

# CA22151: Cyber-Physical systems and digital twins for the decarbonisation of energy-intensive industries



## Deliverable D5

Roadmap for the integration of renewable synthetic fuels in existing energy-intensive industry infrastructures

**Authors:** Viktor Józsa (BME), Pino Sabia (CNR-STEMS), Giancarlo Sorrentino (CNR-STEMS), Federica Ferraro (TUB), Antonio Attili (UoE), Alessandro Parente (ULB)

## Table of Contents

1. Introduction.....	3
2. Utilising renewable synthetic fuels .....	5
2.1. Carbon-free fuels: Hydrogen and Ammonia.....	5
2.2 Renewable hydrocarbon fuels.....	7
2.3 Renewable biogenic fuels .....	8
3. Modelling renewable synthetic fuel combustion .....	9
3.1 High-fidelity simulations.....	9
3.2 Reactor (network) modelling .....	10
4. Advanced sensing .....	10
5. Industrial implementation .....	11
6. CYPHER COST Action activities .....	12
7. Conclusions .....	13
Acknowledgments .....	15
References .....	16

## 1. Introduction

The integration of Renewable Synthetic Fuels (RSFs) poses critical challenges for energy-intensive industries worldwide. The current bottleneck on the upstream side is availability, which is expected to be addressed through excessive renewable energy generation and currently underutilised sources, such as various waste streams. The currently used industrial combustion systems solely utilise hydrocarbon fuels, meaning that burner modification may be required to employ certain RSFs, which necessitates a significant extension of the knowledge base in Combustion Science and Technology (CS&T). If hydrocarbon fuels are used, a Carbon Capture Utilisation/Storage (CCUS) solution is required to suppress CO<sub>2</sub> emissions downstream [1]. Implementing RSFs must be economically competitive, which in turn requires ad-hoc governmental, national, and international policies and investments, along with the harmonization of regulatory guidelines on emissions. Herein, the development of a consolidated Combustion Science and Technology (CS&T) for RSFs mandates the involvement of academic/research institutions and centers as principal actors. The penetration of RSFs into industrial sectors cannot happen without solving the fundamentals of RSFs. These issues have an intrinsically multifaceted nature (involving chemistry, heat and mass transfer phenomena, turbulence, turbulence-chemistry interaction, radiation, etc.), which must be partially or even completely rebuilt with respect to fossil fuels. Within this framework, the first step towards the spread of RSFs is understanding their physical and chemical behaviour. Thermodynamic and physical-chemical (density, viscosity, boiling/fusion temperature, vapor tension, etc.) are fundamental for both combustion processes (adiabatic temperature, heat capacities, atomization, vaporization) and safety regulations. Second, the oxidation/pyrolysis and pollutant formation chemistry should be addressed through experimental tests and numerical simulations to gain relevant information related to combustion system design, pollutant emission regulation, and control. To achieve this target a “scale bridging approach” have to be selected (Fig. 1). The industrial combustion processes are intrinsically multi-physical, i.e. the combustion is governed by complex heat and mass transfer phenomena that are inherently very difficult to characterize at industrial harsh levels, where also the implementation of advanced diagnostic techniques and sensing for data collection is very complex (no physical/optical accesses). Given this scenario, the only adoptable philosophy is to scale down the problem from a multifaceted to a single-faceted process, which can be resolved in time or space with low uncertainty. For instance, model reactors (Jet-Stirred flow Reactor, Tubular Flow Reactors, laminar flames, counter diffusion/co-flow flames, etc), built up over decades in the Chemical/Mechanical Engineering, can be used to fully characterize fuel Oxidation/Pyrolysis chemistry, or lab-scale burners (easily accessible) can be used to solve other aspects (chemical-chemistry interaction, radiation, etc.) through the implementation of advanced chemical and optical diagnostic techniques. System scale-down or scale-up rules encompass a fundamental aspect that preserves the

chemical/physical constraints of real industrial systems. The advantage of lab-scale reactors/burners lies in the possibility of controlling the external parameters of the system and exploiting the effect of various parameters on the combustion process (fuel, mixture composition, pressure, etc.), allowing for the coverage of a wide range of combustion domain conditions. This approach clearly enables the support of developing high-fidelity models for use in the design phase of industrial systems. The scale-bridging approach features a dual reading key, as it can be interpreted both from bottom to top or vice versa. The vice versa logic is driven by the necessity to delimit the combustion domain conditions to real systems. Likewise, in an industrial system, local conditions can be addressed through dedicated experiments at lab-scale levels, once the boundary conditions are correctly identified. Key characteristics, such as safety, combustion efficiency, operational stability, and pollutant emissions, are the targets of the scale-bridging approach, along with the development of high-fidelity models for design purposes.

This approach has been developed over the years for conventional fuels and must be reapplied to RSFs for the development of their CS&T, given different chemical/physical properties. Herein, the scale bridging approach has been developed from the industrial revolution (1850) up to now, stepping also through trial-and-error approaches before maturing conventional fuels CS&T. Considering the target of 2050, following EU guidelines related to the decarbonization of “hard to abate” industrial sectors, the elapsed time consists in a drastically smaller period needed for the fossil fuel CS&T development for industrial segments. This point imposes the implementation of new strategies to accelerate the deployment of RSFs to real systems. In this perspective, the scale bridging approach can be aided by the development of new tools based on digital twin, Artificial Intelligence, and Machine learning. From the other side, the development of these tools requires large amounts of data to serve as “training targets”; thus, it proceeds in parallel with data acquisition and sensing development. Hence, it is necessary to develop advanced data acquisition systems that can bypass the constraints of implementing advanced chemical/optical diagnostic techniques in harsh industrial environments.

All these scenarios are also embittered by the consideration that new fuels may require new combustion concepts (MILD combustion, Oxy-flame combustion, Catalytic combustion, plasma-assisted combustion, etc.), thus a new operating combustion domain [2]. The scale-bridging approach must be integrated with the ML-AI bridging approach, while relying on the advancement of fast and reliable experimental data through sensing and sensor fusion technology.

## Combustion-history timescale

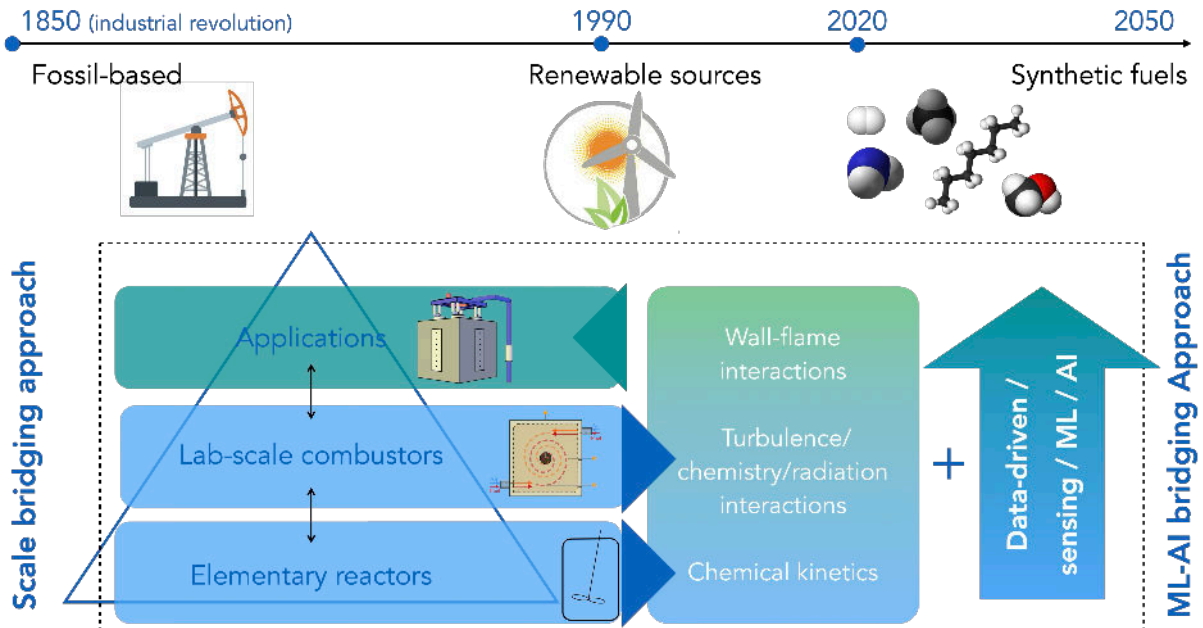


Figure 1 - Timeline of CS&T development from the Industrial Revolution up to 2050. The CS&T for fossil fuels has been developed over the past century, while RSF utilisation needs to catch up in maturity over the next few decades. This is enabled by advanced sensing and ML/AI-based approaches [3].

## 2. Utilising renewable synthetic fuels

Utilising synthetic hydrocarbon fuels has the advantage that the system may remain unchanged, while CCUS can be added. To reduce the CCUS costs, oxyfuel combustion is an option [4], but this requires a system upgrade. The most promising carbon-free fuels are hydrogen and ammonia, as emphasised below. Regardless of the fuel type, the lower heating value (LHV) must be added into the production process of the particular RSF. Based on the required process steps, the LHV/input energy ratio may decrease further. A notable example is the energy required for ammonia production via the Haber-Bosch (HB) process, which necessitates 22.5 MJ/kg of energy, compared to the 18.6 MJ/kg heating value. Even though the HB process is more than a century old, a breakthrough is still awaited [5].

### 2.1. Carbon-free fuels: Hydrogen and Ammonia

The majority of researchers agree that hydrogen will be the fuel of the future [6]. However, the road there is fraught with technical, political, and social challenges. Hydrogen has an extremely wide flammability range, exhibits a laminar flame speed that exceeds that of hydrocarbon fuels, and has an outstanding LHV per kg [7]. On the other hand, burdened by logistics and material compatibility issues. Since ammonia has combustion properties that are much closer to those of hydrocarbon fuels, and its logistics and material compatibility problems have been largely solved [8], it has significant momentum towards industrial penetration. If closed cycles are

considered, sulphur [9] and iron cycles [8] are potential candidates. Since none of the mentioned fuels is considered an ultimate solution in the short or medium term, innovation is highly desired in this field.

Green Hydrogen, produced via electrolysis powered by renewable electricity, is a key chemical energy carrier for decarbonizing Energy Intensive Industries (EII). When used to power furnaces, gas turbines, or engines, hydrogen combustion produces no CO<sub>2</sub> emissions. However, hydrogen combustion differs significantly from conventional hydrocarbons. It exhibits high flame speeds, high adiabatic temperatures, wide flammability limits, and high diffusivity [2]. These properties make the direct use of hydrogen very challenging in conventional burners, due to unsustainable material temperatures and a high tendency to NO<sub>x</sub> production. To handle hydrogen, several strategies have been developed over time, including ultra-lean combustion, which helps contain working temperatures and limit NO<sub>x</sub> emissions. Unfortunately, combustion instabilities can easily occur under this operating mode, particularly near lower flammability limits in high turbulent conditions; thus, extinction phenomena are likely to occur. Further options to handle Hydrogen reactivity rely on novel combustion concepts, such as MILD combustion, which simultaneously guarantee low temperatures, process stability, and low NO<sub>x</sub> emissions.

From a chemical point of view, hydrogen oxidation chemistry has been one of the most studied topics within the combustion community for decades, considering that it forms the basis of any oxidation hydrocarbon kinetic mechanisms, within the hierarchical construction philosophy of detailed schemes. Consequently, detailed kinetic mechanisms are supposed to be reliable and robust. Nonetheless, in view of the advancement of chemical kinetics theory and the exploitation of new combustion modes (different operating conditions), new detailed schemes have been recently proposed, integrating novel combustion roles (mixing roles), declaring novel elementary reactions, and updating third-body efficiencies for pressure-dependent reactions [10–12].

In addition, when moving to diffusive flames, one particularly prominent characteristic of H<sub>2</sub> combustion is its thermodiffusive instability [13,14]. This phenomenon is based on the larger diffusion coefficient of light hydrogen compared to heat (more than a factor of three) and the influence of thermal diffusion (Soret effect), which is much less relevant in hydrocarbon flames. Flame fronts are also affected by hydrodynamic (or Darrieus–Landau) instabilities caused by thermal expansion [3]. The interaction of these intrinsic instability mechanisms is complex and nonlinear, ultimately leading to highly convoluted morphological flame structures [3-5]. In turbulent flow conditions, the interaction between the flow, molecular transport, and chemistry becomes even more complex, with practical implications for flashback, blow-off, and thermoacoustic instability. Given these challenges, modeling and experimental studies are currently being conducted to better understand hydrogen combustion behavior and accelerate its safe and efficient deployment in industrial applications.

Ammonia ( $\text{NH}_3$ ) is emerging as a carbon-free energy carrier and hydrogen carrier, offering a more convenient alternative to hydrogen for transportation and storage. It can be liquefied under moderate pressure ( $\sim 10$  bar at  $25^\circ\text{C}$ ) and temperature ( $-33^\circ\text{C}$  at atmospheric pressure) and benefits from an established global production, storage, and shipping infrastructure for its usage as a fertilizer. For combustion applications, ammonia can be completely or partially cracked to  $\text{H}_2/\text{N}_2$ , enabling either direct ammonia firing or  $\text{NH}_3/\text{H}_2$  blends. While hydrogen is highly reactive and has a high flame speed compared to natural gas, the opposite is the case for ammonia. Blending with hydrogen or other fuels enhances reactivity and flame stability while limiting nitrogen oxides and  $\text{N}_2\text{O}$  production. Specifically, in power generation and marine shipping, the combined use of hydrogen and ammonia is attracting more attention for achieving clean, fuel- and load-flexible energy conversion.

The ammonia oxidation chemistry was developed in the past to model  $\text{NO}_x$  formation routes and to develop flue-gas after-treatments, such as Selective or Non-Selective Catalytic Reduction. Over the last few decades, as the concept of using ammonia as a fuel has gained popularity, numerous (over 60) detailed kinetic mechanisms have been proposed in the scientific literature. While ammonia oxidation chemistry can be considered well-developed (even though kinetic mechanisms are continuously updated and optimized), a significant issue arises from the chemistry related to ammonia mixtures with fuel enhancers ( $\text{CH}_4$ ,  $\text{CH}_3\text{OH}$ , DME, DEE, etc.) in the dual-fuel combustion mode, aimed at enhancing ammonia reactivity [15–17]. Here, the problem is twofold, as the interaction of  $\text{NH}_3$  chemistry with other fuels results in a very complex system with new phenomenological behaviors. At the same time, the lack of dedicated experimental data hinders the development and validation of mechanisms. In this specific context, the role of *ab initio* chemistry is aiding the development of detailed kinetic schemes [18,19].

Recently, in the category of no-carbon fuel, sulphur has also been added to the RSFs [], with a virtual cycle where sulphur is oxidized to  $\text{SO}_2$  and then reduced back into a sulphur state. This concept has been recently proposed; thus, updates will be provided in the near future.

## 2.2 Renewable hydrocarbon fuels

The greatest advantage of synthetic hydrocarbons is their 100% compatibility with our current technologies. Methane production is based on the methanation of  $\text{CO}_2$ . A highlighted platform molecule is methanol, which can be biologically produced. Then, various hydrocarbons can be synthesised by using the Fischer-Tropsch process. As mentioned above, the primary challenge is the development of efficient carbon capture technology.

## 2.3 Renewable biogenic fuels

Other fuels that can be chemically synthesized from renewable sources (biogenic, wastes) are the Sustainable Aviation Fuels (SAFs) [20]. Currently, there are 11 production chains, involving chemical, catalytic, and biochemical processes (Fisher-Tropsch, Hydroprocessed Esters and Fatty Acids (HEFA), Catalytic Hydrothermolysis Jet (CHJ), etc.), which start from crops, lignocellulosic biomasses, solid wastes, sugar, microalgae oils, vegetable/animal fats and oils. SAFs can be used in Gas Turbines and Engines, with a large interest from the aviation sector. They are conventionally composed of linear hydrocarbons with a zero or low aromatic concentration. Given the SAF raw material and process production, the composition may drastically vary. This represents a “weak point” towards standardization. The characterization itself of the SAF composition requires specific lab measurements with (expensive) advanced chemical diagnostic techniques (High Pressure Liquid Chromatography, Nuclear Magnetic Resonance, etc), with a multitude of species not easy to detect and/or quantify, in the absence of standards. In turns, the physical (vaporation curve, distillation, viscosity, density) and chemical properties (formation enthalpy, entropy) may drastically vary, impeding the definition of common rules for combustion system design, as physical (atomization, vaporization, fuel break-up, etc) and combustion (laminar burning velocity, auto-ignition delay times, flammability limits, etc.) processes are SAF dependent composition. Coming from biogenic sources, SAFs can also undergo an aging process, resulting in alterations to their chemical/physical properties. Nowadays, the sooting tendency of SAF is a topic of debate in the combustion community, as the low or no aromatic content should theoretically guarantee lower soot production in real combustion systems. However, the higher hydrogen content, compared to conventional aviation fuels, could lead to higher local temperatures and potentially increase soot production. Additionally, the cost of SAF production remains unaffordable, rendering the “SAF economy” uncompetitive with conventional fuels [21]. This is the reason why they are conventionally mixed with standard fuels (Jet-A1, Jet-A8) at a ratio of 2% to 50%. The category of SAF is the perfect example of how the penetration of RSF into real systems is very complicated, and the related CS&T has to be rebuilt entirely. Given this background, the role of scientific research is fundamental to allow the penetration of this fuel category into the real market. The realization of lab-scale experiments under controlled conditions remains the way forward, while the difficulties in defining the actual composition make the definition of boundary conditions (for example, mixture stoichiometry) very challenging. From this perspective, the role of ML and AI techniques can be fundamental in predicting physical and chemical properties based on reference properties (for example, those derived from functional groups using Nuclear Magnetic Resonance techniques) [22], which can be detected with advanced chemical techniques. The development of detailed kinetic schemes can be initiated with automated tools, based on fuel elemental analyses and averaged composition, and then optimized using experimental evidence.



The SAFs category is also a reference class of fuels on how policies and investments are proceeding from governments to public/private companies; nonetheless, despite all the economic and practical/technological difficulties highlighted in the previous paragraphs, the aviation sector is strongly investing in SAFs, due to its great potential to decarbonize the industry itself.

Other categories of fuels that may play a significant role in the decarbonization of several sectors include oxymethylene ethers (OMEs) and hydrogenated vegetable oils (HVO) [23], which can be used as bio-diesels in engines. Additionally, for these classes, the chemical/physical properties differ from those of conventional fuels, with high production costs and new combustion phenomena and oxidation chemical kinetics that warrant attention before integration into a real economic system becomes feasible.

### 3. Modelling renewable synthetic fuel combustion

#### 3.1 High-fidelity simulations

High-fidelity simulations are essential for advancing the understanding and predictive modeling of renewable synthetic fuel combustion. Regarding hydrogen and ammonia, they are crucial for capturing thermodiffusive instabilities and translating that understanding into reliable models for virtual industrial design. Direct Numerical Simulation (DNS) has become the reference “virtual experiment” for probing fundamental combustion phenomena—flame structure, ignition, and turbulence–chemistry interactions — and for providing benchmarks for Large Eddy Simulation (LES) closures. Due to computational constraints, DNS is typically limited to canonical configurations with simplified geometries and reduced chemistry [13,24,25].

A priori analyses indicate that conventional flamelet manifolds fail to reproduce the coupling between preferential diffusion, curvature, strain, and turbulence in lean hydrogen flames, highlighting the need for extended manifold-based closures [26]. Advanced LES approaches have therefore been developed to incorporate detailed transport and chemistry, supported by machine-learning-assisted tabulated models. These efforts aim to enable predictive simulations of practical systems such as gas turbines and furnaces operating with hydrogen, ammonia, or e-fuel blends.

DNS has also been widely applied to diluted and MILD combustion regimes, increasingly used for low-NO<sub>x</sub> operation. These conditions require special modelling strategies that account for low-temperature chemistry, radiation, and multiphysics coupling [27]. Combined with advances in high-performance computing and data-driven model reduction, these developments are paving the way toward integrated digital twin frameworks for the design and optimization of sustainable combustion technologies.

### 3.2 Reactor (network) modelling

High-fidelity modelling consumes significant computational power; consequently, reduced chemical mechanisms are used to make a compromise in reaction kinetic modelling. However, an alternative approach is to identify characteristic parts of the reaction zone using CFD and build a Chemical Reactor Network (CRN) model to analyze detailed reactions [28], while keeping the computational costs of flow modeling about 3-4 orders of magnitude lower. It works for various burners, including MILD combustion [29]. The number of reactors that decompose the reaction zone can be increased, while the improvement is usually small [29]. In an ideal case, a single Perfectly Stirred Reactor (PSR) describes the reaction zone, which can be the case with a distributed flame [30]. Moreover, PSR models always provide an ideal case, which can be approached by various design considerations, providing a realistic lower boundary for, e.g., pollutant emissions for a given system.

### 4. Advanced sensing

Industrial combustion chambers are typically optically inaccessible, making most laboratory sensor types unusable. However, sensor miniaturisation and cost reduction may enable real-time tracking of various operational parameters. The combined use of various sensors, known as sensor fusion, can significantly enhance accuracy. Navarez et al. [31] concluded that Convolutional Neural Networks (CNN) combined with the spectrogram of the audio signal were the most accurate method for flame classification. This example demonstrates that combining classical and AI hybrid approaches can yield the most accurate results. However, certain environments might benefit from the combined use of image and audio signals for real-time process tracking. CNN also excels in flame identification by OH- Planar Laser-Induced Fluorescence image series [32]. Flame image processing is critical for both lab-scale experiments and industrial process control. Since flames have a finite thickness, image processing under a wide range of conditions may require advanced considerations, where deep learning may lead to outstanding results [33]. Kardos et al. [34] tested 16 binarisation techniques to identify those with good performance in terms of computational effort, accuracy, and consistency for four different flames, using three optical filters. The results are shown in Fig. 2.

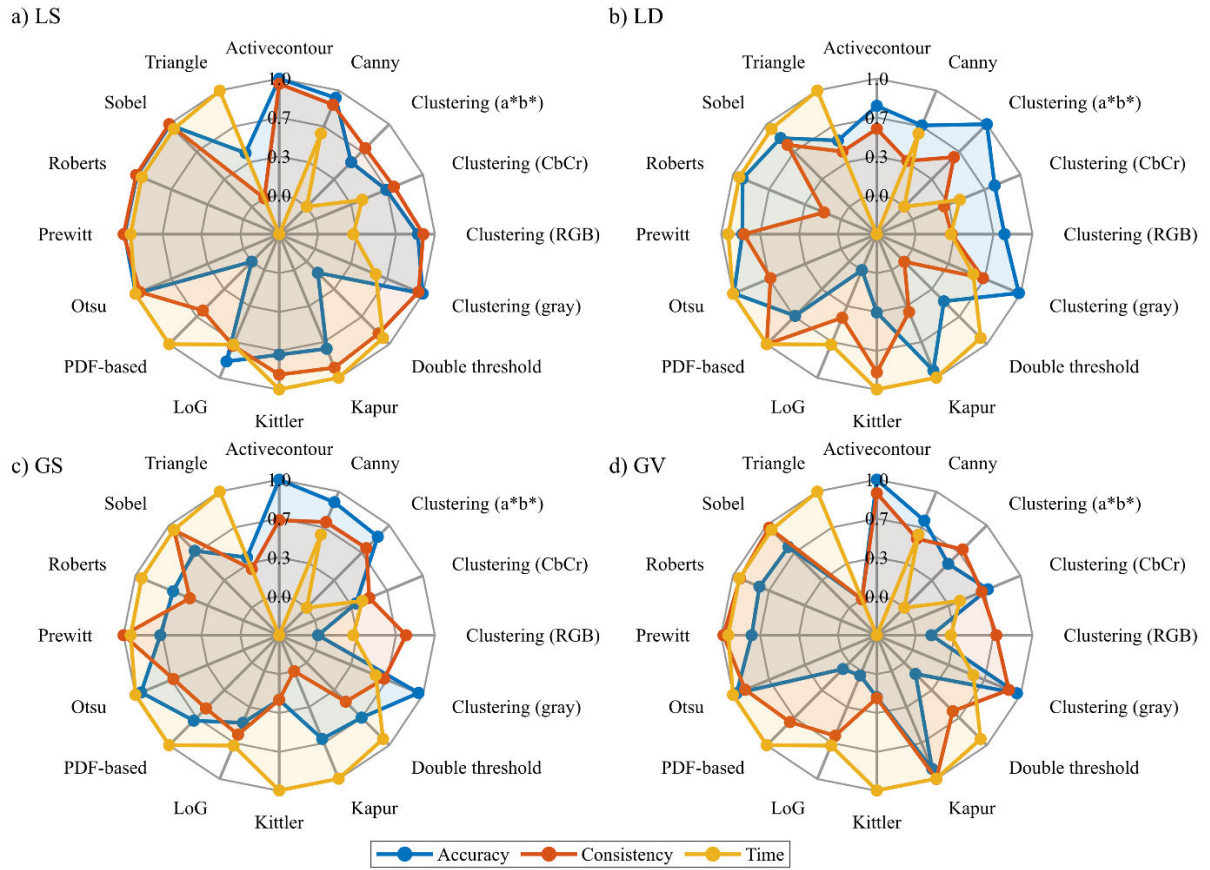


Figure 2 – Relative performance of 16 binarisation methods for different flames. a) liquid fuel – straight flames, b) liquid fuel – distributed flames, c) natural gas – straight flames, and d) natural gas – V-shaped flames.

## 5. Industrial implementation

The industrial implementation of RSFs requires careful consideration of operational safety, system lifetime, and increased concentrations of various pollutants [35]. It is expected that the rakeoff of RSFs will result in further regulations to clarify the complicated and currently unbalanced renewable fuel directives affecting different applications [36]. Among the EIs, it is most probable that the glass and ceramics industry can be the first to become completely carbon-free. Moreover, this industry is looking forward to hydrogen oxyfuel combustion [37], which requires revising emission standards to specify the emissions to the thermal power plant, as only the contaminating species remain if the flue gas from oxyfuel hydrogen combustion is condensed [4]. This pressure on the regulating bodies has been present for decades.

The cement industry is responsible for the largest contribution to global CO<sub>2</sub> emissions. This problem is more complex than that of other EIs, as the majority of the CO<sub>2</sub> emissions originate from calcination. Hence, process carbon capture solutions are also required, in addition to implementing alternative fuels. The results of a comprehensive analysis for the Chinese cement industry up to 2040 are presented in Fig. 3. Even though no realistic scenario exists for pushing the emissions to zero, the effect of the implementation of the advanced technologies in the cement

industry will significantly reduce global CO<sub>2</sub> emissions, as it is responsible for about a quarter of all industrial CO<sub>2</sub> emissions.

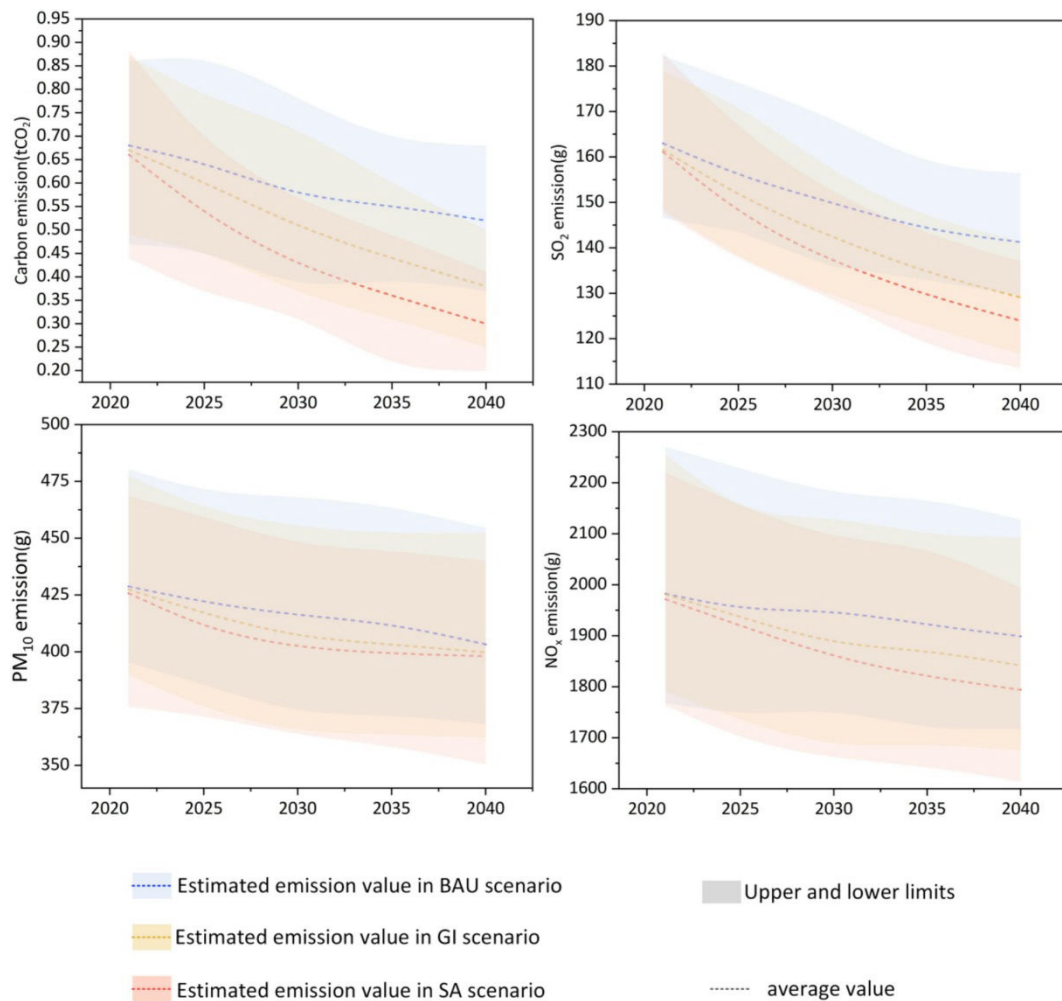


Figure 3 – Uncertainty analysis of pollutant and carbon emission assessments under different scenarios: BAU: business as usual, GI: gradual intensification, and SA: stringent advancement [38].

The steel industry is the second-largest industrial source of CO<sub>2</sub> emissions. Fortunately, carbon-free fuels may contribute to clean combustion. Ending up with the lowest emissions may require relocating the site to the RSF producer site [39], which does not necessarily mean the best political-strategic option in many cases. The future of steel and ironmaking is likely to transition towards Electric Arc Furnaces (EAFs), which will eliminate combustion for the majority of processes, as EAF technologies are expected to become competitive soon [40].

## 6. CYPHER COST Action activities

The CYPHER Cost Action has been highly active across all the aforementioned topics, aiming to identify the most promising fuels for hard-to-abate industries and to address the related challenges. To this end, members of the COST Action have invited experts from various sectors to deliver plenary lectures, fostering proactive

discussions and establishing a joint framework for defining RSF roadmaps and common guidelines.

Below is a list of the contributions presented during the CYPHER Cost Action meetings and workshops:

- "On virtual development of renewable fuels for real and virtual powertrains", 1<sup>st</sup> General Meeting, Ljubljana, 10-12 April 2024, Speaker: Prof. Fabian Mauss, University of Technology, Cottbus-Senftenberg, Germany
- "Ammonia chemistry in a progressively decarbonized world", 2<sup>nd</sup> General Meeting, Krakow, Poland, 19-20 May 2025: Speaker: Prof. Maria Alzueta, University of Zaragoza, Spain
- "Oxygenated Fuels – Recent Experimental Knowledge and Modelling", Cypher Cost Action WG<sub>1</sub> and WG<sub>2</sub>, Naples, Italy, from September 10-12, 2025. Speaker: Prof. Zeynep Serinyel, University of Orléans – CNRS, France
- "Decarbonizing Aviation with Low-Carbon Fuels. Progress, Challenges & Opportunity for Data Intensive Research", Cypher Cost Action WG<sub>1</sub> and WG<sub>2</sub>, Naples, Italy, 10-12 September 2025. Speaker: Prof. Stephen Dooley, Trinity College, Dublin.

Accordingly, the topics addressed have encompassed hydrogen, ammonia, and ammonia-based blends, oxygenated compounds, and Sustainable Aviation Fuel (SAF) combustion. These discussions have covered the state of the art, regulatory frameworks, experimental and numerical approaches, as well as current challenges and future perspectives.

## 7. Conclusions

The decarbonization of "hard-to-abate" industries is an urgent challenge that can be addressed through the widespread adoption of Renewable and Sustainable Fuels (RSFs) across multiple energy sectors. Several RSFs are suitable for meeting this objective in various industrial segments, and their large-scale implementation is feasible, provided that their production costs become competitive with those of conventional fossil fuels and that RSF combustion science and technology continue to advance rapidly.

Zero-carbon fuels such as hydrogen (H<sub>2</sub>) and ammonia (NH<sub>3</sub>) present several challenges before they can be directly employed in combustion systems. For hydrogen, the combination of high laminar flame velocities and elevated adiabatic flame temperatures results in a strong tendency toward thermal NO<sub>x</sub> formation, raising concerns about safety, material durability, and pollutant emissions. Conversely, ammonia exhibits low reactivity—characterized by narrow flammability limits and low laminar burning velocities—along with a high propensity to generate both fuel and thermal NO<sub>x</sub> under conventional combustion conditions. Although the oxidation kinetics of these fuels are relatively well understood, recent studies have

revealed new combustion phenomena governed by  $H_2$  thermo-diffusive effects (e.g., cellular flame structures) in both hydrogen and ammonia flames.

Other RSFs with chemical structures similar to conventional fuels—such as biomethane, bioalcohols, methanol, and ethanol—generally pose fewer challenges in practical applications due to their close analogy with traditional hydrocarbons, aside from their higher production costs. On the other hand, fuels such as Sustainable Aviation Fuels (SAFs), Oxymethylene Ethers (OMEs), and Hydrogenated Vegetable Oils (HVOs) still present significant open issues related to their chemical and physical properties, combustion behavior, pollutant emissions, and the current lack of standardized regulations.

It is evident that dedicated national and international government policies, along with targeted investments, are essential to accelerate the development of Combustion Science and Technology of RSFs. Likewise, the establishment of a robust Combustion Science and Technology (CS&T) foundation for RSFs cannot proceed without academic/industrial scientific research and collaboration, as the integration of these fuels into industrial sectors depends on resolving their fundamental combustion-related challenges to scale up to real combustion systems. These challenges are inherently multidisciplinary, encompassing chemical kinetics, heat and mass transfer, turbulence–chemistry interactions, and radiation phenomena. Many of these aspects must be reformulated in comparison to those of conventional fossil fuels. The first step toward RSF deployment is thus a comprehensive understanding of their physical and chemical behaviour. Thermodynamic and physical-chemical properties are critical for combustion modelling, process safety, and regulatory compliance. To address these objectives, a scale-bridging approach is essential. Industrial combustion systems are multiphysical and highly complex, making detailed diagnostics under operational conditions extremely challenging. Therefore, the problem must be scaled down—from full-scale industrial systems to simplified, single-facet processes that can be studied with reduced uncertainty under controlled conditions. Model reactors provide controlled environments for characterizing oxidation/pyrolysis chemistry. Similarly, laboratory-scale burners enable investigation of turbulence–chemistry interactions and radiative effects using advanced optical and chemical diagnostics. The development of resilient sensing and sensor-fusion technologies, capable of operating under harsh industrial conditions, is then fundamental to extending the “scale-bridging approach” to real combustion systems.

The “scale-bridging approach” must be reapplied and adapted to RSFs due to their distinct chemical and physical properties. Furthermore, RSFs adoption may necessitate novel combustion concepts — including MILD, oxyfuel, catalytic, or plasma-assisted combustion — each defining new systems operational regimes with respect to conventional combustion modes, thus defining new combustion domains to exploit.

In this context, the integration of digital twins, Artificial Intelligence (AI), and Machine Learning (ML) offers promising opportunities to expedite the research and implementation of RSFs. These methods are also capable of processing and post-processing vast numerical datasets derived from CFD simulations. Consequently, the ability of AI and ML techniques to efficiently manage large numerical and experimental datasets provides a synergistic and highly effective pathway toward the rapid advancement of RSF-based combustion systems.

## Acknowledgments

This deliverable is based upon work from COST Action CA22151 – CYPHER, supported by COST (European Cooperation in Science and Technology). COST is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation. For more information, visit [www.cost.eu](http://www.cost.eu).

## References

- [1] Niculescu R, Clenci A, Shirmeshan A, Năstase M. A review of the synthetic transport fuels as a solution for carbon neutrality. *Next Energy* 2025;8:100355. <https://doi.org/10.1016/j.nxener.2025.100355>.
- [2] Cavaliere A, de Joannon M. Mild Combustion. *Prog Energy Combust Sci* 2004;30:329–66. <https://doi.org/10.1016/j.pecs.2004.02.003>.
- [3] Sabia P, Mounaïm-Rousselle C, Józsa V, de Joannon M, Battin-Leclerc F, Sorrentino G. Renewable synthetic fuels: challenges, opportunities, and the need for data (submitted manuscript, part of Roadmap for decarbonizing hard-to-abate industries: the role of renewable synthetic fuels, cyber-physical systems, and digital twins). *J Phys Energy* 2025.
- [4] Hasche A, Krause H, Eckart S. Hydrogen admixture effects on natural gas-oxygen burner for glass-melting: Flame imaging, temperature profiles, exhaust gas analysis, and false air impact. *Fuel* 2025;387:134397. <https://doi.org/10.1016/j.fuel.2025.134397>.
- [5] Martín AJ, Shinagawa T, Pérez-Ramírez J. Electrocatalytic Reduction of Nitrogen: From Haber-Bosch to Ammonia Artificial Leaf. *Chem* 2019;5:263–83. <https://doi.org/10.1016/j.chempr.2018.10.010>.
- [6] Su-ungkavatin P, Tiruta-Barna L, Hamelin L. Biofuels, electrofuels, electric or hydrogen?: A review of current and emerging sustainable aviation systems. *Prog Energy Combust Sci* 2023;96:101073. <https://doi.org/10.1016/j.pecs.2023.101073>.
- [7] Glassman I, Yetter R. Combustion. 4th ed. Burlington: Academic Press; 2008.
- [8] Sepman A, Malhotra JS, Wennebro J, Wiinikka H. Iron as recyclable electrofuel: Effect on particle morphology from multiple combustion-regeneration cycles. *Combust Flame* 2024;259:113137. <https://doi.org/10.1016/j.combustflame.2023.113137>.
- [9] German Aerospace Center (DLR). Sulphurreal: Pioneering Technology: Long-Term Solar Energy Storage in Solid Sulphur. 2025 n.d.
- [10] Burke MP, Klippenstein SJ. Ephemeral collision complexes mediate chemically termolecular transformations that affect system chemistry. *Nat Chem* 2017;9:1078–82. <https://doi.org/10.1038/NCHEM.2842>.
- [11] Burke MP, Song R. Evaluating Mixture Rules for Multi-Component Pressure Dependence:  $H + O_2 (+M) = HO_2 (+M)$ . *Proc Combust Inst* 2017;36:245–53. <https://doi.org/10.1016/j.proci.2016.06.068>.
- [12] Sabia P, de Joannon M. On  $H_2$ – $O_2$  oxidation in several bath gases. *Int J Hydrogen Energy* 2020;45:8151–67. <https://doi.org/10.1016/j.ijhydene.2020.01.134>.
- [13] Berger L, Attili A, Pitsch H. Synergistic interactions of thermodiffusive instabilities and turbulence in lean hydrogen flames. *Combust Flame* 2022;244:112254. <https://doi.org/10.1016/j.combustflame.2022.112254>.
- [14] Gaucherand J, Laera D, Schulze-Netzer C, Poinot T. Intrinsic instabilities of hydrogen and hydrogen/ammonia premixed flames: Influence of equivalence ratio, fuel composition and pressure. *Combust Flame* 2023;256:112986. <https://doi.org/10.1016/j.combustflame.2023.112986>.
- [15] Manna MV, Sabia P, Sorrentino G, Viola T, Ragucci R, de Joannon M. New insight into  $NH_3$ – $H_2$  mutual inhibiting effects and dynamic regimes at low-intermediate temperatures. *Combust Flame* 2022;243:111957. <https://doi.org/10.1016/j.combustflame.2021.111957>.
- [16] Alzueta MU, Ara L, Mercader VD, Delogu M, Bilbao R. Interaction of  $NH_3$  and  $NO$  under combustion conditions. Experimental flow reactor study and kinetic modeling simulation. *Combust Flame* 2022;235:111691. <https://doi.org/10.1016/j.combustflame.2021.111691>.
- [17] Alzueta MU, Abián M, Elvira I, Mercader VD, Sieso L. Unraveling the  $NO$  reduction mechanisms occurring during the combustion of  $NH_3/CH_4$  mixtures. *Combust Flame* 2023;257:112531. <https://doi.org/10.1016/j.combustflame.2022.112531>.
- [18] Tang Y, Lu HH, Sun J, Fu Z, Tao Z, Yang L, et al. Theoretical kinetics study of key reactions



- between ammonia and fuel molecules, part II: H-atom abstraction from alcohols and ethers by  $\dot{\text{N}}\text{H}_2$  radicals. *Combust Flame* 2025;271:113682. <https://doi.org/10.1016/j.combustflame.2024.113682>.
- [19] Giri BR, Shrestha KP, Mai TVT, Giri S, Adil M, Naik RT, et al. A Theoretical Study of  $\text{NH}_2$  Radical Reactions with Propane and Its Kinetic Implications in  $\text{NH}_3$ -Propane Blends' Oxidation. *Energies* 2023;16:5943. <https://doi.org/10.3390/en16165943>.
- [20] Chiaramonti D. Sustainable aviation fuels: The challenge of decarbonization. *Energy Procedia* 2019;158:1202–7. <https://doi.org/10.1016/j.egypro.2019.01.308>.
- [21] Chireshe F, Petersen AM, Ravinath A, Mnyakeni L, Ellis G, Viljoen H, et al. Cost-effective sustainable aviation fuel: Insights from a techno-economic and logistics analysis. *Renew Sustain Energy Rev* 2025;210:115157. <https://doi.org/10.1016/j.rser.2024.115157>.
- [22] Parker RP, Kelly M, Watson-Murphy T, Ghaani MR, Dooley S. Predictive Modeling of Liquid Density and Surface Tension for Sustainable Aviation Fuels Using Nuclear Magnetic Resonance Atom Types. *Energy and Fuels* 2025;39:3690–702. <https://doi.org/10.1021/acs.energyfuels.4c05601>.
- [23] Holzer A, Günthner M, Jung P. Performance of pure OME and various HVO–OME fuel blends as alternative fuels for a diesel engine. *Automot Engine Technol* 2022;7:369–83. <https://doi.org/10.1007/s41104-022-00122-8>.
- [24] Rieth M, Gruber A, Chen JH. The effect of pressure on lean premixed hydrogen-air flames. *Combust Flame* 2023;250:112514. <https://doi.org/10.1016/j.combustflame.2022.112514>.
- [25] Luca S, Attili A, Lo Schiavo E, Creta F, Bisetti F. On the statistics of flame stretch in turbulent premixed jet flames in the thin reaction zone regime at varying Reynolds number. *Proc Combust Inst* 2019;37:2451–9. <https://doi.org/10.1016/j.proci.2018.06.194>.
- [26] Böttler H, Kaddar D, Karpowski TJP, Ferraro F, Scholtissek A, Nicolai H, et al. Can flamelet manifolds capture the interactions of thermo-diffusive instabilities and turbulence in lean hydrogen flames?—An a-priori analysis. *Int J Hydrogen Energy* 2024;56:1397–407. <https://doi.org/10.1016/j.ijhydene.2023.12.193>.
- [27] Rieth M, Gruber A, Hawkes ER, Chen JH. Direct numerical simulation of low-emission ammonia rich-quench-lean combustion. *Proc Combust Inst* 2024;40:105558. <https://doi.org/10.1016/j.proci.2024.105558>.
- [28] Nguyen TH, Kim S, Park J, Jung S, Kim S. CFD-CRN validation study for  $\text{NO}_x$  emission prediction in lean premixed gas turbine combustor. *J Mech Sci Technol* 2017;31:4933–42. <https://doi.org/10.1007/s12206-017-0942-2>.
- [29] Trespi S, Nicolai H, Debiagi P, Janicka J, Dreizler A, Hasse C, et al. Development and application of an efficient chemical reactor network model for oxy-fuel combustion. *Energy and Fuels* 2021;35:7121–32. <https://doi.org/10.1021/acs.energyfuels.0c03560>.
- [30] Borsó J, Papp M, Józsa V, Turányi T. Modelling of JP-8 distributed combustion using a HyChem mechanism under gas turbine conditions. *Results Eng* 2024;23. <https://doi.org/10.1016/j.rineng.2024.102596>.
- [31] Narvaez P, Lopez A, Karam JE, Restrepo A, Amell AA. Development and evaluation of machine learning models for premixed flame classification in different hydrogen-natural gas proportions using images and audio. *Results Eng* 2025;27:106003. <https://doi.org/10.1016/j.rineng.2025.106003>.
- [32] Roncancio R, El Gamal A, Gore JP. Turbulent flame image classification using Convolutional Neural Networks. *Energy AI* 2022;10:100193. <https://doi.org/10.1016/j.egyai.2022.100193>.
- [33] Gharib M, Vogelbacher M, Matthes J, Gräbner M, Richter A. Comparative analysis of image segmentation methods on various flame types and their influence on flame stability assessment. *Therm Sci Eng Prog* 2025:104175. <https://doi.org/10.1016/j.tsep.2025.104175>.
- [34] Kardos R, Tóthpálné Hidegh G, Rác E, Józsa V. Assessment and ranking of 16 binarization methods for turbulent swirl flame images of various flame types 2025. <https://doi.org/10.2139/ssrn.5460714>.

- [35] Anderson LG. Effects of using renewable fuels on vehicle emissions. *Renew Sustain Energy Rev* 2015;47:162–72. <https://doi.org/10.1016/j.rser.2015.03.011>.
- [36] Beiron J, Harvey S, Thunman H. Locked in on RFNBOs – Will EU mandates for drop-in synthetic aviation fuels lead to decreased energy- and cost-efficiency? *Submitt Publ* 2025;406:137181. <https://doi.org/10.1016/j.fuel.2025.137181>.
- [37] Barreiro P, Alava I, Blanco JM. Design and scale-up of a hydrogen oxy-fuel burner for high-temperature industrial processes. *Fuel* 2026;405:136566. <https://doi.org/10.1016/j.fuel.2025.136566>.
- [38] Dang W, Chen S, He B, Song J, Duan Z, Duan H, et al. Decarbonization and clean production in China's cement industry: Strategies from the LEAP-LCA perspective. *Environ Impact Assess Rev* 2026;116:108124. <https://doi.org/10.1016/j.eiar.2025.108124>.
- [39] Caiafa C, Kratena K, Arto I. Macroeconomic and environmental impacts of two decarbonization options for the Dutch steel industry: green relocation versus green hydrogen imports. *Energy Policy* 2025;206:114726. <https://doi.org/10.1016/j.enpol.2025.114726>.
- [40] Wang Y, Yan Y, Liu H, Luo X, Wu T, Zheng C, et al. An integrated assessment model for cost-effective long-term decarbonization pathways in China's iron and steel industry. *Renew Sustain Energy Rev* 2025;216:115639. <https://doi.org/10.1016/j.rser.2025.115639>.