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

Deliverable D6

Guidelines for the implementation of renewable synthetic fuels in combustion experiments and data collection

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1. Introduction

To mitigate anthropogenic carbon dioxide emissions, renewable synthetic fuels (RSFs) are critical for energy-intensive industries and long-range transportation. Both hydrocarbon RSFs, combined with carbon capture solutions, and carbon-free RSFs, such as hydrogen and ammonia, represent essential pathways toward a carbon-neutral energy system. Hydrogen can be produced from purified water, while ammonia can be synthesised from nitrogen extracted from air. The main advantage of ammonia lies in its existing logistics infrastructure, while hydrogen requires significant advances in storage and distribution technologies. However, the presence of nitrogen in ammonia poses a considerable challenge to minimise NOx emissions [1]. In parallel, several hydrocarbon RSFs such as methanol, ethanol, dimethyl ether (DME), diethyl ether (DEE), dimethoxymethane (DMM), and oxymethylene ether (OME) also offer strong potential for decarbonisation [2], [3]. Modelling the combustion of these fuels requires detailed chemical mechanisms that accurately describe their behaviour across a wide range of operating conditions, including boilers, reciprocating engines, and gas turbines.

Understanding and optimising RSF combustion behaviour requires the integration of high-fidelity simulations [4][5][6][7][8][9][10][11][12][13][14][15][16][17], advanced diagnostics [18][19][20],[21],[22],[23], and systematic data collection. These approaches enable the characterisation of fundamental processes such as flame structure, ignition, turbulence–chemistry interaction, and pollutant formation, and they provide the foundation for predictive modelling and digital-twin development. Despite significant progress in numerical and experimental capabilities, several challenges persist. The computational cost of incorporating detailed chemical mechanisms remains high, particularly for complex RSFs, and the inclusion of multiphase effects, radiation, and pollutant formation adds further complexity. On the experimental side, diagnostic techniques originally developed for hydrocarbon fuels must be adapted for carbon-free or nitrogen-containing fuels, while quantitative measurements at high pressure remain limited.

Bridging the gap between laboratory-scale research and industrial applications requires coordinated efforts in data generation, management, and sharing. Aligning experimental and numerical studies under comparable conditions, and ensuring that non-dimensional parameters such as the Reynolds, Karlovitz, and Damköhler numbers are representative of real systems, are crucial for developing reliable predictive models. This deliverable provides guidelines for the implementation of RSFs in combustion experiments and data collection, offering a framework for reproducible, interoperable, and scalable research across the COST network.

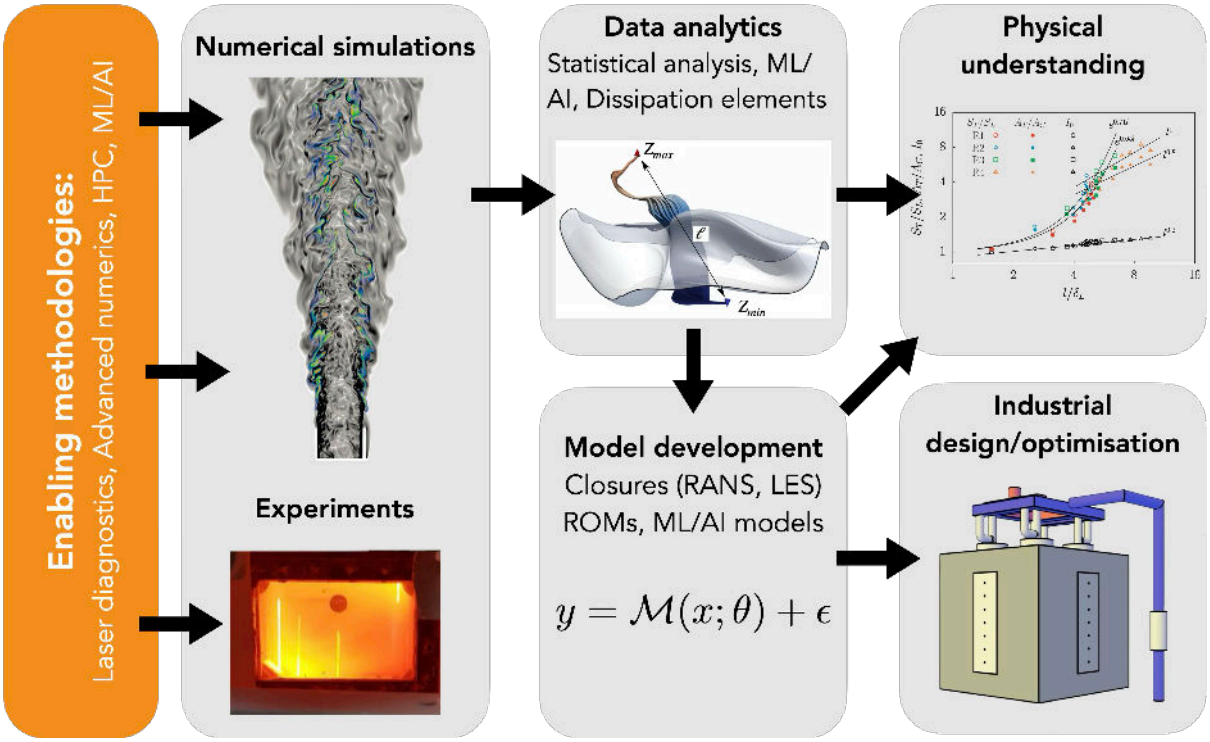

Figure 1 - The integration of high-fidelity simulations, advanced experimental diagnostics, and novel AI-driven data analytics enables a transformative approach to the digital design and optimization of sustainable, clean technologies.

2. Systematic data collection

2.1. Reaction kinetics data

The most versatile chemistry database is the National Institute of Standards and Technology (NIST) Webbook (https://webbook.nist.gov), which is also useful for combustion. Data sets used to develop reaction mechanisms include ignition delay times (IDT) measured in shock tubes (ST) and rapid compression machines (RCM), laminar burning velocities (LBV), and concentration measurements in jet-stirred reactors (JSR), flow reactors (FR), and ST. Since the apparatus for these measurements is similar across laboratories worldwide, reproducibility has been excellent for data over the past few decades. Due to the sufficiently large amount of similar data sets for commonly investigated species, it is possible to locate and highlight problematic measurements [24].

Reaction kinetics data points can be efficiently stored in an .xml file format, and occupy relatively low space. The entire Reaction kinetics, Spectroscopy, and Thermochemistry (ReSpecTh https://respecth.elte.hu/) database is less than one GB and contains more than 160,000 individual data points from more than 5400 data series. A further highlighted resource for reaction mechanisms is the SciExpeM (https://sciexpem.polimi.it) database. An automated reaction mechanism generator has been developed at MIT (https://rmg.mit.edu) to principally help CFD calculations.

2.2 Experimental combustion data sets

Reliable experimental data are essential for developing, validating, and improving combustion models for renewable synthetic fuels (RSFs). Among the most valuable community resources are the Turbulent Non-Premixed Flame (TNF) Workshop datasets (https://tnfworkshop.org), which have established a benchmark for reproducible, high-fidelity measurements in turbulent reacting flows. The TNF database contains systematically acquired and quality-assured data for canonical flame configurations, such as piloted jet flames of methane, hydrogen, and syngas mixtures, covering a wide range of Reynolds numbers, equivalence ratios, and boundary conditions.

These datasets provide detailed measurements of velocity, mixture fraction, temperature, and major and minor species, often obtained through simultaneous application of advanced optical diagnostics such as Raman and Rayleigh scattering and laser-induced fluorescence (LIF). The availability of consistent experimental conditions and well-documented uncertainty quantification makes the TNF data uniquely suited for model validation, comparison of numerical simulations, and machine-learning-based model development.

For renewable and carbon-free fuels, ongoing efforts are extending the TNF database to include ammonia, hydrogen, and e-fuel flames, addressing their distinct combustion characteristics such as strong thermodiffusive effects and low-temperature reactivity. Similar initiatives, including the International Sooting Flame (ISF) Workshop (isfworkshop/data-sets) and the Sydney and Darmstadt flame datasets, complement the TNF effort by providing data for alternative fuels, flame–wall interactions, and pollutant formation.

The systematic organisation of these experimental datasets, their open accessibility, and their alignment with numerical benchmarks are fundamental to accelerating the development of predictive models for RSF combustion.

2.3 Numerical combustion data sets

High-fidelity simulations such as Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) are increasingly used to generate benchmark datasets for model validation and data-driven modelling. DNS provides detailed information on turbulence–chemistry interactions, flame instabilities, and ignition behaviour in canonical configurations with reduced mechanisms, while LES enables the exploration of more complex, engine-relevant conditions.

The growing availability of open-access numerical datasets (e.g. BLASTNet [25]) facilitates cross-validation and model development. Data from DNS and LES are now systematically post-processed to include not only flow and scalar fields, but also

chemical reaction rates, curvature, and conditional statistics, all stored in standardized, machine-readable formats. Integrating these with experimental databases enables hybrid workflows for AI-assisted model training and uncertainty quantification.

3. Advancements in reaction kinetic modelling for NH_3 and NH_3/H_2 flames

Numerous mechanisms have been proposed in the literature to model the oxidation of NH_3/H_2 mixtures [26], [27]. Two large-scale quantitative mechanism comparison works have been carried out in the last two years for NH_3 and NH_3/H_2 combustion: one by Girhe et al. [28] (RWTH Aachen) in 2024, using 3,997 data points, and the other by Szanthoffer et al. [29] (ELTE Budapest) in 2025, using 17,242 data points from 110 papers. The two studies applied different methodologies to assess the performance of the investigated models. Girhe et al. [28] used the curve matching (CM) approach [30] proposed by the CRECK Modelling Group at POLIMI. The CM approach evaluates the similarity between the smoothly interpolated experimental and prediction curves, as well as their first derivatives, based on their deviation and correlation. In contrast, Szanthoffer et al. [29] utilised a root-mean-square error function to evaluate the pointwise agreement between the simulated and measured results, normalised by the uncertainties of the experimental data. This methodology was initially proposed and applied by Turányi et al. [31] (ELTE Budapest). [29] compared 33 mechanisms and concluded that the NUIG-2024 [32] was the best mechanism, followed by the Tsinghua-2024 model [33]. It is clear from these studies [28], [29] that even the best available NH_3 mechanisms are not satisfactorily accurate under all experimental conditions. Therefore, further mechanism development is necessary for NH_3 and NH_3/H_2 fuel mixtures.

In a joint research effort involving groups from the HUN-REN Research Centre for Natural Sciences (RCNS), ELTE Budapest, Cardiff University, and Poznan University, a small-scale, optimised NH_3 combustion mechanism was developed for the oxidation of NH_3/H_2 mixtures [34]. The research was primarily carried out at the HUN-REN RCNS. The initial mechanism of the optimisation was the San Diego mechanism [35], which had medium performance in the mechanism comparison work of Szanthoffer et al. [26]. The peculiarity of this mechanism is that it contains only 21 species and 64 reactions, which is very small relative to a typical detailed NH_3 mechanism (30–40 species and 250–300 reactions). The work aimed to develop a compact, yet robust model for Computational Fluid Dynamics (CFD) simulations.

Recently, Szanthoffer et al. [36] proposed a generally applicable, systematic approach for the development of more accurate combustion mechanisms, which does not require the optimisation of a mechanism. Testing detailed combustion mechanisms typically concludes that some mechanisms reproduce the experimental data well at most conditions but are inaccurate at other conditions. However, other mechanisms

may perform well under these conditions [28], [29]. The idea was that a better mechanism ("mosaic mechanism") may be obtained by identifying the overall best-performing mechanism and adding the most important reaction steps and their rate parameters from another mechanism with good performance at the conditions where the overall best model is ill-performing. A new algorithm based on this approach was presented in this work, which was successfully applied using a comprehensive collection of NH_3/air LBV data (348 data points in 61 data series) and eight recent detailed NH_3 combustion mechanisms. The proposed algorithm can be applied to any chemical kinetics system and any other types of experiments. All data needed to apply the algorithm to various combustion systems are already available or can be generated with minimal human effort using the experimental data files, mechanisms, and codes available on the ReSpecTh (https://ReSpecTh.elte.hu) website.

4. Advancements in numerical modelling and data sharing

Recent advances in high-performance computing and data science have greatly enhanced the capability to model the combustion of renewable synthetic fuels (RSFs). High-fidelity simulations, including Direct Numerical Simulation (DNS) [4][5][6][7][8][9][10][11][12][13][14] and Large Eddy Simulation (LES) [15][16][17] , are increasingly used to generate detailed datasets that resolve the fundamental interactions between turbulence and chemistry. Within the framework of this COST Action, several new DNS studies have been conducted, including high-pressure simulations of hydrogen flames and investigations of turbulent combustion dynamics under conditions representative of energy-intensive industrial systems. These simulations provide valuable reference data for the validation and calibration of reduced-order and machine-learning-assisted models.

A key objective of the Action has been to promote open and reproducible research through data sharing and collaborative platforms. Several high-fidelity datasets have been collected and shared within the network, such as DNS of sooting flames available through the ERCOFTAC repository at: https://www.ercoftac.org/events/machine-learning-for-fluid-dynamics/workshop-test-cases/. These datasets include detailed information on velocity, temperature, species concentration, and soot statistics, and have been widely used by the community for model validation, uncertainty quantification, and data-driven model development.

To further encourage the use of data and foster collaboration across disciplines, the Action has organised open data challenges, such as the CYPHER Data Challenge hosted at: https://cypher.ulb.be/data-challenge/. These initiatives provide an ideal framework to engage both experimental and modelling groups, stimulate the adoption of data-driven and AI-based methods, and demonstrate the potential of shared datasets to accelerate innovation in combustion science.

Together, these efforts contribute to establishing a culture of open, FAIR-compliant data practices within the European combustion community. By linking new high-fidelity simulations, shared databases, and community-driven challenges, the COST Action is promoting a more collaborative, data-driven approach to modeling and optimizing renewable synthetic fuel combustion systems.

5. Systematic experiments and advanced sensing

Systematic and high-quality experiments are crucial for generating the data necessary to validate and improve combustion models for renewable synthetic fuels (RSFs). The reproducibility and accuracy of these experiments depend on the use of well-characterised facilities, advanced diagnostics, and standardised data acquisition protocols.

Recent progress in advanced laser-based diagnostics has significantly enhanced the capability to characterise reactive flows. Techniques such as planar laser-induced fluorescence (PLIF), Raman and Rayleigh scattering, coherent anti-Stokes Raman spectroscopy (CARS), and chemiluminescence imaging enable spatially and temporally resolved measurements of temperature, major and minor species, and intermediate radicals, including OH, CH, and NH. These diagnostics have been extended to high-pressure and high-temperature environments relevant to industrial combustion, providing detailed insights into flame stability, pollutant formation, and thermodiffusive instabilities.

The Action also promotes the integration of multi-sensor and AI-assisted sensing strategies. Convolutional Neural Networks (CNNs) and other machine-learning techniques are increasingly applied to process high-speed imaging or spectroscopic signals for automated flame classification, anomaly detection, and control.

The alignment of experimental and simulation efforts within the COST network strengthens the development of predictive, data-driven models and supports the transition toward digital-twin-enabled RSF combustion systems.

6. Conclusion

The implementation of renewable synthetic fuels (RSFs) in combustion experiments and data collection is a crucial step toward the decarbonisation of energy-intensive industries. The COST Action has fostered significant progress in this direction by promoting a systematic, data-driven approach that integrates high-fidelity simulations, advanced diagnostics, and open data sharing. Reliable experimental datasets, such as those from the Turbulent Non-Premixed Flame (TNF) Workshop, combined with new numerical data from Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES), provide a strong foundation for model validation and mechanism development for hydrogen, ammonia, and e-fuel combustion.

Through the coordinated efforts of its members, the Action has produced and shared new benchmark DNS datasets, including high-pressure hydrogen flames and sooting turbulent flames, and has encouraged the community to use and expand these resources via open initiatives such as the ERCOFTAC test cases and the CYPHER Data Challenge. These activities have strengthened collaboration across Europe, enhanced reproducibility, and accelerated the adoption of data-centric and AI-assisted research methods in the field of combustion science.

Looking ahead, the continued integration of experiments, simulations, and data analytics will be essential to developing predictive tools and digital twins for RSF combustion systems. Establishing common standards for data storage, metadata, and uncertainty quantification will ensure that future research remains interoperable and transparent. The outcomes of this Action lay the groundwork for a new, collaborative paradigm in combustion research, enabling Europe to move closer to a sustainable and carbon-neutral energy future.

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