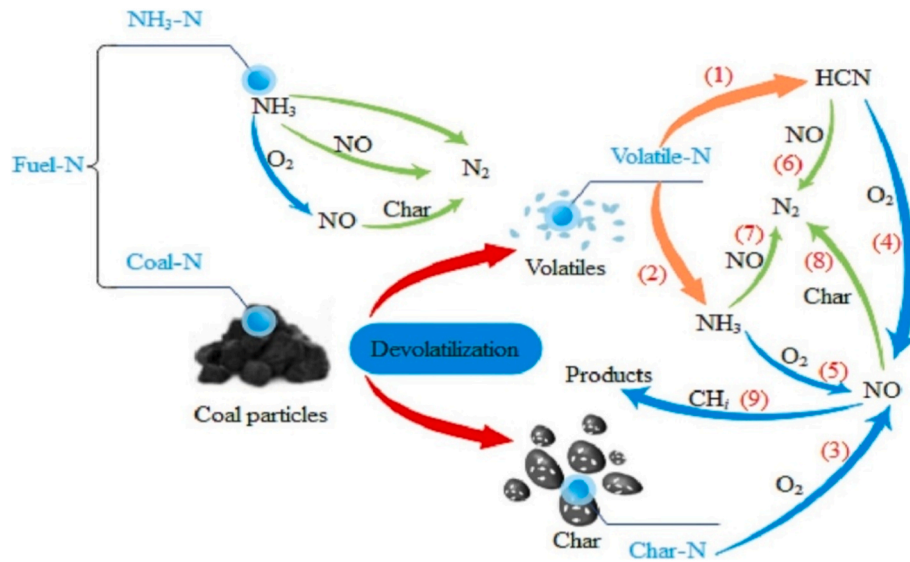


Fig. 10. Fuel NO formation mechanism (Reprint from Ref. [80] with permission).

with various pulverized coal burners and secondary air nozzles, a CFD model run using FLUENT in a 2.02 million cells with the RANS κ - ϵ model was performed. The group found more H_2O production after adding ammonia, which evaporated and absorbed heat from the water, whilst incomplete combustion of solid fuel depended on the position of the ammonia injection (i.e. which is in line with the previously mentioned phenomena of higher ammonia reactivity). It is emphasized that these studies are still under assessment for their further implementation under real industrial conditions.

Liu et al. [79] adopted the low NO_x swirl burner used in a 1000 MWe pulverized-coal boiler for five different blending ratios (0, 10, 20, 30 and 50% based on calorific value). Three different injection locations were evaluated along the boiler (e.g. central, primary, inner or outer secondary) employing a ~ 0.79 million cells mesh. As expected, the temperature distribution across the flame front was highly dependent on the type of injection used and the blend employed, which also had an impact on the final emissions. In summary, the group identified different flame shapes, Fig. 9.

With a swirling flame, the ammonia enters the high temperature region and reacts with oxygen, being oxidized in up to 52% with a high boost in NO emissions. As for the “candle-type”, reactants are mixed early and reacted in the central part of the unit. The process of ammonia consumption occurs by pyrolysis, which leads to H_2 production, rela-

Fig. 10. The 1,050 MW unit presents an industrial layout with a primary combustion zone, the main burner comprised of 6 coal burners, three oil nozzles, and 12 secondary air nozzles. In the burnout zone, six Separated Over Fire Air (SOFA) nozzles are strategically positioned for the burnout of combustibles. The computational domain also included the platen superheater and final superheater. Findings agree with previously raised works, with the rapid ammonia oxidation caused by the high temperature zone which also impacts in the reduction of slip ammonia, whilst the process also reduces the DeNO_xing effect, which seems to be also dependant on the SOFA ratio. While temperatures drop between 100 and 200K with ammonia addition, the higher H_2O content surge in the flue gas boosts coal burnout, an issue that may cause low-temperature corrosion in exhaust gas components. Similar findings were obtained by Ahmad et al. [81] who evaluated a 1GW Ultra Super Critical Coal Fired Power Plan being fired with 5-60% ammonia (thermal) ratios. Results reassure the findings for the decrease in emissions by injecting ammonia at the bottom of the unit. However, in addition to the corresponding reaction analyses and power losses previously addressed, the team evaluated the potential impacts caused by the flue gases product from the process. The acid dew point temperature was also analyzed using the Verhoff and Branchero equation, Eq. (1) [82]. The acid dew point of H_2SO_4 was preferred due its higher dew point than HNO_3 and H_2SO_3 .

$$T_{ADP} = \frac{1000}{2.9882 - 0.13761 \log P_{H_2O} - 0.2674 \log P_{SO_3} + 0.03287 \log P_{H_2O} \log P_{SO_3}} - 273.15 \quad (1)$$

tively controlling NO (although emissions are still higher than pure coal). Finally, the elongated flame shows the best NO performance, as the ammonia is surrounded by the primary air, separating the ammonia from the high temperature zone, inhibiting ammonia oxidation and leading to pyrolysis as the dominant reaction mode, which leads to higher stabilities and moderate NO formation. Details of the modes of reaction are presented in Fig. 9.

Jin et al. [80] also evaluated, for exploratory assessments critically needed before implementation, a boiler unit operating with various ammonia ratios and air staging conditions. NO modelling was performed using a post-processing approach after the converged solution of combustion was obtained. The schematic of the mechanism is presented in

It was found that the acid dew point temperature decreases with ammonia increase due to the reduction of SO_3 , which is an inconvenience at 30% (thermal) co-firing ratio, as the dew point temperature crosses the stack temperature. This can potentially cause severe acid corrosion on the surface of heat exchangers (with impacts on heat transfer efficiency). Further, the acid droplets can react with surfaces and fly ash that can lead to fouling. Therefore, the team suggests modifying heat exchangers if ammonia is employed for coal co-firing.

Recent work produced by Juangsa et al. [83] models a 350 MW power plant via ANSYS. The work investigates the use of 20% ammonia

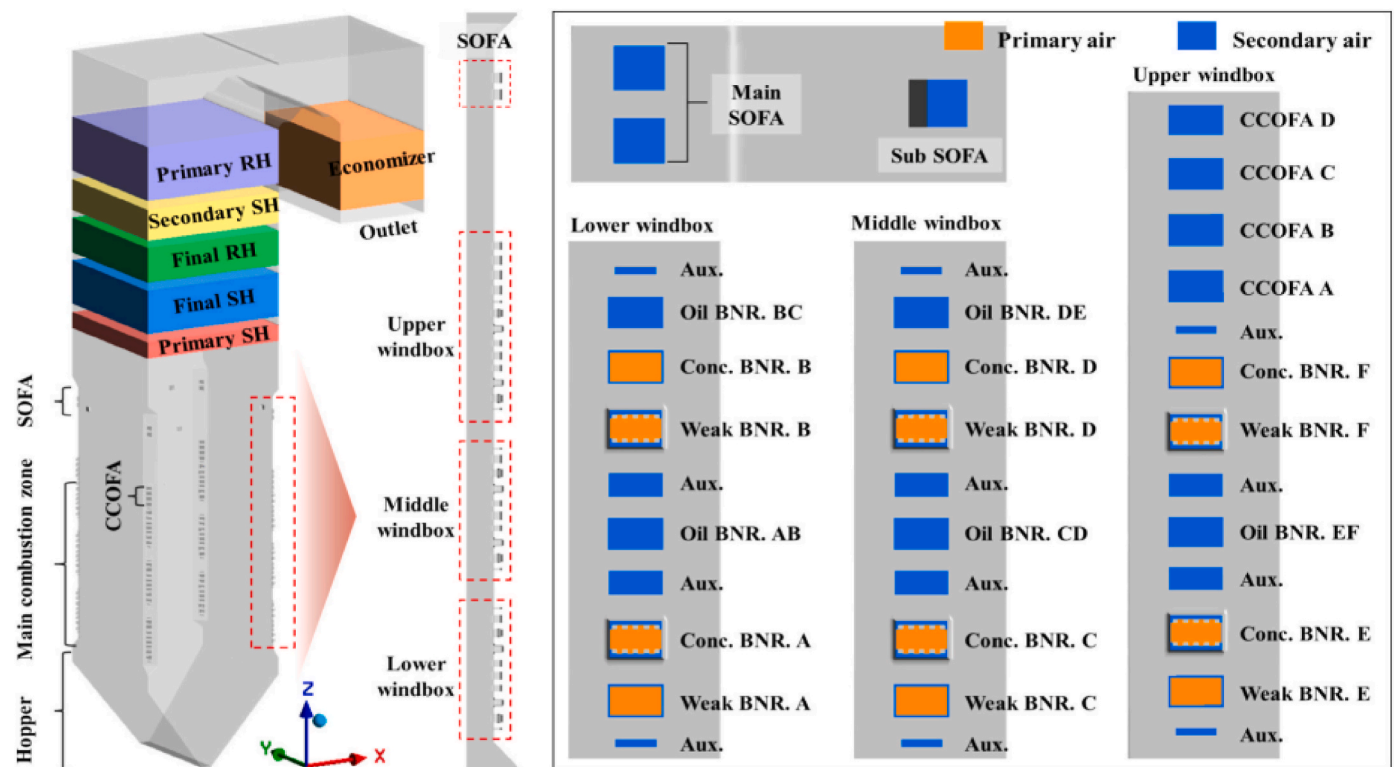


Fig. 11. Schematic of the 550 MW tangentially fired boiler geometry and burner arrangement (Aux.: auxiliary, Conc.: concentrated, CCOFA: close-coupled overfire air, SOFA: separated overfire air, RH: reheater, SH: superheater). (Reprint from Ref. [85] with permission).

and the addition of flue gas recirculation, a method to reduce emissions and maximise product recovery. The concept promises a reduction in furnace peak temperature ($\sim 100^\circ\text{C}$), which added to the recirculation and further recombination of unburned ammonia brings down NO emissions in up to 31%. The work innovated in improving the commonly used Eddy-dissipation model (EDM), which overpredicts emissions, by locally modifying constants based on Re numbers. Similar findings were reported by Zeng et al. [84,85] as various groups in South Korea are currently engaged with the topic of ammonia combustion for coal replacement in power plants. Their results, obtained through simulations in a 550 MW boiler unit via Realizable $k-\epsilon$ and DO models, showed the complexity of using many alternatives for injection strategies, hence justifying the modelling tools employed. Initially, 12 different ammonia blending methods and scenarios were used, with ammonia being injected at different locations of the combustion zone. Efficiency losses and heat absorption values were defined, showing how the injection of ammonia in different cases can increase losses in up to $\sim 4.6\%$ whilst also sacrificing heat absorption in walls and heat exchangers. However, on a positive side, it was found that the injection of ammonia at the bottom of the burner can promote a more extensive distribution of high-temperature zones and maintain lower levels of NO_x emissions. The effect was associated to the surge of a DeNO_xing area formed below the main combustion zone. The area seems to appear because some of the ammonia enters the hopper zone along with the sinking coal, where the lower temperature and oxygen concentration in this region favor the reaction of ammonia for reducing NO [84]. Additional findings [85] denoted how the use of 20% ammonia was less intense in the reduction of CO₂ but also in the increase of NO and temperature drop. However, when the unit was operated at 50% ammonia substitution, higher NO were detected. Although it was recognised that large CO₂ mitigation is achieved by this high ammonia concentration, it was also evident that the use of ammonia at high concentrations is a technical challenge. It was also found that by adjusting SOFA up to 23% could drastically reduce NO and improve coal burnout, although maintaining thermal

performance was the main drawback of the study. The complexity of the burner can be seen in Fig. 11, thus justifying numerical works to find the ideal conditions for operation at large power generation using the proposed blends. Overall, the team found in the iteration process that the best solution would be the use of a single burner injection at mid furnace level (Case 4), as this configuration creates an extensive high temperature zone while maintaining coal burnout efficiency, which leads to furnace outlet temperatures of 1514.18 K and NO emissions of 124.76 ppm.

Other works address the use of desulfurization systems to support ammonia/coal co-combustion. Coal presents several elements, including carbon, hydrogen, oxygen and sulphur. Depending on the quality of the coal, the content of each element would vary. However, considering most practical cases, there would be always a portion of sulphur in the selected coal. Although free-sulphur-ammonia would reduce emissions product of the combustion of sulphur (e.g. H₂S), the reality is these will still be present in the flue gases. Therefore, Tong et al. [86] numerically assess and optimize a system for desulfurization of the streams products of ammonia/coal co-firing inside a burner. Through Response Surface Methodology (RSM) and Multi-Objective Optimization Design (MOD), the study optimized parameters such as desulfurization efficiency, pollutant emissions, and combustion performance. The system consisted of a swirl burner, a combustor case and a porous media made of calcium oxide. A simplified reaction model was used for the calcium reaction, whilst for the combustion process a RANS realizable $k-\epsilon$ model with Eddy Dissipation Concept and a simple reaction mechanism (using main ammonia and coal reactions) was employed. It was found that the ratio of ammonia/coal had an impact on SO₂ production, as expected. However, the conclusions depict that this increase will also lead to greater pressure losses, potentially leading to unstable combustion, an important parameter to consider for future designs (as explained by the authors).

Circulating fluidized bed (CFB) reactors have also been assessed for their utilization with ammonia blends at large power [4], although

Table 1

Various CFD methods for the resolution of the relevant literature (NR: Not Reported).

Reference	System/study	Turbulence model	Turbulence-chemistry/ combustion model	Radiation	CFD solver	Chemical kinetic mechanism	Validation
[37]	CH ₄ /NH ₃ premixed micro-planar combustor	Laminar	NR	Robin-type condition	OpenFoam 5.X	GRI-Mech 3.0	Numerical/experimental basis reported
[38]	NH ₃ /H ₂ -O ₂ micro-power system	Laminar	Detailed chemistry	Mixed Thermal	ANSYS Fluent 18.1	Drake et al. (1989)	Validated against available experimental data
[39]	Perforated-plate NH ₃ /O ₂ micro-combustor	Laminar	Detailed chemistry with Finite Rate Model	Conjugate Heat Transfer	ANSYS Fluent 18.1	Drake et al. (1989)	Experimental validation from previous works
[40]	Perforated-plate NH ₃ micro-power system	Laminar	Detailed chemistry with Finite Rate Model9	Conjugate Heat Transfer	ANSYS Fluent 18.1	Drake et al. (1989)	Validated using experimental data from methane/air tests
[41]	NH ₃ /CH ₄ reversed-flow MILD furnace	RANS (Standard k-ε)	EDC	Discreate Ordinate	ANSYS Fluent 19.2	Okafor et al. (2018)	Experimental emissions
[42]	NH ₃ /pulverized-coal MILD	RANS (Realizable k-ε)	EDC	Discreate Ordinate with WSGG	NR	Several sources/ bespoke mechanism	Experimental values using pure coal
[43]	MILD reactors/ reactive structures	RANS (RSM)	Timescale/reactive-structure analysis	Discreate Ordinate with WSGG	ANSYS Fluent	Shrestha et al. (2021)	Fundamental/model comparison
[46]	Pure NH ₃ MILD furnace	RANS (Standard k-ε)	Dynamic PaSR	Discreate Ordinates	OpenFOAM	Mendiara & Glarborg (2009)	Experimental combustion validation
[47]	3-D NH ₃ /H ₂ reversed-flow MILD	RANS (RNG k-ε)	SAGE detailed chemistry	Discreate Ordinate with WSGG	CONVERGE	CEU-NH ₃ (2020) + dynamic mechanism reduction	Previous works by the research team
[48]	H ₂ O ₂ -enriched NH ₃ combustion	RANS (Realizable k-ε)	EDC	Discreate Ordinate with WSGG	ANSYS Fluent R22	Otomo et al. (2018)	Experimental validation from existing literature
[49]	NH ₃ co-firing + air staging	RANS (RNG k-ε)	EDC	Discreate Ordinate with WSGG + CHT	OpenFOAM-based customized solver	Okafor et al. (2018)	Experimental NO validation
[50]	CH ₄ /NH ₃ swirl flames	RANS (RSM and SST k-ω)	EDC	Discrete Ordinate	ANSYS Fluent 22 R2	Okafor, Xiao & San Diego mechanisms compared	Experimental NO/CO validation
[53]	CH ₄ /NH ₃ premixed swirl flames	RANS (RSM)	EDC	NR	ANSYS Fluent 2019 R3	Xiao et al. (2016)	Experimental
[54]	Compact NH ₃ /H ₂ kinetic mechanism	Model-dependent)	EDC	Discrete Ordinates	ANSYS Fluent 2024 R1	New mechanism proposed	Experimental validations from previous works
[55]	Laminar NH ₃ /air flame radiation	Laminar	Detailed chemistry	Radiation heat-loss model	PREMIX Chemkin-Pro v17.2	Nakamura et al. (2017) and AramcoMech 2.0	Experimental/previous flame data
[56]	Biomass/NH ₃ co-firing	RANS (Standard k-ε)	Multi-Phase	P-1 Model	ANSYS Fluent 2020 R2	Biomass/NH ₃ reduced mechanism/various sources	Experimental validation from the literature
[70]	NH ₃ /coal pyrolysis & ignition	NR	Detailed pyrolysis/ignition chemistry	NR	OpenFOAM-V2112	New mechanism proposed	Experimental
[71]	Coal/NH ₃ MILD combustion	RAN S (Realizable k-ε)	EDC	Discrete Ordinates with WSGG	ANSYS Fluent 18.0	Reduced Coal/NH ₃ mechanism/various sources	Experimental coal combustion
[72]	NH ₃ -N conversion in coal co-firing	RANS (Realizable k-ε)	Detailed N conversion chemistry	Discrete Ordinates with WSGG	ANSYS Fluent 18.0	Reduced Coal/N/ NH ₃ mechanism/various sources	Experimental/numerical
[73]	Low-NO NH ₃ /coal burner	RANS (Realizable k-ε)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent	NH ₃ /coal mechanism	Experimental NO emission from literature
[74]	Semi-industrial NH ₃ /coal burner	LES	Particle-Source-in-Cell (PSI-Cell)	Discrete Ordinates with WSGG	NuFD/FFR	Okafor et al. (2018)	760-kWth semi-industrial experimental validation
[75]	Pulverized-coal combustion facility	RANS (Realizable k-ε)	EDC	Discrete Ordinates with WSGG	ANSYS Fluent 15.0	Reduced Coal/NH ₃ mechanism/various sources	NR
[76]	210-MW coal-fired plant	RANS (Standard k-ε)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent 2023 R2	Reduced Coal/NH ₃ mechanism/various sources	Plant-scale case study with coal
[77]	600-MW utility boiler	RANS (Standard k-ε)	Finite-rate/eddy-dissipation	P-1 Model	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Utility-boiler application
[78]	NH ₃ /sludge/coal utility boiler	RANS (Standard k-ε)	NR	P-1 Model	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Design conditions (Case 0)

(continued on next page)

Table 1 (continued)

Reference	System/study	Turbulence model	Turbulence–chemistry/ combustion model	Radiation	CFD solver	Chemical kinetic mechanism	Validation
[79]	NH ₃ /coal low-NOx swirl burner	RANS (Realizable k- ϵ)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent 2021 R1	Reduced Coal/NH ₃ mechanism/various sources	NR
[80]	1050-MW boiler, ultra-low load	RANS (Realizable k- ϵ)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Experimental condition using coal
[81]	1000-MWe boiler, NH ₃ injection	RANS (Standard k- ϵ)	EDM	P-1 Model	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Large boiler at 8.5 MW and full load with coal
[83]	350-MWe boiler with Flue Gas Recirculation	RANS (Standard k- ϵ)	Zonally selective Re-scaled adjusted EDM	Discrete Ordinates	ANSYS Fluent 2023 R2	Kobayashi Mechanism/Modified reaction	Plant-scale case study with coal (Case 1) and other NH ₃ studies (Case 2).
[84]	Tangentially fired boiler	RANS (Realizable k- ϵ)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Experimental using pure coal data
[85]	Tangentially fired boiler optimization	RANS (Realizable k- ϵ)	Finite-rate/eddy-dissipation	Discrete Ordinates with WSGG	ANSYS Fluent	Reduced Coal/NH ₃ mechanism/various sources	Experimental using pure coal data
[86]	NH ₃ /coal burner + desulfurization	RANS (Realizable k- ϵ + Wall function)	EDC	Discrete Ordinates with WSGG	ANSYS Fluent 2020 (Mesh)	Reduced Coal/NH ₃ mechanism/various sources	Experimental validation from the literature
[87]	50-kWth CFB	Multi-Phase Particle-in-Cell	NR	NR	Barracuda VR	Reduced mechanism from various sources	Experimental validation

limited work still exists on using CFD modelling. The trend is taking a turn particularly in Asia, where South Korean institutions are evaluating the concept in depth for large ammonia replacements. Kweon et al. [87] modelled a 3D CFB rig operating at 50 kWth. The results were of critical importance to the development of these systems, as it was recognised the nonlinear NO pattern along the burner, with a sharp rise near the bed, selective non-catalytic reduction through the burner, and an ammonia-concentration dependency (as previously observed in other furnace systems). Unsurprisingly, and as in other studies, 20% ammonia replacement showed the lowest NO production, a phenomenon previously described along the recombination of species. However, and different to other works, the bed conditions appeared to increment reactivity and the yield of emissions as a consequence of higher residence times combined with H₂O increased pools. Caution should be exercised when considering additional optimization methods such as air staging, strategic injection, and co-firing ratios.

From the previous discussions, it is evident that there are strategies that can be implemented in larger industrial systems thanks to their validation at lower power ratios. Particularly, the methodologies developed to improve geometrical parameters for fluid enhancement and better reactivity are consistent features in the scalability process. Additionally, the use of RANS, LES and Hybrid turbulence approaches appear to deliver consistent results from small to large scale expansion, whilst embedding solid-fluid strategies for complex phenomena such as radiation/convection/conduction heat transfer appears to be the most realistic, better validated approach, a method that needs to consider non-adiabatic scenarios to account for heat losses highly relevant to ammonia combustion when scaling up designs are performed. However, the works also show a complex interaction between reaction models and their applicability to different scales, as most reaction mechanisms have been developed under different conditions to those used in industrial settings, hence potentially posing a constraint in the validation of results. Additionally, geometrical simplification, easy to accomplish under low power ratios, might not be as effective in larger systems that show complex interactions between components and atmospheric conditions. This is recurrent in the works previously addresses, which tend to simulate the entire system rather than simplified versions. These are points that need to be considered for the use of CFD when scaling up is attempted for ammonia combustion systems.

Table 1 presents a comparison between cases and their resolution methods. Table 2 summarizes these works and also addresses a few

points relevant to estimated computational costs (from low to high based on turbulence/combustion resolution methods), accuracy with validated methods, applicability scenarios, and key design parameters. Additionally, Table 3 provides a Cross-cutting assessment that reveals the stage at which these models have been generated and implemented for real industrial purposes.

3.3. Gas turbines

As discussed, the challenge to decarbonize power generation is driving ammonia (NH₃) into the focus of attention as a potentially carbon-free energy carrier and fuel. The application of NH₃ in gas turbines (GT) is, however, limited by its rather challenging combustion characteristics such as low laminar flame speed, high ignition energy, high NOx emissions potential, and a very narrow flammability limit inducing the propensity for instabilities and blow-off [88]. As a result, current discussion and effort have mainly focused on ammonia blends with more reactive fuels like H₂ or CH₄ because they can improve flame stability and operability. Therefore, this section focuses on the challenges associated with accurately predicting flame characteristics in ammonia-based gas turbines units, while a deep focus on challenges related to the NOx prediction by CFD models can be found in a recent work by Mashruk et al. [89].

To fill the gap between laboratory-scale burners and full-scale engines, micro gas turbines (mGT) and complex combustor geometry investigations offer key information for design. These geometries extend to more advanced flows including those used in engines, hence adding detailed engine features such as staged air injections, complex cooling arrangements, and multi-dimensional deflection of the fuel. For example, Bastani et al. [90] studied a can combustor featuring a central swirler and azimuthally distributed secondary and dilution air holes designed to enable a staged combustion strategy aimed at improving flame stability and controlling emissions. Their study demonstrated that a RANS approach coupled with a Flamelet Generated Manifold (FGM) model was able to capture the overall temperature distribution trends. However, noticeable flow asymmetries were observed, with the discrepancies attributed to the limitations of the RANS turbulence model and the high sensitivity of ammonia flames to geometric variations. Okafor et al. [88] investigated emissions control in micro gas turbines, achieving remarkably low emissions—49 ppm of NOx, 2 ppm of CO, and nearly zero N₂O, HCN, and NH₃—along with a combustion efficiency of

Table 2

Comparison between references, showing estimated accuracy, applicability, key design parameters and industrial validation challenges.

Reference	Computational costs	Accuracy/predictive capability	Applicability	Key design parameters	Industrial validation challenges
[37]	Low–moderate: 3-D/CFD combustion modelling at micro-scale; relatively small domain but coupled heat transfer and NOx chemistry increase cost	Good for resolving thermal performance and NOx trends; accuracy depends strongly on kinetic mechanism and wall heat-transfer treatment	Micro-combustors and distributed small-scale power generation	NH ₃ fraction, equivalence ratio, inlet velocity, wall thermal conductivity, combustor geometry	Scaling micro-combustor results to industrial combustors; wall heat losses and detailed chemistry must remain representative
[38]	Low: coupled combustion/heat-transfer simulations with parametric fuel and wall-property studies	Useful for identifying sensitivity to fuel composition and wall conductivity; quantitative prediction requires validated kinetics	Micro-power systems and compact NH ₃ /H ₂ combustion	H ₂ /NH ₃ ratio, O ₂ concentration, equivalence ratio, wall thermal conductivity	Limited direct transferability to large industrial furnaces and boilers
[39,40]	Moderate: Detailed chemistry with complex flow through perforated structures, but under laminar conditions.	Strong for evaluating NOx mitigation mechanisms and temperature fields	Compact combustors and NOx-control concepts	Plate geometry, hole diameter/pitch, fuel/oxidizer ratio, velocity, equivalence ratio	Manufacturing tolerances, fouling, durability and scale-up of perforated structures
[41]	Moderate: reacting CFD with detailed NO chemistry and complex MILD flow	Good mechanistic prediction of fuel-NO formation/reduction; sensitive to turbulence–chemistry interaction	MILD combustion furnaces using NH ₃ -containing fuels	NH ₃ /CH ₄ ratio, recirculation, temperature, oxygen concentration, residence time	Validation under industrial-scale recirculation, non-uniformity and transient operating conditions
[42]	Moderate: multiphase reacting flow and MILD-combustion modelling	Useful for comparative trends between coal particle sizes and NH ₃ addition	Coal-fired industrial furnaces employing MILD combustion	Coal particle size, NH ₃ fraction, O ₂ dilution, temperature, residence time	Particle-scale processes, heterogeneous reactions and scale-up to utility boilers
[43]	Moderate: detailed analysis of multiple chemical and flow timescales	Strong for fundamental identification of controlling regimes rather than direct plant prediction	MILD reactors with different energy carriers	Chemical timescale, mixing timescale, residence time, temperature, fuel type	Translating idealized timescale relationships into highly heterogeneous industrial furnaces
[46]	Moderate: detailed reacting-flow modelling involving NOx/N ₂ O chemistry	Good for reaction-zone and emissions analysis; detailed nitrogen chemistry is computationally demanding	NH ₃ -fired MILD industrial combustion	Equivalence ratio, temperature, dilution, residence time, NH ₃ concentration	Accurate simultaneous prediction of NOx and N ₂ O under real furnace conditions
[47]	High: 3-D reacting flow, recirculation and detailed chemistry	Higher geometric fidelity than simplified models; still mechanism/turbulence dependent	Reversed-flow MILD furnaces	NH ₃ /H ₂ ratio, recirculation, geometry, inlet conditions, air staging	Experimental validation at scale; computational expense increases substantially with industrial geometry
[48]	Moderate: CFD with modified oxidizer chemistry	Good for assessing sensitivity of NH ₃ combustion to oxidizer enrichment	NH ₃ combustion enhancement and burner optimization	H ₂ O ₂ concentration, equivalence ratio, inlet temperature, NH ₃ concentration	Safe/controlled oxidizer implementation and validation under industrial operating conditions
[49]	High: conjugate heat transfer couples gas-phase combustion with solid-wall heat transfer	Stronger thermal prediction because wall heat transfer is represented; emissions remain mechanism-sensitive	Industrial burners and furnaces requiring thermal/NO control	NH ₃ co-firing ratio, staging ratio, air distribution, wall properties, temperature	Accurate wall-property data, cooling conditions, deposits and plant-specific air distribution
[50,53]	Moderate–high: turbulent reacting-flow CFD; multiple swirl configurations increase parametric cost	Useful for predicting flame shape and emissions trends; turbulence/chemistry model selection is critical	Industrial burners and retrofit methane systems	Swirl number, NH ₃ fraction, equivalence ratio, injection configuration	Maintaining flame stability and low emissions during load changes
[54]	Low–moderate: reduced/compact mechanism substantially lowers chemistry cost	Designed to preserve important flame behaviour while reducing computational burden	CFD of NH ₃ /H ₂ burners and larger systems	Mechanism species/reactions, NH ₃ /H ₂ ratio, pressure, temperature	Demonstrating mechanism validity over industrial pressure, temperature and composition ranges
[55]	Low: radiation adds another heat-transfer calculation	Improves prediction of laminar NH ₃ flame temperature/structure where radiation is important	Fundamental burner modelling and validation	Radiation properties, flame temperature, equivalence ratio, burner geometry	Accurate radiative properties and extension from laminar flames to large turbulent furnaces
[56]	Moderate–high: multiphase biomass combustion + NH ₃ chemistry	Useful for co-firing trends and effects of stoichiometry	Biomass-fired boilers transitioning toward carbon reduction	NH ₃ fraction, biomass composition, stoichiometric ratio, air supply	Fuel variability, ash behaviour, NH ₃ conversion and plant-specific combustion conditions
[70]	Moderate: detailed pyrolysis/ignition chemistry	Strong for ignition and early conversion mechanisms	Burner design and fuel preparation	Particle composition, NH ₃ /coal ratio, temperature, heating rate	Connecting particle-scale ignition data with furnace-scale behaviour
[71]	Moderate: MILD with reduced bespoke mechanism using RANS	Adequate with experimental validation using coal combustion	Industrial coal units	MILD improvements, temperature, burner stages	Reliable scalability using NH ₃ with accurate mechanisms for large power
[72]	Moderate: combined experimental/numerical nitrogen chemistry	Particularly valuable because modelling is supported by experiments	NH ₃ /coal co-firing and NOx-control development	Coal properties, NH ₃ fraction, temperature, oxygen availability	Obtaining reliable nitrogen-speciation data under realistic furnace conditions
[73]	Moderate–high: integrated pyrolysis, staging and burner-flow modelling	Promising because design is explicitly oriented toward NO reduction	Industrial coal boilers and retrofit burners	Air-jet velocity, NH ₃ pyrolysis, staging ratio, injection location	Demonstrating durability, controllability and emissions performance at commercial scale
[74]	Very high: LES + finite-rate chemistry + multiphase coal/NH ₃ + multiple air streams	Potentially high spatial/temporal fidelity; validation remains essential	Semi-industrial and industrial burner development	NH ₃ fraction, secondary/tertiary air, staging,	Very large computational cost; need extensive experimental data for validation

(continued on next page)

Table 2 (continued)

Reference	Computational costs	Accuracy/predictive capability	Applicability	Key design parameters	Industrial validation challenges
[75]	High: industrial-scale CFD of NH ₃ co-firing	Useful for predicting boiler-scale effects of NH ₃ fraction	Utility boilers	preheat temperature, turbulence NH ₃ co-firing ratio, injection position, boiler geometry, air distribution	Full-scale measurements of temperature, burnout and NOx/N ₂ O
[76]	Very high: plant-scale CFD with complex boiler geometry	High practical applicability; accuracy constrained by plant operating data	Existing 210-MW coal-fired power plant retrofit assessment	NH ₃ fraction, injection configuration, coal properties, boiler operating conditions	Access to plant data, validation measurements and uncertainty in fuel/air distribution
[77]	Very high: full utility-boiler CFD	Strong industrial relevance; numerical results require plant-scale validation	Large coal-fired power generation	NH ₃ blending ratio, injection location, air distribution, furnace temperature	Full-scale experimental validation and prediction across different loads
[78]	Very High: full utility-boiler CFD	Strong industrial relevance at large scale	Scalability and burner unit improvements	NH ₃ blending ratio, injection strategy, additional components (sludge)	Full-scale experimental validation with feasible stream recovery
[79]	High: full utility-boiler CFD at 1000 MW	Useful assessment for the impact of different air injection strategies	Scalability and plant improvement with various retrofitting challenges	Air injection strategy, ammonia content	Accurate implementation through the various retrofitting challenges
[80]	Very high: large-scale boiler CFD with low-load operating conditions	Useful for assessing operational limits and low-load behaviour	Large utility boilers and flexible operation	NH ₃ ratio, air staging, load, injection location	Highly non-uniform low-load flow, flame stability, incomplete burnout and emissions
[81]	Very high: large-scale CFD and injection-position parametric study	Strong engineering applicability for optimizing ammonia injection	Ultra-supercritical utility boilers	NH ₃ injection location, mixing, coal properties, furnace conditions	Reliable prediction of NH ₃ mixing, corrosion/deposition and emissions in full-scale systems
[83]	High: large-scale CFD with various zones.	Strong applicability for the use of Flue Gas Recirculation	Boilers using Flue Gas Recirculation	Improved strategy to model more accurate emissions with local Re changes.	Validation required for future works.
[84,85]	Very high: full-boiler CFD with multiple injection/blending scenarios	High engineering value for optimization of ammonia injection and blending	Carbon-free/low-carbon retrofit of existing Korean utility boilers	Burner configuration, NH ₃ injection strategy, blending ratio, air distribution	Validation at full scale; maintaining furnace temperature, burnout, NOx and equipment integrity; validity of reaction mechanism at scale
[86]	Very high: coupled combustion and pollutant-control optimization	Broadens modelling from combustion to downstream pollutant control	Industrial burners and integrated emission-control systems	NH ₃ /coal ratio, burner geometry, flow distribution, desulfurization conditions	Coupled effects among combustion, pollutant formation/removal, deposits and equipment operation
[87]	Moderate: low power but coupled with solid/fluid interaction	Approaches the use of fluidized beds and solid/fluid interactions	Small heating units with potential for ammonia utilization	NH ₃ /coal ratio, burner geometry, flow distribution, NO abatement	Scalability to larger scales coupled with adequate reaction mechanisms that include reliable material interaction

Table 3

Cross-cutting assessment of current state for each subject.

Criterion	Micro/laminar models	MILD/flameless CFD	Turbulent burner CFD	Coal/NH ₃ boiler CFD	Industrial-scale priority
Computational cost	Low-moderate	Moderate-high	Moderate-high	High-Very high	Reduced-order/reduced-chemistry models are highly desirable
Accuracy	High for fundamental flame properties	High for mechanism studies	Strongly dependent on turbulence/chemistry models	Strong engineering capability but significant uncertainty	Validation against plant measurements is essential
Applicability	Fundamental and micro-power systems	Low-emission industrial combustion	Burner design/retrofit	Utility-scale co-firing and retrofit	Boiler-scale models have greatest immediate industrial relevance
Most influential design parameters	Equivalence ratio, fuel composition, wall properties	Recirculation, dilution, residence time, temperature	Swirl, injection, staging, turbulence	NH ₃ ratio, injection location, air staging, mixing, load	Multi-parameter optimization rather than single-variable studies
Main validation challenge	Scale-up	Reproducing industrial recirculation	Flame stability and turbulence modelling	Reliable full-scale measurements and heterogeneous furnace conditions	Coupled validation of temperature, burnout, NOx/N ₂ O, NH ₃ slip and heat transfer
Major research gap	Limited industrial transfer	Scale-up uncertainty	Model uncertainty	Limited full-scale experimental datasets	Integrated CFD-experiment-plant validation framework

99.8% using a rich-lean staged combustion strategy. This performance contrasts with a single-stage configuration, which produced up to 5000 ppm NOx at equivalence ratios, $\phi = 0.8$ –1.1. Somarathne et al. [91] introduced a novel radial swirl combustor (swirl number, $Sn = 2.34$) specifically designed for liquid ammonia sprays co-fired with methane.

The combustor employs strong swirl to stabilize a two-phase flame under stringent operating conditions, Fig. 12. Their results point out the importance of pressure (as depicted in the liquid injection section), whilst large recirculation zones in the combustor played a vital role in enhancing the mixing of hot combustion products and NH₃ vapours,

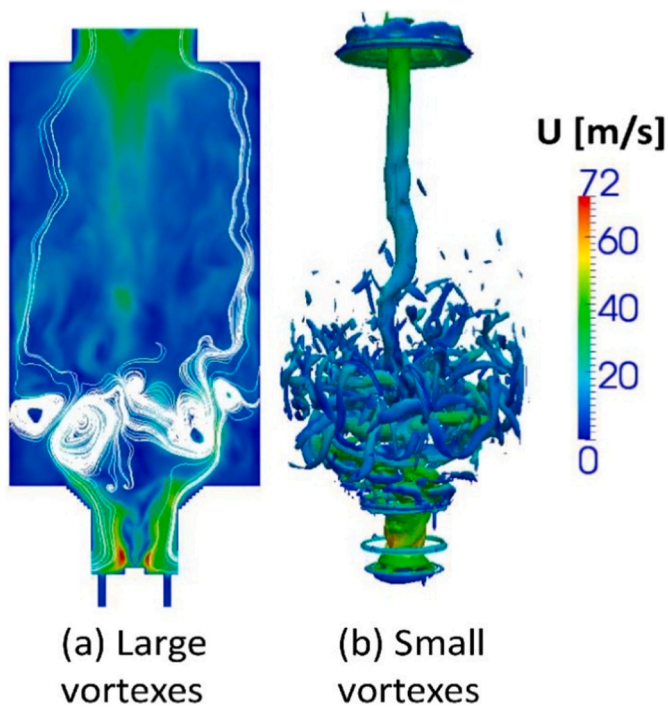


Fig. 12. Reacting flow structures in the combustors (Reprint from Ref. [91] with permission).

which promoted flame stabilization. This is additionally addressed in the work produced by Kumuk et al. [92], who investigated the influence of annular cooling slot angles (15–45°) on flame structure and NOx emissions in a heavily-swirling, high-temperature combustor. Their findings highlight that directly integrated cooling air interacts with the reaction zone, and that the slot angle (e.g., 30°) can affect flame shape and NOx formation by modifying the recirculation zone.

It is important to raise that for the analyses of NO emissions, it was

observed that the use of liquid ammonia (blended with hydrogen) followed the same trends as those with gaseous ammonia. The finding is quite encouraging for NO abatement due to the potential trade-off relation between NO and unburned NH_3 . A clear distinction should be made between NOx formation mechanisms driven by the intrinsic chemistry of ammonia and those influenced by controllable design and operating parameters. From a chemical perspective, ammonia combustion inherently promotes the formation of fuel-NOx through intermediate species such as NH , NH_2 , HNO and N radicals [89]. These pathways are strongly affected by pressure, temperature, equivalence ratio and fuel composition. Conversely, several combustion and design parameters can be optimized to mitigate NOx emissions, including staged combustion strategies, fuel cracking, swirl intensity, air staging, dilution air distribution and wall thermal management.

Fatehi et al. [93] compared premixed and non-premixed fuel injection using ammonia. Pressure, fuel slip, emissions and aerodynamic patterns at the flame front were evaluated. It was concluded that the mixing regime was the primary contributor for the combustion performance, with the premixed flame showing more compact features that also led to higher temperature profiles with elevated NO at lean equivalence ratios. Stronger, more compact recirculation zones promote further recirculation of fuel/oxidizer that within thin layers promote further fuel NO. Comparatively, non-premixed cases denote how oxidizer resides in shear/wall layers, a phenomenon that reduces NO formed at the shear layers.

The validation strategies adopted in these GT studies differ substantially in both scope and strength. Bastani et al. [90] validated the Realizable $k-\epsilon$ /steady-flamelet calculation against thermocouple measurements in the secondary zone of the same can combustor. Grid independence was assessed using approximately 0.7, 1.5 and 3.6 million cells; the 1.5-million-cell mesh produced axial-velocity and CO_2 profiles close to those obtained with 3.6 million cells and was therefore selected. The predicted and measured temperature profiles showed similar overall distributions, but the numerical solution was more axisymmetric than the experiment. The measured asymmetry was attributed to the fuel injector, manufacturing tolerances and three-dimensional

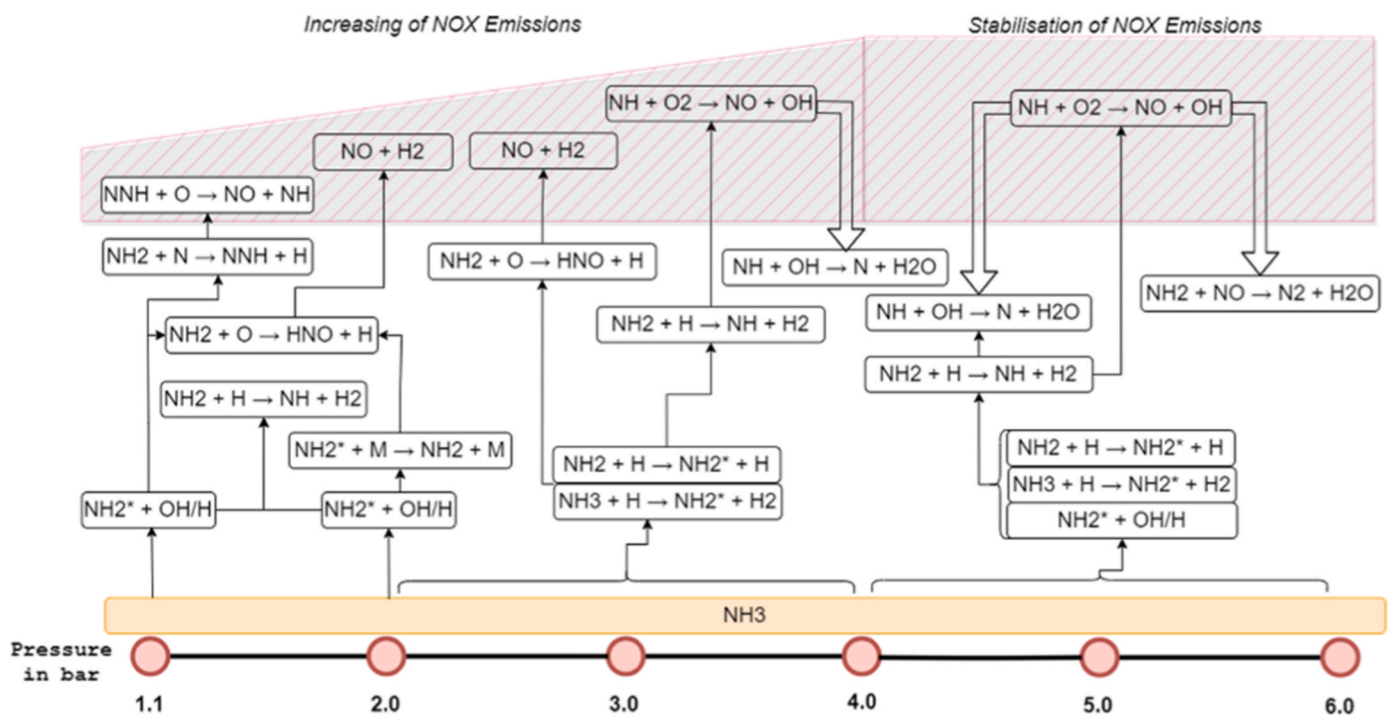


Fig. 13. Pressure-induced shift in NH_2^* , NH^* , and OH^* dominance and NO_x stabilization pathways in 99% cracked ammonia combustion (Reprint from Ref. [94], licensed under CC BY 4.0).

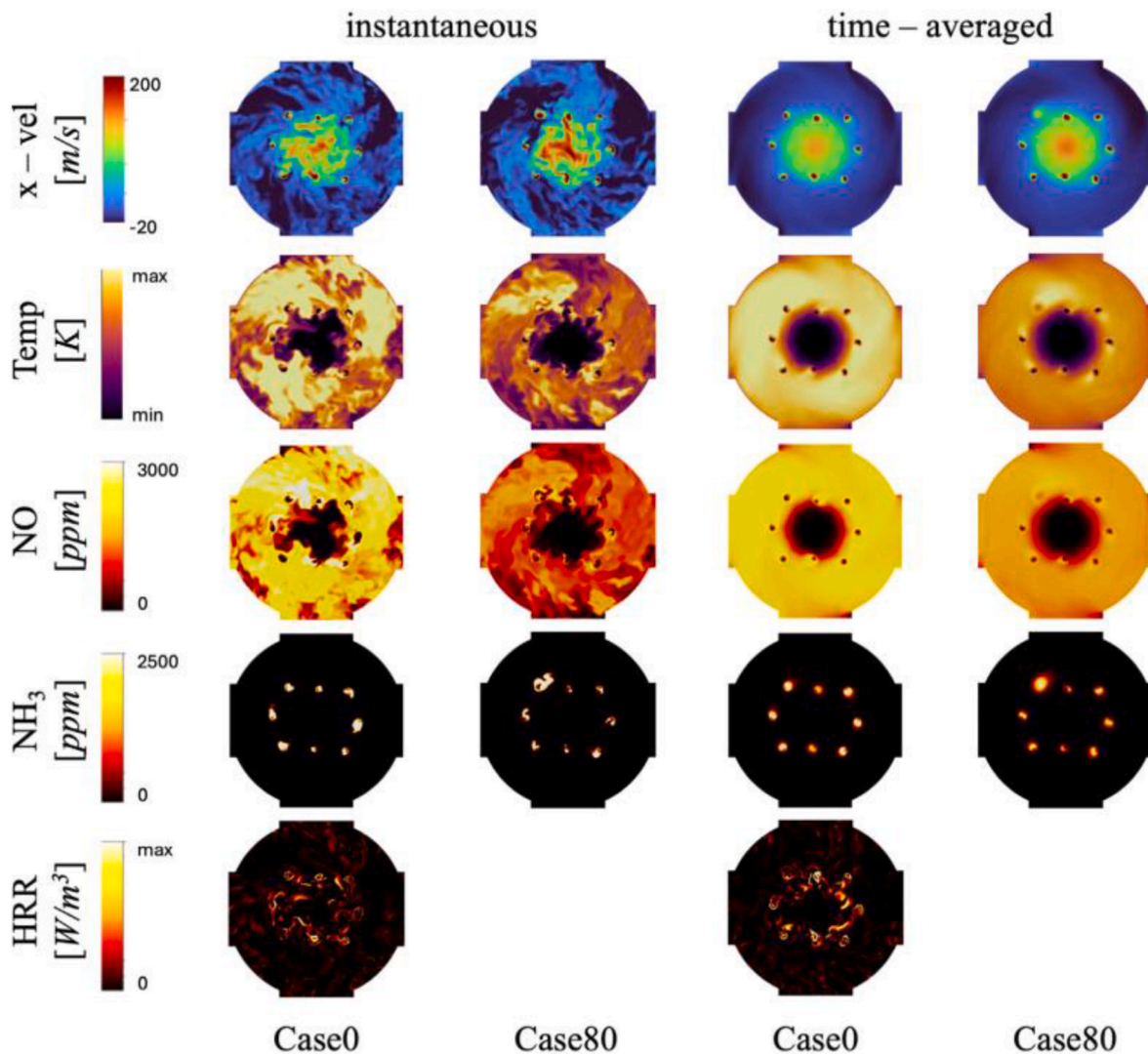


Fig. 14. Instantaneous and time-averaged contours comparing the axial velocity, temperature, NO, NH₃ and HRR between uncracked (Case0) and cracked (Case80) ammonia flames in a transversal plane at $x = 15$ mm from the burner outlet (Reproduce from Ref. [22] with permission).

geometric imperfections. This comparison demonstrates that steady RANS-flamelet modelling can reproduce the mean thermal field and ammonia-induced flame displacement, but it does not establish equivalent accuracy for instantaneous coherent structures, local extinction or pollutant chemistry because the validation was primarily temperature-based [90].

A more comprehensive validation hierarchy was used by Okafor et al. [88], combining PIV, OH-PLIF, simultaneous OH/NO-PLIF, FTIR exhaust measurements and LES-PaSR calculations. The LES employed the WALE subgrid-scale model and finite-rate chemistry, whereas the experiments independently characterized the velocity field, reaction-zone location, spatial association between OH and NO, and exhaust emissions. The measured emission uncertainty was generally below ± 8 ppmv, although the uncertainty increased for species present close to the lower measurement limit. This multi-observable validation is particularly valuable because agreement in outlet NO_x alone does not guarantee that the model predicts the correct flame structure or NO-formation pathway. Nevertheless, the comparison remained strongest at atmospheric or moderate pressure, and the use of adiabatic walls limits its ability to represent heat-loss-sensitive NH₃ consumption and post-flame NO reduction in an actual engine liner [88].

To further illustrate the effect of pressure on nitrogen conversion pathways, Fig. 13 summarizes the dominant reaction routes leading to

NO formation when increasing in pressure, from 1.1 to 6 bar. The analysis highlights the increasing role of NH₂-mediated pathways at elevated pressures and supports the experimentally observed stabilization of NO emissions above 4 bar. This behaviour suggests that pressure alters the balance between fuel-NO_x generation and NO reduction mechanisms, ultimately affecting the attainable emissions levels.

Regarding equivalence ratio, investigations into ammonia combustion and NO_x emissions, at both laboratory and industrial scales, have identified NO_x production peaks at equivalence ratios of 0.8–0.9 for ammonia/hydrogen blends [89].

In addition, the studies reviewed consistently indicate that fuel staging and rich-lean combustion concepts currently represent the most effective mitigation strategies, allowing a significant reduction of NO_x emissions while maintaining flame stability. Similarly, ammonia cracking increases hydrogen availability, enhancing combustion reactivity. Combustor design also plays a critical role, as recirculation zones promote fuel-air mixing and can favor NO reduction through local reburning mechanisms. Therefore, while the fundamental nitrogen chemistry sets the lower bound of achievable emissions, the final NO_x levels remain highly dependent on combustor design and operating conditions.

Among the NO emission mitigation strategies in GT applications, rich-lean staging and air staging have consistently demonstrated the

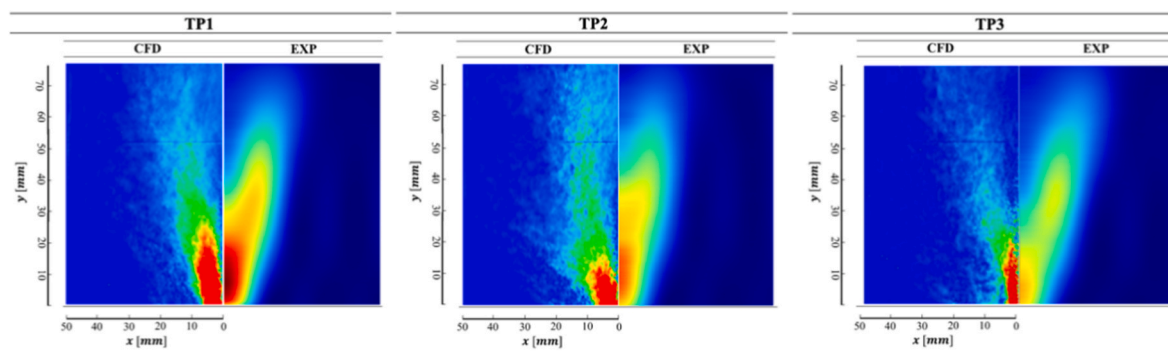


Fig. 15. Comparison between numerical HRR and experimental OH* (Reproduce from Ref. [97] with permission).

greatest potential for reducing NO_x emissions while maintaining flame stability, by varying equivalence ratio and consequently NO formation pathways. Similarly, fuel cracking and enhanced swirl-induced recirculation promote fuel-air mixing and reburning effects, limiting the formation of fuel-NO_x precursors and improving overall combustion performance. Therefore, although NO_x formation is intrinsically linked to ammonia nitrogen chemistry, its final emission levels can be significantly influenced through appropriate combustor design and operating conditions.

In studies with more realistic geometric resolution, such as those by Yu et al. [95] on a 9E heavy-duty gas turbine combustor and Mazzotta et al. [22] on an industrial Baker Hughes burner, the entire system was modelled, including primary and dilution zones, complex swirler assemblies, and compressor discharge chambers. Such detailed geometries are essential to accurately simulate the highly turbulent, three-dimensional, and non-premixed flow conditions characteristic of practical gas turbine engines. Mazzotta et al. [22] combined Large Eddy Simulation and Chemical Reactor Network (CRN) methodologies to analyse NO_x emissions and flame characteristics, operating with hydrogen-ammonia and cracked ammonia fuel blends. Both modelling approaches reproduced the velocity and exhaust temperature fields and the key emission trends with NO_x and temperature overpredicted by approximately 11% and 3%, respectively. This work also allowed to appreciate the use of cracked ammonia to reduce NO_x emissions; in particular, the use of 80% cracked ammonia resulted in a 25% reduction in emissions when compared to the uncracked case. Fig. 14 shows instantaneous and time-averaged main flame characteristics comparing uncracked ammonia flame (Case 0) to cracked one (Case 80).

Sheykbaglou et al. [96] advanced on the concept of using partially cracked ammonia against pure ammonia/hydrogen blends (as the removal of nitrogen from the cracking process is extremely expensive, not only due to additional equipment, but also due to the complexities of hydrogen sieving and nitrogen/ammonia separation). By injecting the fuel via different methods with and without oxygenated conditions, flame structure was assessed to defined better stability methods with reduced NO emissions, with cracked blends showing a better heat release rate distribution consequence of the reduced reactivity of the blends. Flame height heavily influenced emissions in recirculation zones altered by their size change (hence their straining potential), whilst emissions paths shift at higher cracking ratios due to higher temperatures representative of hydrogen flames (shifting NO Fuel production to Thermal NO mechanisms).

The validation strength of the full-engine study by Yu et al. [95] should be interpreted more cautiously. The 9E combustor calculation included the transition piece, primary and secondary nozzles and the associated air distribution, and a grid study covering approximately 1.04–3.47 million cells was performed; solutions above 1.76 million cells were broadly consistent, and a 2.41-million-cell grid was selected. However, the combustion model was validated against temperature data taken from an operating condition reported in the literature rather than

against simultaneous measurements from the simulated 9E geometry. Although the predicted temperature trend was reproduced, a noticeable deviation in its magnitude remained, and direct validation of the predicted NO_x emissions was not presented. Therefore, the model is useful for identifying relative effects of hydrogen fraction and nozzle arrangement, but the absolute NO_x values should not be regarded as engine-validated predictions [95].

In a subsequent study [97], the same research group applied the coupled CFD–CRN framework to a laboratory-scale, optically accessible burner at the Cardiff University Gas Turbine Research Centre, assessing the effect of pressure (1–6 bar) on flame morphology and validating it by comparing OH* chemiluminescence with simulated heat-release-rate (HRR) fields, as shown in Fig. 15. The results denoted the impact of highly cracked ammonia (99%) in the production of NO and other emissions under lean conditions representative to gas turbines. The 1% left of ammonia in the blend triggered HNO reactions that led to moderate NO emissions (~200 ppm). However, the most interesting finding was that at pressure between 1 and 3 bar, the trend on emissions followed that of H₂-based gas turbines (with NO raising linearly), whilst from 4 to 6 bar the emissions stabilised and flattened out to a constant value of 190 ppm. Similarly, unburned ammonia from the process reached a constant value ~40 ppm. While NH₂* considerably increased with pressure, OH* and NH* remained stable between 4 and 6 bar. The differing behaviour of NH* and NH₂* with pressure indicates shifts in combustion pathways. NH* reactions dominate at lower pressures, while NH₂* formation increases at higher pressures. This suggests that either NH₃ and NH react with OH and H₂ to enhance NH₂ signatures, or a balance between De-NO_xing effects and thermal NO_x production occurs at higher pressures. These assertions require further analyses.

Model comparison across the attached studies further demonstrates that chemical-mechanism performance is fuel- and operating-range dependent. In the CFD–CRN assessment of industrial NH₃/H₂ and NH₃/CH₄ flames, the KAUST, POLIMI, Okafor, Tian and GRI-Mech 3.0 mechanisms reproduced different portions of the experimental NO_x trends. For NH₃/H₂, all mechanisms captured the qualitative trend, with the KAUST mechanism providing the closest prediction up to approximately 50 wt% NH₃; above this fraction, NO_x was substantially overpredicted. For NH₃/CH₄, the Tian and Okafor mechanisms captured the trend up to approximately 50 wt% NH₃, whereas GRI-Mech 3.0 significantly overpredicted NO_x. After adjusting the pilot-zone equivalence ratio, the CRN reproduced most experimental points with an average error below 10%; however, this improvement represents calibration rather than fully blind validation. Consequently, a mechanism validated for ignition delay, laminar flame speed or a limited fuel-composition range should not automatically be assumed to predict NO_x accurately across the complete GT operating envelope [23,98].

Somaratne et al. [99] employed LES to compare the effects of liquid ammonia injection combined with gaseous hydrogen (LNH₃/GH₂) against fully gaseous ammonia–hydrogen mixtures at a pressure of 3 bar. The study also examined different equivalence ratios ($\phi = 0.90$ to $\phi =$

Table 4

Various CFD methods for the resolution of the relevant literature (NR: Not Reported).

Reference	Turbulence model	Combustion/turbulence-chemistry model	CFD solver	Chemical kinetic mechanism	Validation
[88,88]	LES (WALE model)	Partially Stirred Reactor (PaSR) model	OpenFOAM	Okafor mechanism	PIV, PLIF, FTIR
[93]	RANS (Realizable k- ϵ)	Flamelet Generated Manifold	ANSYS Fluent	Stagni et al. (2020) mechanism	No validation of the burner. Methodology validated from relevant literature.
[90]	RANS (Realizable k- ϵ)	Flamelet Generated Manifold + Finite-rate method	NR	Okafor reduced mechanism	Experimental micro-GT
[91]	LES (WALE model)	Partially Stirred Reactor (PaSR) model	OpenFOAM	Okafor reduced mechanism	High-pressure experiments
[92]	RANS (RNG k- ϵ)	EDC	ANSYS Fluent	NH ₃ /H ₂ mechanism	Experimental
[95]	RANS (Realizable k- ϵ)	EDC	ANSYS Fluent	NH ₃ /H ₂ mechanism	Industrial GT study
[22]	LES	Tabulated chemistry, NO/NO ₂ scalar transport + CRN	ANSYS Fluent	Stagni et al. (2020) mechanism	Experimental NOx; $\leq 10\%$ deviation
[96]	RANS (k- ω SST)	EDC	ANSYS Fluent v2021 R2	Reduced Li et al. (2019)	Experimental measurements of LBV and OH radicals
[97]	LES (WALE model)	Flamelet Generated Manifold + Finite-rate method + CRN	ANSYS Fluent	Stagni et al. (2020) mechanism	Experimental OH* and NOx emissions
[99]	LES (WALE model)	Partially Stirred Reactor (PaSR) model	OpenFOAM	Miller et al. mechanism	Micro-GT experiments
[29]	LES (Dynamic-Smagorinsky Lilly model)	Extended Turbulence Flame Speed Closure model (ETFC)	ANSYS Fluent	Okafor's mechanism	Experimental OH* and NOx emissions
[100]	RANS (k- ω SST)	Laminar Flame Concept (LFC)	STAR-CCM+ 19.3	Reduced Okafor et al. mechanism	NOx, NH ₃ , H ₂ , base-plate temperature
[101]	RANS (RNG k- ϵ)	SAGE detailed chemical-kinetics model with species transport	CONVERGE CFD 3.0	Reduced Li et al. (2019) NH ₃ /H ₂ /CH ₄ mechanism	Experimental PIV
[102]	RANS (RNG k- ϵ)	SAGE detailed chemical-kinetics model with species transport	CONVERGE CFD 3.0	Reduced Li et al. (2019) NH ₃ /H ₂ /CH ₄ mechanism	Experimental PIV
[98]	RANS (Realizable k- ϵ)	Flamelet Generated Manifold + Finite-rate method, NO/NO ₂ scalar transport	ANSYS Fluent	Zhang et al. mechanism	Experimental NOx emissions
[23]	RANS (Realizable k- ϵ)	Flamelet Generated Manifold + Finite-rate method, NO/NO ₂ scalar transport	ANSYS Fluent	Otomo et al. mechanism	Experimental NOx emissions
[103]	RANS (Realizable k- ϵ ; RNG k- ϵ ; k- ω SST); RSM; LES (Dynamic-Smagorinsky Lilly - WALE models)	FGM + detailed chemistry; NO/NO ₂ scalar transport	ANSYS Fluent	Otomo et al. mechanism	Experimental NOx emissions
[104]	LES (Dynamic-Smagorinsky Lilly model)	Flamelet Generated Manifold (FGM) + Finite Rate Closure model	ANSYS Fluent	ANSYS Model Fuel Library (MFL) mechanism	Experimental temperature/NOx/NH ₃
[105]	RANS (Realizable k- ϵ)	General Gas Phase Reaction (GGPR) model	AVL FIRE	Konnov, Okafor, San Diego mechanisms	Experimental NO/CO
[106]	LES	Thickened Flame Model	ANSYS Fluent	Reduced CRECK mechanism	Experimental OH* and NOx emissions
[107]	RANS (Standard k- ϵ)	EDC	ANSYS Fluent	Reduced mechanism derived by GRI-Mech 3.0 + Otomo	PIV, Experimental NOx

1.43), assessing their influence on temperature distribution, NO formation, unburned NH₃, and OH radicals. Increasing the equivalence ratio resulted in a substantial reduction in NO emissions and a decrease in combustor temperature. No significant differences in NO emissions were observed between liquid and gaseous ammonia injections. LNH₃/GH₂/air flames exhibited an optimum equivalence ratio of approximately 1.36, corresponding to the minimum NO emissions. A major limitation is that such high-fidelity geometric models are typically computed at low pressures [29].

Taken together, the studies previously described indicate that the predictive capability of CFD models in ammonia-fuelled gas turbines strongly depends on the degree of geometric fidelity, the turbulence-chemistry interaction model, and the availability of validation data under pressure conditions representative of real engines.

The CFD challenges for GTs are therefore twofold: (i) managing the considerable computational cost associated with resolving intricate geometries, particularly when LES is employed—often requiring sector models, as demonstrated by Viguera-Zuniga et al. [100]; and (ii) accurately capturing the coupled physics of complex swirling flow fields, wall heat transfer and cooling flows, along with the finite-rate chemistry of ammonia-based blends in industrially (with limited validation) conditions.

Predicting the lean blow-off limit is also critical for ensuring safety in

gas turbine applications. Due to ammonia's low reactivity, flames become highly sensitive to flow fields and mixing conditions. In such cases, LES approach is essential to capture the unsteady nature of the phenomenon. Supporting this, Chaudhury et al. [101,102] observed flame roll-off at lower pilot fuel; however, the steady-state RANS model used was unable to reproduce the transient blow-off behaviour. The assumption of adiabatic walls, adopted in several studies, has been identified as a significant source of error. Viguera-Zuniga et al. [100] showed that combustor wall temperature greatly influences post-flame ammonia decomposition and emissions. Chaudhury et al. [102] also reported strong variations in NOx prediction for adiabatic vs. isothermal wall conditions. Predicting convective heat transfer in this context is critical but computationally expensive.

Overall, for rapid design exploration and parametric studies—such as varying ammonia content in the fuel mixture, equivalence ratios, or geometry—a well-validated RANS approach represents a practical tool. Specifically, RANS models (e.g., Realizable k- ϵ or Reynolds Stress Model, RSM) combined with a detailed combustion chemistry framework and a skeletal mechanism offer a reasonable compromise between accuracy and computational cost. The combined findings of Mazzotta et al. [22,97] and Meloni et al. [29] demonstrated that LES with a sophisticated combustion model (TFM, EDC or PaSR) and a carefully selected mechanism is the only way to quantitatively predict the

Table 5

Comparison between references, showing estimated accuracy, applicability, key design parameters and industrial validation challenges.

Reference	Computational cost	Accuracy/predictive capability	Applicability	Important design parameters	Industrial validation challenges
[88]	High: detailed turbulence using LES	Strong flow/flame/emission resolution; LES complemented experiments	Micro-GT and low-NOx combustor development	NH ₃ fraction, equivalence ratio, rich/lean staging, swirl, pressure	Full-scale GT extrapolation; NOx chemistry and NH ₃ slip
[93]	Moderate: Inclusion of representative GT conditions	Good for temperature/velocity trends	Pressurized gas turbines	Pressure, equivalence ratio, diffusive/premixed configurations	Real-combustor geometry and secondary-air flows
[90]	Moderate-high: Real combustor geometry	Numerical results supported by experiments	Actual micro-GT combustor	NH ₃ fraction, thermal power, equivalence ratio	Real-combustor geometry and secondary-air flows
[91]	High: Complex fuel and air injection at high pressure	Detailed analysis of OH/temperature/NO	Pressurized gas turbines	Pressure, OH concentration, temperature, staging	High-pressure NOx validation
[92]	Moderate-high: cooling included in the model	Good for flame/cooling sensitivity	Gas-turbine combustor design	H ₂ /NH ₃ ratio, swirl, cooling angle	Cooling/thermal-stress effects at scale
[95]	High: Industrial representative conditions	Industrial-scale numerical assessment	Heavy-duty GT	NH ₃ /H ₂ ratio, operating load, burner conditions	Commercial-scale emissions validation
[22]	Very high: LES with detailed turbulence; moderate CRN	NOx within ~10% of experiment	GT burner optimization and NOx pathway analysis	NH ₃ cracking, blend composition, equivalence ratio	Broader pressure/load validation
[96]	Moderate: Addition of cracked blends and various oxygen ratios	Good OH Radical location	Cracked blends in GT systems	Central fuel injection with various delivery methods and oxygen contents	Addition of in-situ cracking with oxygenated blends
[97]	High: Industrial conditions with detailed geometry	Strong experimental/numerical validation	Semi-industrial burner design	Cracking level, NH ₃ /H ₂ /N ₂ composition, operating point	Scale-up and long-duration operation
[99]	High: Evaluation of novel methods for NOx control	Experimental + numerical development	Low-NOx micro-GT	Fuel ratio, staging, equivalence ratio	Maintaining low NOx without combustion instability
[29]	Very high: LES with high NOx fidelity approach	High-fidelity NOx prediction	GT emissions prediction	NH ₃ /CH ₄ ratio, operating condition	LES cost and chemistry uncertainty
[100]	Moderate: Detailed geometrical patterns	Good for temperature/species trends; validated against experiments	GT combustor screening	NH ₃ /H ₂ ratio, pressure, inlet T, swirl	Limited temperature measurements and complex chemistry cost
[101]	Moderate-high: representative industrial operation	Experimental characterization	Gas-turbine burner/pilot design	Pilot percentage, NH ₃ fraction, equivalence ratio	Pilot/main flame interaction
[102]	Moderate: Evaluation of operating regimes	Experimental combustion characterization	GT can combustors	Pilot flame, fuel ratio, operating condition	Stability and emissions over load range
[98]	Moderate: FGM based approach	CFD-CRN supported by experiments	Gas-turbine preliminary design	Blend ratio, operating condition, reactor zones	Translating CRN zones to full combustor
[23]	High: Stratification included in the analysis	Experimental + numerical	Stratified GT combustion	Stratification, cracking, swirl, equivalence ratio	Reproducing stratification at scale
[103]	Low-very high: depending on model	LES <10% emission error; RANS can underestimate emissions ~35%	Model-selection for GT burners	Turbulence model, NH ₃ /H ₂ ratio, swirl	Computational cost vs emission accuracy
[104]	Very high: LES with complex geometry	Good agreement with measured flame/temperature/NOx/NH ₃	Non-premixed GT burners	NH ₃ cracking, H ₂ /N ₂ , bluff-body geometry	Transfer to swirl/industrial geometries
[105]	Low-moderate: Fast, generic burner resolved with RANS	Satisfactory NO agreement; CO prediction less reliable	Fast CFD and engineering screening	Mechanism selection, equivalence ratio	Reduced chemistry may miss CO/intermediate species
[106]	Moderate-high: Industrial representative operation with LES	Detailed NOx prediction	Pressurized GT combustion	Pressure, NH ₃ /H ₂ , equivalence ratio	Pressure-dependent NOx chemistry
[107]	Moderate: use of reduced mechanism	Good flame/temperature/species prediction	Industrial DLN GT	NH ₃ fraction, equivalence ratio, burner geometry	Full-scale validation

complex turbulence-chemistry interactions governing ammonia combustion. The hybrid CFD-CRN methodology [23,98] represents an effective compromise for NOx prediction. Unlike workflows that require multiple LES runs for parametric exploration, the hybrid methodology significantly reduces the number of high-fidelity simulations needed, thereby making systematic parametric studies feasible. Key remaining challenges include the development of robust and computationally efficient chemical mechanisms, the acquisition of high-pressure experimental data for model validation, and the further refinement of models capable of accurately capturing heat-loss effects and transient combustion phenomena. Addressing these challenges is essential to advance the design of efficient, low-emission ammonia-fuelled gas turbines.

Table 4 presents a comparison between cases and their resolution methods. Table 5 summarizes these works and also addresses a few points relevant to estimated computational costs (from low to high based on turbulence/combustion resolution methods), accuracy with validated methods, applicability scenarios, and key design parameters. Finally, Table 6 provides a Cross-cutting assessment that summarizes the findings performed by all groups mentioned in this review.

4. Major challenges and way forward

As learned from all the previous sections, ammonia combustion modelling of medium to large units has reached all corners of the combustion field. However, major challenges still remain to keep progressing with the concept, thus delivering modelling strategies that can be used for faster implementation and evaluation of concepts whilst reducing time consumption and deployment costs.

The choice between RANS and LES represents a fundamental trade-off between computational cost and predictive accuracy; the RANS approach gives steady-state solutions at an affordable level of computational cost and is appropriate for parametric analysis and preliminary design scoping. Most of the work with design implications [92,95,97, 101,102] used RANS models to facilitate parametric analysis and support design-oriented investigations. Nevertheless, RANS is unable to capture unsteady phenomena that play a critical role in combustion, such as transient local phenomena, particularly in ammonia or hydrogen combustion, as previously described. Confirming this, Chaudhury et al. [101,102] reported discrepancies between axial velocity prediction and

Table 6

Cross-cutting assessment of current state for resolution method.

Criterion	Fundamental/ kinetic studies	RANS CFD	High-fidelity LES	LES + FGM/ CRN	Industrial GT CFD	Overall assessment
Computational cost	★	★★	★★★★★	★★★	★★★★– ★★★★★	Reduced chemistry/CRN offers major savings
Flow-field accuracy	N/A	★★★	★★★★★	★★★★	★★★★	LES best resolves unsteady flow
Flame prediction	★★★★★	★★★	★★★★★	★★★★	★★★★	Strongly dependent on turbulence closure
NOx prediction	★★★★★	★★★	★★★★– ★★★★★	★★★★	★★★★	Chemistry is as important as turbulence
NH ₃ -slip prediction	★★★★★	★★★	★★★★	★★★★	★★★	Requires detailed intermediate chemistry and component interactions
N ₂ O prediction	★★★★★	★★–★★★	★★★★	★★★	★★★	Significant research gap
Radiation treatment	Usually N/A	★★★	★★★	★★★	★★★	Needs systematic validation – most literature approached in this review do not consider radiation in GTs, hence making this an interesting area of research
Pressure effects	★★★★★	★★★	★★★★	★★★★	★★★★★	Essential for GT applications
Fuel flexibility	★★★★★	★★★★	★★★★★	★★★★★	★★★★	Cracked NH ₃ is an important emerging area
Experimental validation	★★★★★	★★★★	★★★★	★★★★	★	Full-scale validation remains scarce
Industrial applicability	★★	★★★★	★★★★	★★★★★	★★★★★	Industrial GT studies are increasingly mature compared to other areas (ie. boilers and furnaces)
Ease of optimization	★★★★★	★★★★★	★★	★★★★	★★★	RANS/CRN useful for design-space exploration
Best use	Mechanism development	Engineering design	High-fidelity physics	Industrial emission prediction	Final design/ retrofit	Hierarchical modelling is preferable

PIV measurements, attributing these differences to the limitations of the steady-state model. Mazzotta et al. [103] performed a direct comparison between RANS models (including the Reynolds Stress Model) and LES using a 70% H₂ - 30% NH₃ (by vol.) blend, finding that although large-scale flow structures were captured by RANS models such as RSM, all of the RANS-based approaches under-predicted NO_x emissions when compared with LES (~35% error vs. an error below 10% in LES). The reason is mainly attributed to the capacity of LES to resolve large, energy-containing turbulent features and their unsteady interaction with the flame that drives the slow formation of pollutants such as NO_x. Therefore, LES is currently recognised as the tool of choice for high-fidelity analysis and final design validation which can be employed for more detailed engineering. Similarly, RANS provides faster resolution, critical for large infrastructure improvement that otherwise would require massive computational requirements. Studies by Somaratne et al. [91], Okafor et al. [99], and Mazzotta et al. [22] successfully employed LES to gain detailed insight into flame structure, vortex breakdown, and turbulence–chemistry interactions, often supported by customized User-Defined Functions (UDFs), as demonstrated in the work of Meloni et al. [29]. While RANS-based approaches remain valuable for preliminary parametric screening, their ability to predict NO_x formation, flame asymmetries and transient stability limits is limited when compared with LES-based frameworks, particularly in strongly swirling ammonia-hydrogen flames.

Based on the studies reviewed, turbulence-chemistry interaction models and chemical kinetic mechanisms have the strongest influence on NO_x predictions, owing to the complexity of ammonia nitrogen chemistry. In contrast, geometric fidelity and turbulence modelling mainly govern flame morphology, anchoring, recirculation patterns and temperature fields, making LES preferable to steady-state simulations for these aspects. Heat transfer modelling and wall boundary condition assumptions become increasingly important for predicting wall temperatures, ammonia slip and post-flame chemistry. In particular, the coupling between turbulence and chemistry lies at the core of any combustion model. For ammonia-based blends, this coupling is particularly challenging due to the intricate nitrogen chemistry involved. The kinetic formation mechanisms are extremely sensitive to the temperatures and concentrations of radicals (O, OH, HNO). Across the modelling spectrum—from tabulated to finite-rate chemistry—approaches such as the FGM, employed by Bastani et al. [90] and Xia et al. [104], represent

an intermediate solution for large power system development. However, such models can struggle to capture extinction and re-ignition phenomena and may inadequately represent flame characteristics and the full range of NO_x formation pathways. Detailed chemistry approaches, such as the EDC or PaSR models, directly integrate chemical kinetics into the simulation. Therefore, the choice of chemical mechanism becomes critical and a subsequently recurring theme across all CFD studies, a particular issue for gas turbine and pressurized boiler analyses due to their high-pressure conditions. It is noted that high pressures promote NO-reburn reactions at different ratios depending on the ammonia content of the blend. Mikulčić et al. [105] reported the San Diego model [108] to be most precise in predicting NO effects, and Romano et al. [98] suggested the Zhang et al. [109] model for NH₃/H₂ mixtures. Meloni et al. [106] employed high-fidelity LES combined with a custom-reduced mechanism (12 species), achieving accurate NO_x prediction (<5% error). As shown by Sun et al. [107] using RANS with a skeletal mechanism predicted that NO₂ lower by two orders of magnitude. Furthermore, predictions of other nitrogenous species like N₂O and HCN are often poor due to a lack of validation data and uncertain kinetics, as noted by Okafor et al. [88].

This apparent discrepancy between mechanisms reflects a broader limitation of reduced-order chemistry. Skeletal and reduced mechanisms are calibrated against a finite set of experimental targets (e.g., laminar flame speed, ignition delay time, or species profiles from jet-stirred and burner-stabilised reactors) collected over a bounded range of temperature, pressure and equivalence ratio; their accuracy cannot be assumed to hold once the simulated conditions fall outside this calibration envelope. Reduction inherently trades chemical completeness for computational speed: Alnasif et al. [54] derived a compact NH₃/H₂ mechanism from the San Diego model and reported that physically realistic rate coefficients had to be sacrificed to preserve predictive accuracy for practical CFD use, with good agreement against NO, N₂O and NO₂ measurements confirmed specifically for the 70/30 NH₃/H₂ blend and equivalence ratio range they tested. This sensitivity is more pronounced for minor nitrogenous species than for major flame parameters: temperature, velocity and NO are generally well reproduced because they are governed by the dominant heat-release chemistry that reduction schemes are designed to preserve, whereas species such as NO₂, N₂O and HCN originate from low-concentration radical pathways that are more easily lumped or removed during reduction. This explains why

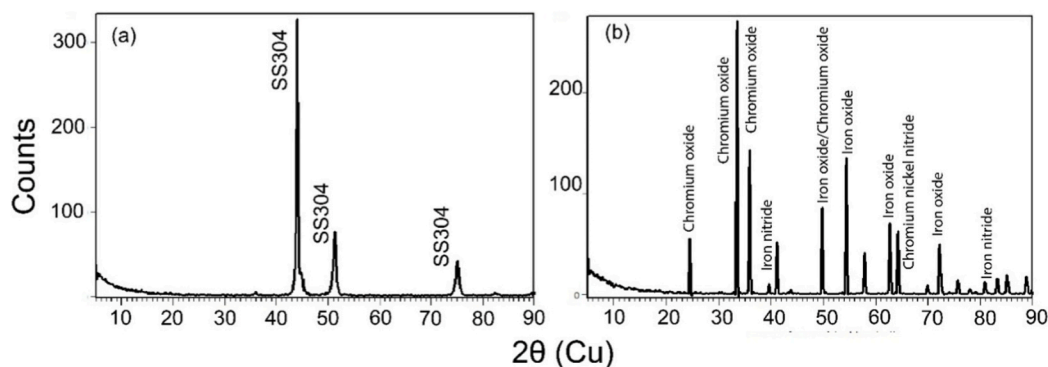


Fig. 16. (a) XRD images of SS304 (a) and exposed at 500 kW [XX11].

comparable modelling approaches can yield very different accuracy levels for different pollutants, under/overpredicting some emissions up to two orders of magnitude.

Through these tools, developments of industrial burners and furnaces will see an expansion thanks to the use of advanced CFD models. However, one of the main obstacles that need to be resolved is the accurate definition of the radiation models and reliable boundary conditions within these systems to properly resolve large scale combustion systems. Different to conventional lab-scale burners, the higher power, lower heat losses, greater radiation and different third reaction mechanisms occurring within the components of the units of interest, will present a real challenge for ammonia fuelled units >100 kW. The implications of having solid-liquid-gaseous co-firing with other fuels such as diesel, coal or hydrogen will also increase the complexity of these models, hence requiring novel strategies for their resolution, strategies that attempt to resolve turbulence with precision similar or greater to LES. As part of the foreseeable futures for these systems, it is believed that RANS modelling will serve to support data generation, which in turn will expand the capabilities of machine learning codes. The codes, validated via limited experiments (to reduce time and cost), will serve to create datasets which will support advanced modelling for scalability and analyses of transient scenarios (ie. turn on, ramp up, shut down). These modelling advancements, combined with models that incorporate gasification, droplet breakup, boiling, thermal interactions, etc. will then have to be resolved via new low computational methods that likely will be based on machine learning strategies.

Concurrently, for ammonia-containing fuels to enter commercial gas turbine utilization in the near future, three main areas must be addressed within the next few years. First, there is a significant demand for robust but computationally efficient chemical kinetic mechanisms that can predict chemical kinetic and flame propagation processes convincingly in high-pressure, high-temperature real-engines conditions. These can be facilitated by focused experimental campaigns as there is a lack of high-pressure validation data. Although most validation datasets currently originate from laboratory-scale facilities, they remain essential to identify the governing mechanisms controlling flame stability, emissions formation and optimal operating conditions. Several of the reviewed studies [22,98] employ industrially representative burner designs, bridging the gap towards practical gas turbine applications. Furthermore, the trends governing NO_x emissions, ammonia slip and flame morphology have shown consistent behavior across different scales, suggesting that these phenomena may be scalable when the dominant combustion features are preserved. Second, modelling frameworks need to advance in their treatment of heat transfer, moving beyond adiabatic assumptions to incorporate conjugate heat transfer and accurately predict wall cooling effects on emissions and flame stability. Finally, it is necessary to scale up validated numerical methods from laboratory-sized test chambers to full-scale and complex engine geometries, including advanced staging and new fuel injection strategies. Addressing these challenges will be essential for the reliable design

of efficient, low-emission ammonia gas turbines that employ validated models.

As for accurate emissions prediction and mitigation, control modelling will require substantial advancements; current understanding of N₂O formation mechanisms in ammonia combustion remains incomplete, with comprehensive mechanism development studies necessary to capture competing pathways producing nitrous oxide through intermediate species and temperature-dependent reaction sequences [110]. Accurate ammonia slip prediction will also require improved sub-models for wall film dynamics, crevice flow contributions, and post-oxidation processes in cooler cylinder boundary regions where unburned ammonia accumulates. As in the previous assessments, it is evident that these and other pollutants play an important role in ammonia-blends combustion. Carbon emissions, which are expected to be part of the exhaust gases produced during the transition to pure ammonia fuelling, will also have to be tackled to mitigate environmental impacts. The higher equivalence ratio that leads to ammonia slip is also culprit of the higher production of carbon monoxide, which due to the reduced oxygen concentration, leads to reduced combustion efficiencies and environmental concerns. Thus, the trade-off between emissions needs to be properly assessed via advanced numerical methods that also integrate Life Cycle Assessments that adequately elaborate on the decarbonisation, oxygen depletion, acid rain effect, and greenhouse gas potential of the systems fired using ammonia-blends. It must be recognised that there will be cases in which the ammonia molecule will not be the best to fulfil the stringent requirements expected by 2050 energy transition scenarios. However, it is also clear that there will be niche applications where power will meet with lower emissions, and the overall trade-off will be better than current fossil applications -and even electrification approaches-, thus making ammonia part of the energy mix of a cleaner future. Therefore, additional computational efforts to unveil the complexities of these pollutant interactions will be needed in the following years.

4.1. Real impacts at large scales

It is also critical that further assessments via CFD and other numerical methods are conducted on the impacts of ammonia firing at large power scales. Recent studies performed by Wang et al. [111] suggest that by using ammonia blends, the integrity of stainless steel (SS) components can suffer detrimental impacts as a consequence of the nitration effect. The latter, which directly impacts the recrystallization of the material and various layer impurities, can have drastic consequences at larger scales. This was a problem recognised recently in the AMBURN program conducted at Cardiff, in which SS pipelines were employed as part of the components designed to deliver hot ammonia into a novel cracking system [112]. The results from Xray analyses and electronic microscopy revealed a drastic change in morphology and species formation at the outer layers of these components, Fig. 16. The challenge raises the importance of further development for coatings that through

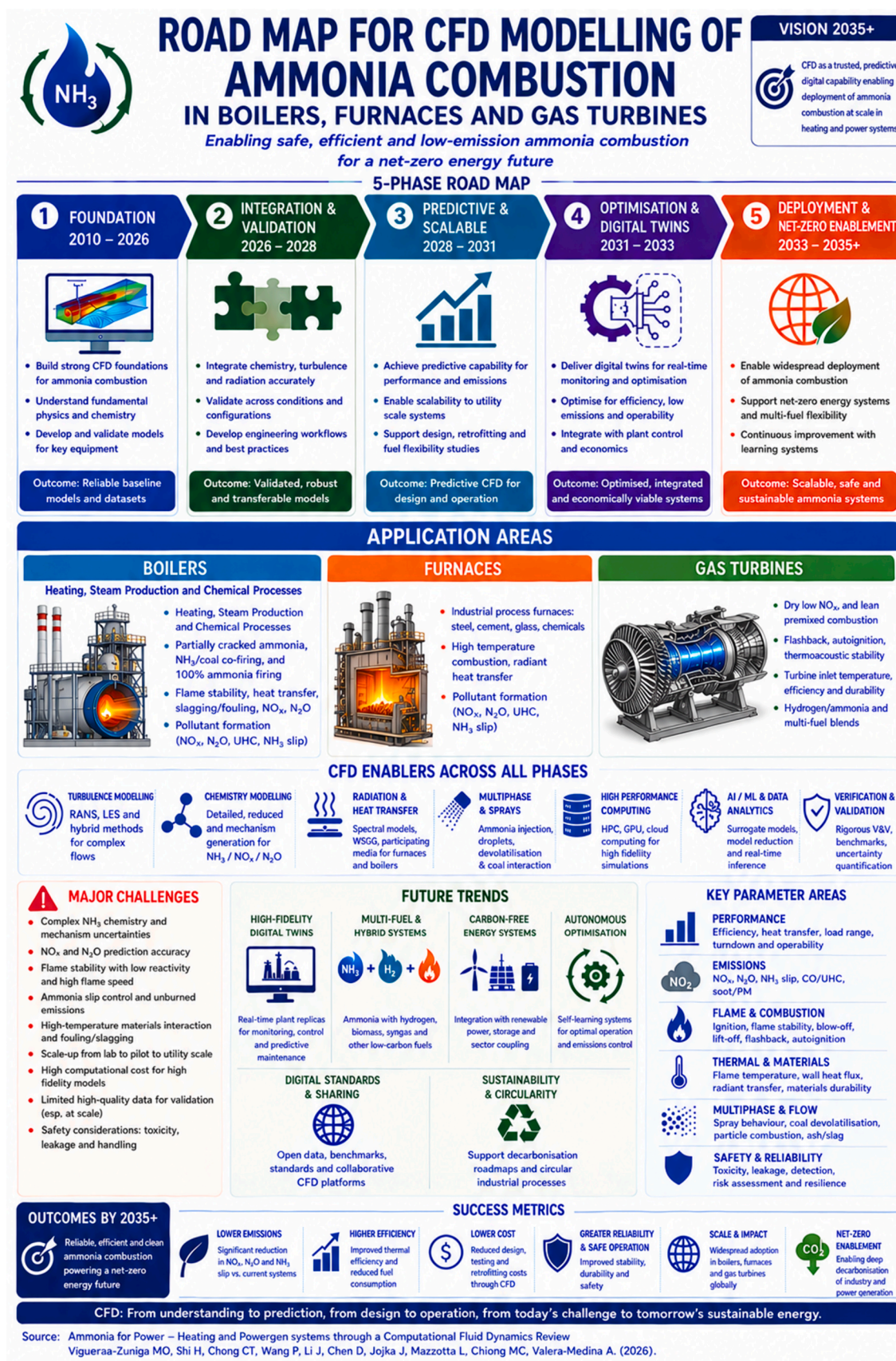


Fig. 17. Summary Roadmap acknowledging the works cited in this manuscript.

numerical modelling can be improved and maximised for ammonia firing purposes whilst reducing costs and augmenting component resilience.

Additionally, recent studies performed by Alnaeli et al. [113,114] also show that the impact of ammonia, hydrogen and methane in turbine materials (ie. Inconel, Hastelloy) represent an area of industrial concern. The nitration problem comes accompanied by hydrogen embrittlement processes that reduce ductility whilst also making the components more brittle and easier to reach failure at lower loads. The high interaction between H/N species with Ni-based materials appears to be the culprit of the effect, a phenomenon that will require large numerical support to overcome the potential safety impacts caused by these changes in material properties.

4.2. Summary Roadmap

The analyses of these works have enabled the production of a Roadmap that summarizes this manuscript, Fig. 17.

5. Conclusions

Ammonia combustion modelling is expected to keep growing not only in number of publications but also in impact for the understanding of fundamental concepts, delivery of improved modelling techniques and support for industrial implementation of ammonia as an energy vector. International conglomerates keep expanding to establish corridors and industrial hubs capable of using ammonia efficiently for climate abatement and energy resilience. Behind many of these expansions, CFD modelling has and will keep playing a critical role, thus making evident the importance of the concept and the need for a review like the one presented.

As for the use of CFD in large burners and furnaces, results show that mainly using RANS can be an option with good deliverables for practical applications. Low computational cost combined with relatively simple configurations have shown the capabilities of current methods, although further advancements and more complex geometries will require more advanced resolution methods. The correct selection of heat transfer modes with the right mechanism is critical for the adequate resolution of these models, which can show disparities of several orders of magnitude if the selection is not adequately performed. Radiation, being a complex parameter that is still under the scope of several research programs, needs to be validated with better experiments, hence delivering robust data for more reliable modelling approaches. Similarly, the use of coal co-firing will continue to expand due to the great interest of Asian countries in using ammonia for coal displacement. Multi-burner units will be modelled at various scales, injection strategies and emissions control modes, hence showing not only the complex nature of high temperature/low heat losses systems on ammonia decomposition/pyrolysis/oxidation processes, but also intrinsic phenomenology of multi-flame interactions for control and scalability.

Similarly, gas turbines have benefitted from the use of CFD modelling when using ammonia fuelling. The implementation of advanced codes, mainly LES, has ensured that configurations previously validated experimentally can be expanded and improved by maximising fuel efficiency through geometrical reconfigurations. Simultaneously, emissions abatement and process integration appear feasible in the short term through RANS studies that can deliver faster analyses with the potential of more complex system configurations. These advantages have delivered physical systems that have demonstrated that ammonia can be combined with methane (ie. natural gas) and hydrogen to support the transition towards a carbon-free industry. However, more accurate models are still required, whilst the use of reduced mechanisms and User Defined Functions in combination with more reliable turbulence models and machine learning strategies are in the scope of current research groups to generate methodologies that can reduce implementation costs whilst commercially supporting an industry that has realised the

potential of ammonia as a turbine fuel. In particular, reduced mechanisms offer a fantastic solution for the resolution of more complex turbulence methods. However, their accuracy highly depends on the power load, temperatures and heat transfer conditions present in the evaluated systems. Additionally, third body reactions, complex radical interactions, and improperly resolved residence times can drastically affect the performance of these mechanisms, making the case too complex for standing methods, an issue that takes us back to the large number of standing mechanisms in the literature. The challenge could be an area where machine learning can be successfully applied, supporting the creation of bespoke, easily generated reduced mechanisms for specific conditions – although, this is another story.

CRedit authorship contribution statement

M.O. Viguera-Zuniga: Conceptualization, Writing, Reviewing and Editing. **H. Shi:** Reviewing, Data curation, Image Copyrights, Writing. **C. T. Chong:** Reviewing, Editing, Writing (Chapter 6). **P. Wang:** Reviewing and Writing. **J. Li:** Writing and Reviewing. **D. Chen:** Writing and Image review. **J. Jójka:** Reviewing, Data curation, Writing. **L. Mazzotta:** Writing and Reviewing. **M.C. Chiong:** Writing. **A. Valera-Medina:** Supervision, Reviewing, Final Editing, Writing.

Declaration of competing interest

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Data availability

No data was used for the research described in the article.

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