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A roadmap for decarbonizing energy-intensive industries with renewable synthetic fuels and digital technologies

Alessandro Parente^{1,2,3,31,*} , Giancarlo Sorrentino^{4,31} , Pino Sabia⁴ , Christine Mounaïm-Rousselle⁵ , Viktor Józsa⁶ , Mara de Joannon⁴ , Frédérique Battin-Leclerc⁷ , Antonio Attili⁸ , Federica Ferraro⁹ , Pasquale Eduardo Lapenna¹⁰ , Daniel Mira¹¹ , Alberto Cuoci¹² , Gaetano Magnotti¹³ , Nguyen Anh Khoa Doan^{14,15} , Katarzyna Bizon¹⁶ , Paola Cinnella¹⁷ , Miguel Alfonso Mendez^{18,1,19} , Luc Vervisch²⁰ , Eduard Petlenkov²¹ , Abiodun Emmanuel Onile²² , Peter Gorm Larsen²³ , Raffaele Ragucci⁴ , Anes Kazagic²⁴ , Alessandro Della Rocca²⁵ , Jörg Leicher²⁶ , Ingrid El Helou²⁷ , Thiago Lima Silva²⁸ , George Skevis²⁹ and Chiara Caccamo³⁰

¹ Aero-Thermo-Mechanics Laboratory, École Polytechnique de Bruxelles, Université Libre de Bruxelles, Brussels, Belgium

² Brussels Institute for Thermal Energy (BRITE), Brussels, Belgium

³ WEL Research Institute, Wavre, Belgium

⁴ Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS-CNR), Naples, Italy

⁵ University Orléans, INSA-CVL, EA 4229—PRISME, F-45072 Orléans, France

⁶ Department of Energy Engineering, Faculty of Mechanical Engineering, Budapest University of Technology and Economics, Műegyetem rkp. 3, H-1111 Budapest, Hungary

⁷ Université de Lorraine, CNRS, LRGP, Nancy F-54000, France

⁸ School of Engineering, Institute for Multiscale Thermofluids, The University of Edinburgh, EH9 3FD Edinburgh, United Kingdom

⁹ Institute of Jet Propulsion and Turbomachinery, Technische Universität Braunschweig, Braunschweig, Germany

¹⁰ Department of Mechanical and Aerospace Engineering, Sapienza University of Rome, Rome, Italy

¹¹ Barcelona Supercomputing Center (BSC), Barcelona, Spain

¹² Institute CRECK Modeling Lab, Department of Chemistry, Materials, and Chemical Engineering, Politecnico di Milano, Milan, Italy

¹³ INSA Rouen-Normandie, CNRS UMR6614-CORIA, Saint-Etienne du Rouvray 76801, France

¹⁴ Department of Aeronautics, Imperial College London, London, United Kingdom

¹⁵ Faculty of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands

¹⁶ Faculty of Chemical Engineering and Technology, Cracow University of Technology, Krakow, Poland

¹⁷ Institut Jean Le Rond D'Alembert, Sorbonne University, Paris, France

¹⁸ von Karman Institute for Fluid Mechanics, Sint-Genesius-Rode, Belgium

¹⁹ Aerospace Engineering Department, Universidad Carlos III de Madrid, Madrid, Spain

²⁰ CORIA-CNRS, INSA Rouen Normandie, Saint-Etienne-du-Rouvray 76800, France

²¹ Centre for Intelligent Systems, Department of Computer Systems, Tallinn University of Technology, Akadeemia tee 15A, Tallinn 12618, Estonia

²² Department of Software Science, Tallinn University of Technology, Akadeemia tee 15A, Tallinn 12618, Estonia

²³ Electrical and Computer Engineering Department, Aarhus University, Denmark

²⁴ JP Elektroprivreda Bosne i Hercegovine d.d., Sarajevo, Bosnia and Herzegovina

²⁵ Tenova S.p.A., Genoa, Italy

²⁶ Gas- und Wärme-Institut Essen e.V., Essen, Germany

²⁷ Marble I, 75011 Paris 11, France

²⁸ SINTEF Industry, 7031 Trondheim, Norway

²⁹ CLEOS, 175 64 P. Faliro, Athens, Greece

³⁰ SINTEF Energy Research, 7031 Trondheim, Norway

³¹ Guest Editors of the Roadmap.

* Author to whom any correspondence should be addressed.

E-mail: Alessandro.Parente@ulb.be, giancarlo.sorrentino@stems.cnr.it, pino.sabia@stems.cnr.it, christine.rousselle@univ-orleans.fr, jozsas@energia.bme.hu, maras.dejoannon@stems.cnr.it, frederique.battin-leclerc@univ-lorraine.fr, antonio.attili@ed.ac.uk, federica.ferraro@tu-braunschweig.de, pasquale.lapenna@uniroma1.it, daniel.mira@bsc.es, alberto.cuoci@polimi.it, gaetano.magnotti@coria.fra, n.doan@imperial.ac.uk, katarzyna.bizon@pk.edu.pl, paola.cinnella@sorbonne-universite.fr, miguel.alfonso.mendez@vki.ac.be, luc.vervisch@insa-rouen.fr, eduard.petlenkov@taltech.ee, pgl@ece.au.dk, raffaele.ragucci@cnr.it, a.kazagic@epbih.ba, alessandro.dellarocca@tenova.com, joerg.leicher@gwi-essen.de, ingrid@marble.studio, thiago.silva@sintef.no, gskevis@cleos.gr and chiara.caccamo@sintef.no

Keywords: digital twins, renewable synthetic fuels, energy-intensive industries, hard-to-abate sectors, combustion, data-driven science, machine learning

Abstract

Decarbonizing energy-intensive and other hard-to-abate sectors remains essential for meeting climate targets, yet these sectors continue to depend on fuels for high-temperature heat, chemical feedstocks, and energy-dense transport applications. This roadmap assesses the potential role of renewable synthetic fuels (RSFs) in supporting this transition, with a primary focus on the European context and on sectors including steel, cement, glass, aviation, shipping, and power generation. It reviews the current status of RSF combustion science, the high-fidelity experimental and numerical data needed to understand fuel behavior under relevant conditions, and the emerging hybrid physics-based and data-driven modeling approaches that can accelerate progress. Particular attention is given to digital twins and related cyber-physical tools as enabling technologies for process optimization, monitoring, scale-bridging, and industrial implementation. The roadmap also examines practical deployment barriers, including fuel availability, infrastructure, safety, regulatory and policy barriers, and data integration challenges. Developed in the framework of the CYPHER COST Action (CA22151), it highlights that large-scale RSF deployment will require coordinated action across research, industry, and policy, together with stronger business cases, policies that stimulate demand, and workforce development.

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1. Introduction

Alessandro Parente^{1,2,3} and Giancarlo Sorrentino⁴

¹ Aero-Thermo-Mechanics Laboratory, École Polytechnique de Bruxelles, Université Libre de Bruxelles, Brussels, Belgium

² Brussels Institute for Thermal Energy (BRITE), Brussels, Belgium

³ WEL Research Institute, Wavre, Belgium

⁴ Institute of Science and Technologies for Sustainable Energy and Mobility, STEMS-CNR, Italy

E-mail: Alessandro.Parente@ulb.be and giancarlo.sorrentino@stems.cnr.it

Achieving global climate goals requires deep decarbonization across all sectors of the economy [1], including limiting global warming to well below 2 °C above pre-industrial levels, as outlined in the Paris Agreement, and reaching net-zero emissions by mid-century. Among the most difficult sectors to decarbonize are energy-intensive industries (EIIs), for which the transition is particularly challenging because many current and emerging technologies are either not yet available or not cost-effective enough to provide the high-density, localized energy sources currently supplied by fuels [2].

EIIs are vital to the economy, as emphasized in the European Green Deal, because they underpin several key value chains in Europe. Sectors such as steel, cement, and chemicals supply materials essential to modern infrastructure, manufacturing, and a wide range of consumer goods, while heavy transport remains crucial for trade and mobility. Their decarbonization and modernization are therefore a major priority [3]. In this context, the present roadmap focuses primarily on Europe, where ambitious policy frameworks such as the European Green Deal and the Fit-for-55 package are shaping transition pathways for these industries.

EIIs, also known as ‘hard-to-abate’ sectors, pose unique challenges for decarbonization. They collectively account for a substantial portion of global greenhouse gas (GHG) emissions, often estimated at around 30% [2], and without tackling their emissions, overall climate targets are impossible to reach. These industries are of fundamental economic importance. Decarbonizing these sectors is difficult due to several technical challenges [4]. Many industrial processes, such as in cement kilns or steel furnaces, require extremely high temperatures that are currently generated most efficiently by burning fossil fuels. Some emissions are also inherent chemical byproducts of the production process itself, for example, the carbon dioxide released from limestone in cement production. This is distinct from emissions from energy use. Certain sectors also rely on fossil fuels not just for energy but also as raw materials or feedstocks, such as natural gas in ammonia production.

While solutions like green hydrogen and electrification with renewables are emerging [5], they are often not yet technologically mature, cost-competitive, or scalable enough to fully replace current methods. Finally, another major obstacle is the long investment cycles of industrial infrastructure. These facilities have long operational lifetimes spanning decades, so investment decisions made today can lock in emissions for a very long time [4]. Delaying action risks either relying on increasingly expensive retrofits later and outdated assets, with severe and irreversible impacts on climate change [6].

The use of renewable synthetic fuels (RSFs) offers a promising solution to reduce GHG emissions, particularly in hard-to-abate sectors such as industry, aviation, and shipping. These sectors are characterized by high energy demands and limited alternatives to fossil fuels, making decarbonization particularly challenging. In the context of this roadmap, RSFs are understood primarily as renewable fuels of non-biological origin, namely synthetic fuels produced using renewable electricity (e-fuels), including hydrogen and its derivatives such as e-ammonia, e-methanol, and e-methane. However, other renewable fuel pathways, including biofuels and waste-based fuels, are also considered where relevant, as they are addressed in the roadmap’s specific chapters.

The heavy industry sector, including steel, cement, glass, and chemical production, can benefit significantly from RSFs [4], as these industries rely heavily on high-temperature processes that are difficult to electrify. In such applications, biofuels and green hydrogen can provide low-carbon alternatives to traditional fossil fuels, helping reduce emissions without compromising operational efficiency. Aviation, a sector widely considered difficult to decarbonize [2], is increasingly focused on sustainable aviation fuels (SAFs) as a key solution. Produced from diverse feedstocks such as waste oils, agricultural residues, and captured carbon combined with green hydrogen, SAFs are expected to achieve 70% of the aviation sector’s emission reductions by 2050 [7]. SAFs offer environmental benefits, with lifecycle GHG reductions

ranging from 20% to 100% compared with conventional jet fuels, depending on the feedstock and production pathway [8]. Importantly, SAFs are categorized as ‘drop-in’ fuels, meaning they are fully compatible with existing aircraft and fueling infrastructure. However, despite these advantages, their current rate of development remains insufficient to meet decarbonization goals [9]. Similarly, the maritime industry is exploring biofuels, ammonia, and methanol derived from renewable sources to replace heavy fuel oil (HFO), thereby significantly reducing emissions [10].

To conclude, while many macroeconomic models highlight the importance of RSFs for decarbonizing hard-to-abate sectors [11], current technologies still pose significant limitations to their scalability. This underscores the potential of digital technologies as enablers of decarbonization. A complete understanding of the impact of RSFs on EII systems is still being developed, primarily due to a lack of comprehensive methods and specialized, multidisciplinary knowledge. The knowledge gap in understanding the impact and penetration of RSFs in EIIs can be addressed by integrating data-driven and physics-based modeling, enhanced by sensing and digital twins (DTs), while also considering techno-economic aspects, the need for collaborations with industry and other stakeholders, and the impact of policy and social acceptance. In this framework, the main aim of the CYPHER COST Action [12] is to propel collaborations between European researchers and industrial stakeholders to foster the use of cyber-physical systems (self-updating DTs) and ultimately promote a safe and sustainable adoption of RSFs as a critical path for EII decarbonization, in agreement with the ‘Sustainability by Design’ principles [13].

This roadmap provides a comprehensive overview of the current status, challenges, and future directions of RSF adoption in hard-to-abate industries. It is designed to be relevant to a broad audience, including researchers, policymakers, and industry leaders. Although grounded in the European context, the analysis highlights generalizable challenges and opportunities relevant to global decarbonization pathways.

The document is structured into six sections, each addressing a critical aspect of RSF implementation. It begins with a presentation of the scientific fundamentals of RSF combustion, followed by an exploration of how high-fidelity data from simulations and experiments can accelerate model development. The third section outlines the transformative potential of hybrid physics-based machine learning (ML) models and DTs as enablers for decarbonization. The fourth section provides a current landscape of industrial projects, detailing real-world applications and pilot programs across various sectors. The final sections address other critical factors: the techno-economic feasibility and social acceptance, including the need for supportive policy and workforce development. This roadmap, which also showcases the progress of the CYPHER COST Action and its members, aims to provide a clear path forward, emphasizing the urgent need for multidisciplinary collaboration to achieve a sustainable energy transition.

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2. Renewable synthetic fuels: challenges, opportunities, and the need for data

Pino Sabia¹, Christine Mounaïm-Rousselle², Viktor Józsa³, Mara de Joannon¹, Frédérique Battin-Leclerc⁴ and Giancarlo Sorrentino¹

¹ Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS-CNR), Naples, Italy

² University Orléans, INSA-CVL, EA 4229—PRISME, F-45072 Orléans, France

³ Department of Energy Engineering, Faculty of Mechanical Engineering, Budapest University of Technology and Economics, Műegyetem rkp. 3, H-1111 Budapest, Hungary

⁴ Université de Lorraine, CNRS, LRGP, Nancy F-54000, France

E-mail: pino.sabia@stems.cnr.it, christine.rousselle@univ-orleans.fr, jozs@energia.bme.hu, mara.dejoannon@stems.cnr.it, frederique.battin-leclerc@univ-lorraine.fr and giancarlo.sorrentino@stems.cnr.it

Status

RSFs are chemically synthesized fuels designed to mimic the chemical/physical properties of fossil fuels, with a high potential to lead the transition to a carbon-neutral energy production system [14, 15] and to guarantee energy security [16]. The breakthrough concept is to treat CO₂ (from direct air extraction or combustion flue gases) as a new source for converting into valuable fuels through reactions with H₂. A plethora of RSFs can be produced via thermochemical conversion processes, enabling chemical (long-term) energy storage, like traditional fuels. Because of these similarities, storage/transportation infrastructures are not an issue for gaseous/liquid RSFs, with some exceptions (H₂). RSFs can penetrate many EIIIs (aviation, shipping, heavy-duty trucks, steel, glass, cement, etc). Synthetic methane, methanol, or Fischer–Tropsch (FT) liquids can be used in boilers, furnaces, and kilns (cement, glass, etc), and syngas, hydrogen, ammonia, synthetic methane, or SAFs can be used in gas turbines (GTs). Heavy-duty truck sectors can benefit from FT liquids, such as methanol, ammonia, biodiesels (fatty-acid-alkyl esters), or hydrotreated vegetable oil derived from biomass thermochemical processes. Dehydration reactions can also convert methanol into alternative biodiesels (Dimethylether (DME), oxymethylene ethers (OMEs), etc) [15]. Also, biomass residues, such as Biochar and Torrefied Biomass, can replace coal in co-firing applications.

Depending on the RSFs' chemical/physical properties, marginal or extreme industrial process modifications are required through academic/industrial efforts to advance combustion science and technology (CS&T). Constraining the discussion to five RSFs, as representative candidates for EIIIs, table 1 shows that the chemical/physical properties of RSFs may differ significantly from those of conventional fuels: H₂ has the lowest boiling point and volumetric mass density, with the highest lower heating values (LHV) and laminar burning velocity (LBV). Ammonia, the second carbon-free RSF, also has combustion properties different from those of methane, methanol, and DME, with lower LHV and LBV. Methanol is the only liquid RSF under standard conditions, with LHV and LBV close to DME; Methanol and DME LHVs are lower than methane's due to the presence of an oxygen atom. RSF's combustion kinetics for simple molecules [17–20] have been investigated for a long time, and several detailed kinetic models are available (table 1). In contrast, for complex and newly developed fuels (bio-oils, OMEs, SAFs), dedicated experimental/numerical studies are mandatory.

Table 1 also reports the technology readiness level (TRL) of synthesis processes and their associated production costs. While green methane and H₂ have reached technical maturity (TRL 9), sustainable alternatives like ammonia, methanol, and DME electrochemical reduction synthesis remain at lower readiness levels (TRL 4) and lack cost competitiveness. According to the cost analysis, the future of RSFs hinges on cost reductions for green hydrogen and e-fuels. Market entry currently depends on financial leveling mechanisms such as the EU Emissions Trading System (EU ETS) (Directive 2003/87/EC), carbon border adjustment mechanism (CBAM) (Regulation EU 2023/956), or carbon contracts for difference (CCfDs). However, beyond policy incentives, two factors are critical for economic feasibility:

- Process Optimization: continuous industrial refinement to lower production costs.
- Multi-stakeholder networks: A synchronized ecosystem is essential to ensure a competitive return on investment (ROI). This requires aggregating demand from multiple buyers, securing surplus energy from various providers to cut costs, and establishing a certified, standardized feedstock supply chain.

Table 1. Example of RSFs relevant for EII, main synthesis technologies, cost of production per fuel/e-fuel, chemical/physical properties, and Examples of oxidation detailed kinetic mechanisms. SR: steam reforming; TRL: technology readiness level; HB: Haber–Bosch; EC: electro-chemical; LHV: low-heating value; LBV: laminar burning velocity.

Chemical properties	Methane	Hydrogen	Ammonia	Methanol	Dimethylether (DME)
Formula	CH ₄	H ₂	NH ₃	CH ₃ OH	CH ₃ OCH ₃
Main current synthesis way	Fossil fuel	Methane SR	H ₂ + N ₂ (catalytic HB)	Catalytic hydrogenation of CO + H ₂	Catalytic reaction of CH ₃ OH/CO + H ₂
Current production cost	0,4–0,6€/m ³	1,5–2,5€/Kg	400–600€/t	250–450€/t	450–650€/t—800–1200€/t
Alternative synthesis way	Catalytic CO ₂ Methanation	Water electrolysis	EC reaction of N ₂ + H ₂ O	EC CO ₂ Reduction	EC CO ₂ reduction
TRL level	TRL9	TRL9	TRL4	TRL5	TRL4
Alternative synthesis cost	1,20–2,50€/m ³	3,5–7€/kg	1200–2500€/t	1200–2500€/t	>2500€/t
Normal boiling point (°C)	−161	−253	−33	64	−25
Liquid density at normal boiling point (kg m ^{−3})	423	71	682	792	735
LHV (MJ kg ^{−1})	50	120	18.6	19.9	28.7
Max LBV @ 298 K and 1 atm (cm s ^{−1})	36 [18]	285 [18]	7 [18]	45 [18]	44 [18]
Detailed kinetic mechanism	Stagni <i>et al</i> [19]	Stagni <i>et al</i> [19]	Stagni <i>et al</i> [19]	Konnov <i>et al</i> [18]	Dong <i>et al</i> [20]

Without this integrated framework, RSFs cannot achieve successful ‘real market’ integration. In relation to these two points, DTs and artificial intelligence (AI) can act as the ‘technological glue’ needed to bridge the gap between low TRL and full market integration. DT and AI directly address process optimization, guaranteeing (dynamic) efficiency, predictive maintenance, and virtual prototyping. In turn, they could create a solid market through an efficient, transparent, and low-risk ecosystem.

Current and future challenges

EIIs need to transition to RSFs to reduce their carbon footprint [21]. Their integration poses substantial challenges in terms of engineering, combustion stability, efficiency, safety, and emissions control before large-scale industrial deployment. In addition, their availability remains marginal compared to global energy demand. Besides updating combustion systems for RSFs, it is also critical to advance existing combustion concepts and retrofit existing units; this latter opportunity has the highest potential to cut CO₂ emissions in the short- to medium-term. Advanced combustion systems must be retrofitted or redesigned to address several critical requirements:

- **Adaptive combustion performance:** Systems must accommodate the distinct properties of RSFs. Unlike conventional fossil fuels, RSFs often exhibit poor combustion characteristics, such as low laminar flame speed and high auto-ignition temperatures, which can compromise stability and overall process efficiency.
- **Enhanced fuel flexibility:** It is essential to ensure fuel flexibility to manage the significant variety and intermittent availability of RSFs effectively. Nowadays, blending conventional fuels is a key strategy for operating conventional combustion systems and partially reducing carbon footprints.
- **Optimization strategies:** Combustion properties can be enhanced by blending RSFs or modifying the environment. For example, ammonia’s performance is often improved through oxygen enrichment or blending with hydrogen (via ammonia cracking [22]) or other e-fuels (methanol, DME [23, 24], etc).
- **Management of complex phenomena:** Designs must account for new combustion behaviors, such as thermo-diffusive instabilities [25] in ammonia/hydrogen mixtures, which can trigger damaging thermo-acoustic oscillations.

- **Advanced emissions control:** Systems must mitigate new pollutant classes, including N₂O and nitrate particulates from ammonia combustion, as well as formaldehyde from methanol. Implementing strategies such as moderate or intense low-oxygen dilution (MILD) combustion [26] and advanced emissions control systems are required to minimize NO_x and particulate matter emissions [27]. In addition, these new classes of pollutants need new regulations.

The five highlighted fuels in table 1 offer promising low-carbon solutions, but further research is needed to address combustion stability, efficiency, and emissions. The design of RSF-based combustion systems necessitates the development of a robust CS&T framework that transitions from laboratory to pilot-scale facilities under controlled conditions to a real system. Given the problem complexity, DTs and AI will play a fundamental role.

A further aspect of the penetration of carbon-free RSFs into the real market concerns safety risk analysis and fuel toxicity. Hydrogen enhances combustion characteristics but introduces significant logistical constraints, whereas methanol, DME, and ammonia necessitate stringent handling protocols due to their inherent toxicity. Ammonia is by far the most toxic, even though it is the second-largest chemical produced worldwide, and it is handled with defined safety procedures in industrial synthesis plants. Its transfer to EII sectors imposes new safety rules and protocols, specialized personnel, and dedicated infrastructure for safe storage and delivery.

Advances in science and technology to meet challenges

Developing CS&T for RSFs necessitates high-fidelity data collection from model reactors under strictly controlled conditions, incorporating rigorous uncertainty quantification. This approach is fundamental to implementing detailed kinetic mechanisms and robust validation/optimization methods. Critical data, including auto-ignition delays, laminar flame speeds, and speciation profiles obtained through advanced optical and chemical diagnostics, are indispensable. While traditional model reactors serve as benchmarks, these tools must be re-engineered to address the distinct properties of emerging fuels.

Reference databases are WebBook of the National Institute of Standards and Technology (<https://webbook.nist.gov/chemistry/>), ReSpecTh (<http://respecth.elte.hu/>), and SciExpeM (<https://sciexpem.polimi.it>). They are continuously updated as soon as new experiments are available.

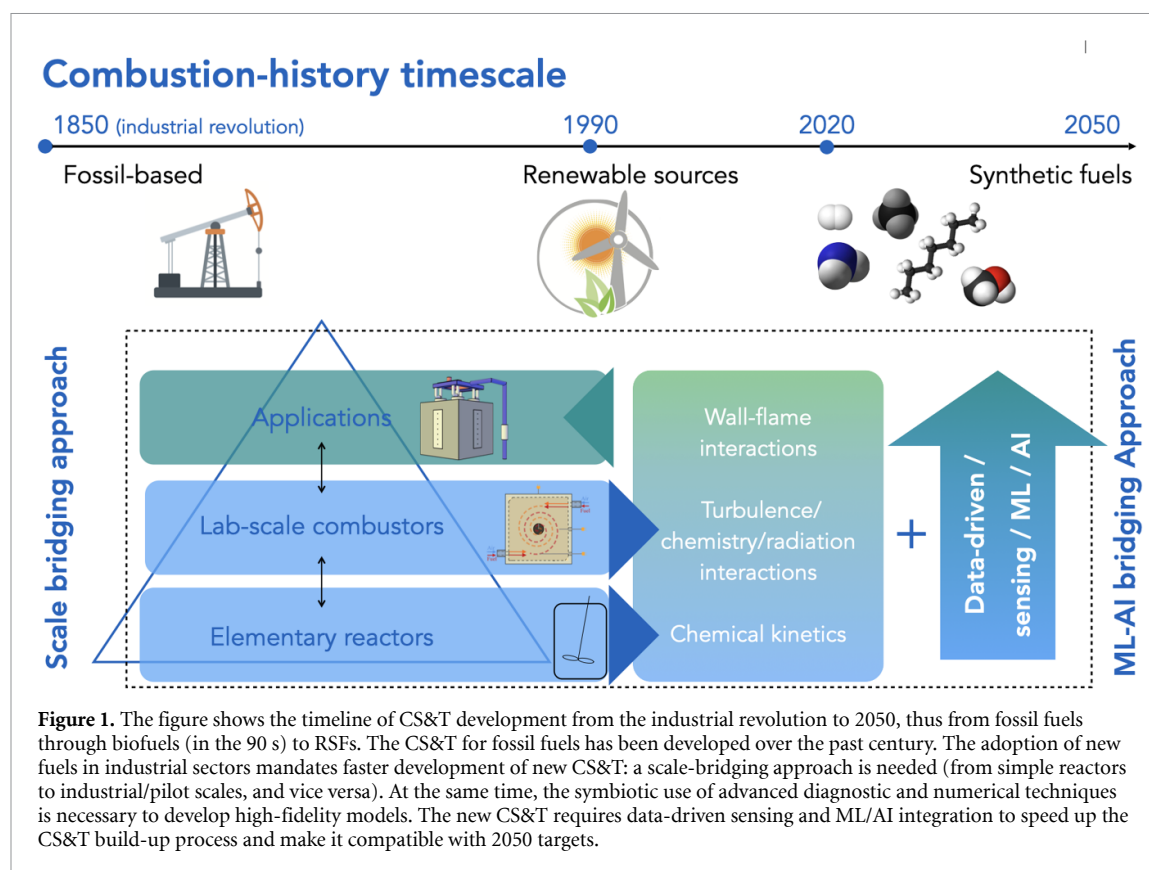
Specifically for liquid RSFs (bio-oils, SAF, etc), knowledge of their physical/chemical properties is necessary to capture physical processes (vaporization, atomization). This is a very challenging issue, as the composition of derived liquid fuels strongly depends on the original biomass and the thermochemical treatment processes. To address this challenge, several software tools have recently been proposed for the estimation of physical/chemical properties (ignition, distillation curves, etc) of molecules based on elemental analyses or rules derived from molecular structure analogies (www.molecularknowledge.com/Cranium/Cranium.html).

For very complex molecules or blends, automated detailed kinetic model generation tools (<https://rmg.mit.edu>) based on molecular structure similarities and/or ML/AI methods have been proposed.

Real systems cannot be categorized as benchmarks because of unique geometries and operating conditions (pressure, stoichiometry, temperature, premixed/non-premixed) in which chemical/physical phenomena (atomization, vaporization, oxidation) occur under turbulent conditions, necessitating the development of turbulence and turbulence-chemical kinetics models [28]. Also, radiative heat transfer phenomena/models for no-carbon fuels are substantially different from those of conventional fossil fuels.

Scale-bridging approaches (from lab- to pilot-scales) must be undertaken to accurately address all facets of real processes [29] (figure 1). Models must be extended to real conditions through further implementation: real combustors are closed, which warrants a better understanding of flame-wall interactions.

The need to monitor/collect a wider array of process variables/data demands more sophisticated sensing solutions: optical sensing in critical industrial applications is generally limited to tunable diode laser absorption spectroscopy [30] or photoacoustic sensors [31]. Laser-induced fluorescence (LIF) (info on selected species) or laser-induced breakdown spectroscopy (atomic composition) are more suited for laboratories. Advancements in micro-electromechanical systems, sensor miniaturization, and cost reduction (laser components, fiber optics) may enable real-time tracking of various properties relevant to the industry [32]. In this perspective, sensor fusion (e.g. coupled optical, chemical, or acoustic sensors or sensor systems) with edge computing may enable a more holistic understanding of combustion states.



Concluding remarks

RSFs are currently regarded as promising fuels for decarbonizing EILs. However, achieving large-scale industrial deployment without relying heavily on fossil fuels will require substantial academic and industrial research to develop robust, cost-effective green hydrogen production routes. This, in turn, depends on further progress in supplying decarbonized electricity from renewable and low-carbon sources, such as concentrated solar power, wind, and nuclear energy. Given the strong potential of RSFs to support the decarbonization of hard-to-abate sectors and the urgency created by EU regulations, their rapid development is essential. The prospect of using this broad and relatively novel class of fuels in hard-to-abate systems also requires, in many cases, a reassessment of combustion science and technology. The chemical and physical properties of RSFs can differ substantially from those of conventional fossil fuels, meaning that fundamental combustion processes, including physical sub-processes such as atomization and vaporization, as well as chemical sub-processes such as reaction kinetics and pollutant formation, may differ significantly.

In this context, high-fidelity models capable of capturing a wide range of coupled chemical and physical phenomena under conditions relevant to hard-to-abate sectors can play an important role in improving understanding of these differences. Such progress may be supported by established approaches, including the generation of high-fidelity data in laboratory- and pilot-scale systems and the use of advanced diagnostic techniques. At the same time, given the urgency of the challenge, faster progress may be achieved by developing and integrating ML and AI methods, DT approaches, and advances in sensor fusion.

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3. The role of high-fidelity data for developing combustion technologies for renewable synthetic fuels

Antonio Attili¹, Federica Ferraro², Pasquale Eduardo Lapenna³, Daniel Mira⁴, Alberto Cuoci⁵
and Gaetano Magnotti⁶

¹ School of Engineering, Institute for Multiscale Thermofluids, The University of Edinburgh, EH9 3FD Edinburgh, United Kingdom

² Institute of Jet Propulsion and Turbomachinery, Technische Universität Braunschweig, Braunschweig, Germany

³ Department of Mechanical and Aerospace Engineering, Sapienza University of Rome, Rome, Italy

⁴ Barcelona Supercomputing Center (BSC), Barcelona, Spain

⁵ Institute CRECK Modeling Lab, Department of Chemistry, Materials, and Chemical Engineering, Politecnico di Milano, Milan, Italy

⁶ INSA Rouen-Normandie, CNRS UMR6614-CORIA, Saint'Etienne du Rouvray, 76801, France

E-mail: antonio.attili@ed.ac.uk, federica.ferraro@tu-braunschweig.de, daniel.mira@bsc.es, alberto.cuoci@polimi.it, pasquale.lapenna@uniroma1.it and gaetano.magnotti@coria.fra

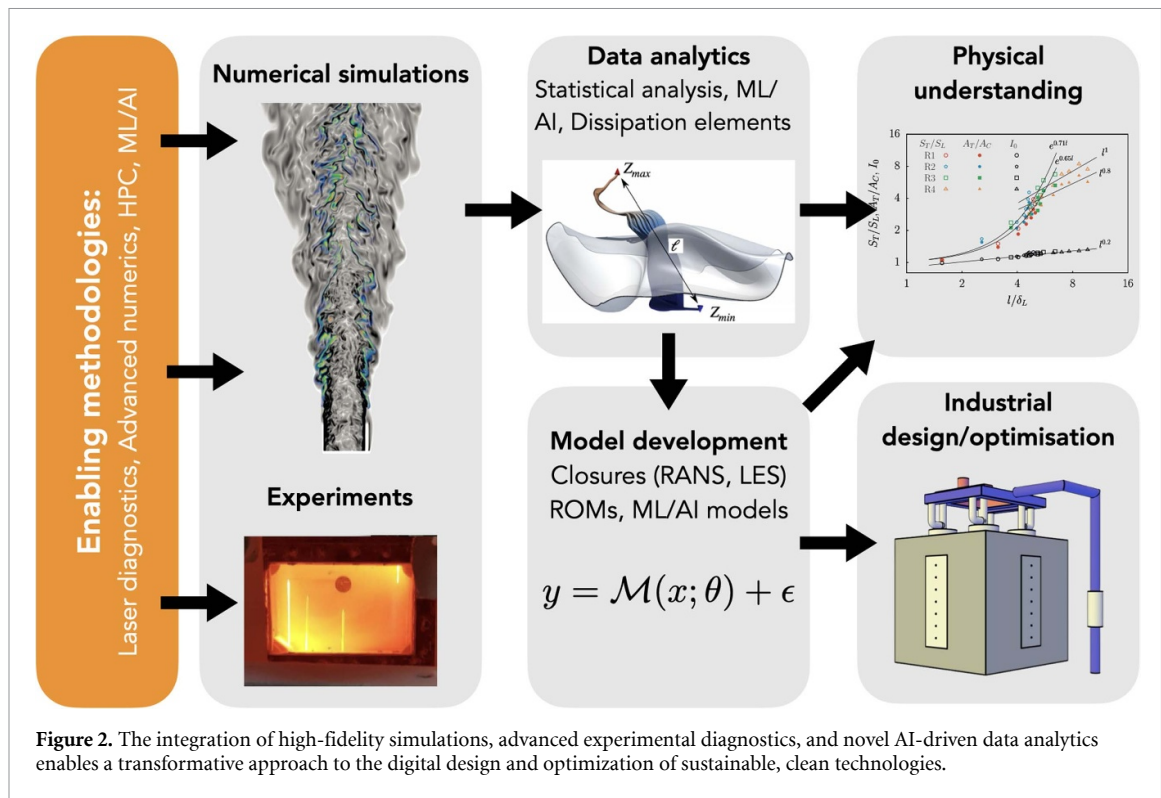
Current status

High-fidelity simulations such as direct numerical simulation (DNS) and large eddy simulation (LES), along with advanced experimental diagnostics, are increasingly applied to study the combustion of RSFs, including ammonia, hydrogen, e-fuels, and bio-derived compounds. DNS provides detailed insights into fundamental combustion phenomena, such as flame structure, ignition, and turbulence-chemistry interaction, and is primarily used in canonical configurations with simplified geometries and reduced chemistry [33]. LES, in contrast, is applied to complex, engine-relevant configurations, enabling the study of turbulent combustion dynamics, pollutant formation, and flame stabilization [34]. To manage the computational expense of detailed kinetics, simulation strategies often rely on reduced mechanisms [35], tabulated chemistry [34], or emerging acceleration techniques, such as machine-learning-assisted surrogates [36]. On the experimental side, significant progress has been made in characterizing RSF combustion in canonical configurations. Advanced diagnostics are being used to investigate RSF combustion experimentally. High-fidelity measurements from shock tubes, rapid compression machines, jet-stirred reactors, and laminar flames provide extensive datasets for the development and validation of chemical kinetics models for RSF [37]. High-resolution, multi-parameter measurements in turbulent, canonical flames are critical for understanding RSF combustion behavior under increasingly realistic conditions and for validating numerical models [38]. Collectively, simulations and diagnostics are becoming more integrated, with experiments informing model development and simulations guiding experimental design, accelerating progress toward a predictive understanding of RSF combustion (figure 2).

Current and future challenges

Despite recent advancements, several challenges persist [39]. A central issue for simulations is the high computational cost of incorporating detailed chemical mechanisms. While hydrogen's chemistry is relatively simple [40], most RSFs exhibit complex reaction pathways [41], necessitating model reduction that may compromise fidelity. Multiphase flows, radiative transfer, and pollutant modeling [42] also remain difficult to simulate robustly. On the experimental side, many diagnostic techniques originally developed for conventional hydrocarbon fuels must be adapted or re-engineered. Raman measurements of temperature and major species, coupled with LIF of minor species, provide high-fidelity data in turbulent flames of hydrogen [43], ammonia [44], dimethyl ether (DME), methanol, ethanol, and OMEs. For more complex molecules and in the presence of soot precursors or liquid droplets, coherent anti-stokes Raman spectroscopy (CARS) is a more promising approach, though it is limited to specific temperature conditions and selected species ratios. Much-needed, high-fidelity quantitative measurements of minor species remain challenging, especially at industry-relevant pressures. In addition, novel fuels such as ammonia require the development of ad hoc diagnostics to accurately measure key radicals such as NH_2 and NH , and pollutants including NO [45], N_2O , and NO_2 .

A shared and persistent challenge across both high-fidelity simulations and advanced experiments is the difficulty of matching the physical regimes typical of real-world combustion applications. Practical systems such as GTs, internal combustion engines, and industrial furnaces operate under extreme



conditions characterized by high pressures, high Reynolds numbers, and a wide range of other non-dimensional parameters, including the Karlovitz, Damköhler, and Weber numbers. Accurately capturing these regimes is essential. However, both DNS and LES, as well as many experimental setups, are often conducted at reduced scales or simplified conditions due to computational cost, facility limitations, or diagnostic accessibility. As a result, there is a gap between the conditions under which most current studies are conducted and those relevant to applications. For instance, the Reynolds number provides a clear example of this disparity. While practical combustors can exhibit very high Reynolds numbers, the state-of-the-art for DNS is limited to values several orders of magnitude lower, and even LES and large-scale experiments often fall short of achieving the fully turbulent asymptotic regime seen in real systems [34]. This affects the turbulence structure, mixing dynamics, and flame-turbulence interactions, potentially leading to models or interpretations that do not fully generalize. To address this issue, it is essential not only to push the boundaries of accessibility but also to conduct careful parametric studies that allow extrapolation to application-relevant regimes [34]. Aligning simulation and experimental studies with these target conditions, either directly or by ensuring the governing non-dimensional numbers are appropriately scaled, will be critical for bridging the gap between laboratory research and practical combustion system design.

High-fidelity data at industry-relevant pressures and Reynolds numbers remain limited due to the complexity and cost of operating high-pressure facilities in academic settings, as well as the challenge of implementing advanced laser diagnostics with restricted optical access and greater spatial resolution requirements. At elevated pressures, increased quenching, signal trapping, and laser absorption complicate the interpretation of the LIF signal [46] and reduce the accuracy of the minor species concentration measurements. The rapid increase of soot formation with pressure restricts the application of Raman scattering in high-pressure turbulent flames. Notable exceptions are carbon-free fuels, for which soot cannot form, and the Raman signal increases linearly with pressure, enabling improved spatial resolution, two-dimensional imaging [47], and kHz-rate acquisition. Despite the significant increase in signal-to-noise ratio and the minimal optical access required, CARS measurements remain challenging at elevated pressure due to increased spectral modeling complexity, stronger beam steering, and higher spatial resolution requirements [48].

Furthermore, there is a growing need for advanced data management [49], model validation, and the development of predictive tools to support the optimization and real-time control of RSF systems. This

includes uncertainty quantification, surrogate modeling, and ML to extract insights from large, multidimensional datasets.

Advances in science and technology to meet challenges

Recent advances are actively pushing the boundaries of what is possible in both simulation and experimental investigation, offering promising avenues to overcome many existing challenges. On the simulation front, the development of high-performance computing architectures and scalable algorithms has significantly increased the accessible resolution and domain size for DNS and LES. Modern codes are now optimized for GPU-accelerated platforms and exascale systems, such as Pele [50] and nekRS [51], enabling larger parametric sweeps and more complex geometries. At the same time, combustion chemistry has benefited from automated mechanism reduction [52], machine-learning-assisted surrogate models [53], and tabulated approaches that preserve critical kinetics while dramatically reducing computational cost [34]. These developments are allowing LES to approach more realistic engine conditions with increasing fidelity. Multiphysics modeling capabilities, such as those that couple combustion with sprays, radiation, and pollutant formation, are also maturing [42], enabling a more comprehensive treatment of practical fuels and systems.

In experimental diagnostics, breakthroughs in laser systems are enabling higher fidelity data. Pulse-burst lasers have extended traditional laser diagnostics to kHz rate, while maintaining elevated precision [54]. Femtosecond lasers [55] have enabled 1D CARS measurements at kHz rate at elevated pressures [48], unprecedented spatial and temporal resolution, multiple species, and 2D measurements. Ultrashort pulses are spectrally broad, enabling innovative approaches to detecting minor species and pollutants [56]. Recently developed, dual-frequency comb spectroscopy provides high-fidelity measurements of all components of the mass flux (velocity, temperature, pressure, and composition) in challenging environments, including shock tubes and scramjet engines, and is a powerful new tool for studying the chemical kinetics of RSF.

Moreover, data science is increasingly central to both domains. ML and uncertainty quantification techniques are being integrated with both simulations [57] and experiments [58] to improve model calibration, interpret large datasets, and guide adaptive experimentation.

In absorption spectroscopy, physics-informed neural network approaches have enhanced data-processing algorithms, providing more effective strategies for high-fidelity, time-resolved, multi-speciation measurements in shock tubes. Similar strategies are being investigated to remove fluorescence interference, extract detailed composition from experimental Raman spectra, and improve and accelerate CARS data analysis [55].

Data assimilation methods are being developed to fuse simulation outputs and experimental observations, closing the loop between modeling and measurement [59]. These technologies, when combined with collaborative platforms and open databases, are fostering a more integrated, efficient, and scalable approach to understanding the combustion of RSFs.

Concluding remarks

The combustion of RSFs presents both a critical opportunity and a formidable challenge for advancing clean energy technologies. While high-fidelity simulations and advanced diagnostics have made significant strides, fully capturing the complex physics and chemistry of these fuels under realistic operating conditions remains an open frontier. Detailed experimental data and high-fidelity simulation datasets are enablers for progress. Datasets shared through community platforms in a standardized format are essential for model development and benchmarking across fuels, combustion regimes, and configurations. Such data also provide the foundation for modern data-driven approaches, surrogate modeling, reduced-order methods, and machine-learning-assisted closures. Bridging the gap between laboratory-scale research and practical applications will require continued advancements in computational efficiency, diagnostic innovation, and interdisciplinary collaboration. By aligning simulation and experimental studies more closely with the regimes of real-world systems and leveraging emerging tools in data science and high-performance computing, the community is well-positioned to accelerate the development of predictive models and scalable solutions for sustainable combustion technologies.

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4. Hybrid physics-based machine learning approaches for renewable synthetic fuels modeling

Nguyen Anh Khoa Doan^{1,2}, Katarzyna Bizon³, Paola Cinnella⁴, Miguel Alfonso Mendez^{5,6,7} and Alessandro Parente^{7,8,9}

¹ Department of Aeronautics, Imperial College London, London, United Kingdom

² Faculty of Aerospace Engineering, Delft University of Technology, Delft, The Netherlands

³ Faculty of Chemical Engineering and Technology, Cracow University of Technology, Krakow, Poland

⁴ Institut Jean Le Rond D'Alembert, Sorbonne University, Paris, France

⁵ von Karman Institute for Fluid Mechanics, Sint-Genesius-Rode, Belgium

⁶ Aerospace Engineering Department, Universidad Carlos III de Madrid, Madrid, Spain

⁷ Aero-Thermo-Mechanics Laboratory, École Polytechnique de Bruxelles, Université Libre de Bruxelles, Brussels, Belgium

⁸ Brussels Institute for Thermal Energy (BRITE), Brussels, Belgium

⁹ WEL Research Institute, Wavre, Belgium

E-mail: n.doan@imperial.ac.uk, katarzyna.bizon@pk.edu.pl, paola.cinnella@sorbonne-universite.fr, miguel.alfonso.mendez@vki.ac.be and alessandro.parente@ulb.be

Status

Innovative modeling techniques are necessary to support the rapid simulation and design of RSFs-based power, manufacturing, and transportation systems, given their complex, multiscale, reactive behavior. Specifically, improved models are needed at various levels: (i) at the chemistry scale, to model the chemical kinetics, (ii) at the flow/combustion interaction level, to capture turbulence and reaction rates, and (iii) at the surrogate modeling level, to provide building blocks for future digital twinning of large-scale RSF systems.

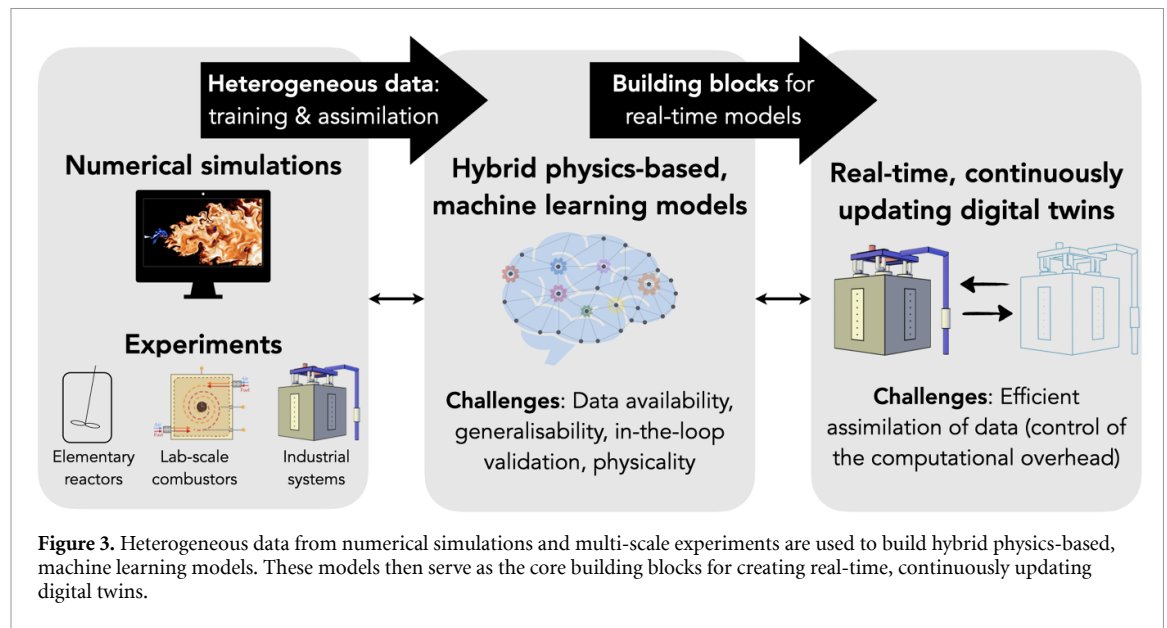
Traditionally, combustion models have been devised from first principles and physical intuition [60]. More recently, the rise of ML techniques, combined with increased access to high-fidelity simulations and advanced diagnostics, has enabled promising advances in RSF modeling [61]. Notable examples include neural network-based models that learn hydrogen combustion kinetics to accelerate chemistry calculations [62, 63], ML-based subgrid scale models using generative adversarial networks [64], and surrogate models combined with data assimilation to produce reduced-order models (ROMs) of furnaces [65].

These approaches remain largely data-driven, relying on high-fidelity data to train ML models, and typically do not leverage existing physics-based models or physical priors. In contrast, recent ML advances for non-reacting flows, particularly in Reynolds-averaged Navier–Stokes (RANS) modeling, have increasingly incorporated physical priors through gray- or open-box approaches that learn corrections to a baseline turbulence model using appropriate bases [66, 67]. Correction fields have been obtained using field inversion [68] or frozen methods [67, 69]. Yet, data-driven ML models often generalize poorly outside the class of flows for which they were trained, and special care must then be taken in complex flow applications, where multiple flow processes may coexist. Strategies for improving generalizability involve multi-objective training [70], model mixtures [71–74], and progressive augmentation [75]. Notably, these hybrid techniques show promise for extension to reacting flows and turbulence/chemistry interactions, for example, with recently developed ML-enhanced physics-based combustion closure [76], but this introduces additional challenges.

Current and future challenges

Despite the promise of ML-driven methods, major challenges hinder their broader application to RSF modeling.

First, while high-fidelity datasets are increasingly available, these are typically *sparse* and limited to one (or a few) specific flow or combustion condition(s). A major challenge is thus the creation of a comprehensive database of high-fidelity RSF data covering a wide range of operating conditions. In addition, even if sparse data is available, it will generally be noisy, either because of experimental diagnostic tools or because of a simulation setup where the effects of numerical schemes and solution convergence may affect the data [77–79]. Thus, treating these with appropriate filtering or adapted data assimilation techniques is a necessary first step in developing ML-based models [78, 79]. It should be noted that the problem of validating an ML-based model goes beyond generalizability and concerns how to effectively assess model performance and estimate the potential gap between the training and deployment phases.



For example, in turbulence/combustion modeling, while many models have been developed and tested in an *a priori* setting, few have been tested *a posteriori* [61, 64, 80, 81]. Furthermore, ensuring consistency of the ML outputs with the necessary corrections requires an *a posteriori* framework in which training is directly embedded within the computational fluid dynamics (CFD) solver, resulting in a highly costly training process [82–84].

In addition, given the multiscale nature of combustion systems, data is often obtained at different scales, resolutions, and fidelities, and from heterogeneous sources (experimental, simulation, ...), necessitating ML modeling to leverage such diverse data. Moreover, ML surrogate models are to be used to construct DTs of large-scale RSF systems, virtual replicas that can forecast their evolution in real time (figure 3).

Since DTs must have this real-time ability, they will necessarily rely on fast surrogate or system-level models. As a result, high-fidelity data may not always be required, particularly when such models are combined with data assimilation techniques that continuously adapt the model. Thus, it becomes important to develop methods that generate training data with appropriate fidelity [85], aligned with the accuracy requirements of the surrogate model. This could greatly simplify data acquisition and reduce computational costs. Real-time deployment will also require these models to efficiently assimilate live data, introducing additional algorithmic challenges due to the need to control computational overhead [86].

Finally, most ML models used in combustion are black boxes, offering no guarantees of physical consistency in extrapolated conditions. Their opacity also prevents physical interpretation of predictions, making it difficult to anticipate model behavior outside the training range. This lack of interpretability poses a major barrier to their use in practical design—especially in safety-critical applications, where physical insights and *a priori* trust are essential.

Advances in science and technology to meet challenges

In recent years, several initiatives have emerged to address the challenges above. To tackle data availability, the fluid mechanics and combustion communities have begun creating large, diverse datasets for training and benchmarking in areas such as surrogate modeling for aerodynamic applications [87, 88], reduced-order modeling [89], and combustion modeling [90].

In combustion modeling, growing attention is being given to hybrid physics-based ML approaches to improve generalizability in RSF applications. For instance [64], examined the extrapolation capabilities of such models for hydrogen combustion, showing that careful dataset design can enhance generalization across different Reynolds numbers and filter sizes.

Beyond combustion and turbulence modeling, progress has been made in hybrid physics-based/ML surrogate modeling, leveraging sparse sensing and data assimilation to improve prediction accuracy [59, 65, 91]. For example [59], developed a real-time DT of an annular hydrogen combustor by combining a physically derived low-order model with a data assimilation framework, using experimental pressure measurements to infer model parameters and enhance predictions alongside a reservoir computer

modeling bias and measurement drift. The resulting framework accurately predicted pressure fluctuations across a range of equivalence ratios, including both stable and thermoacoustically unstable regimes. Additionally, efforts toward model interpretability have advanced through gray- or open-box approaches, such as symbolic regression [67, 69], and explainable AI methods, such as the Shapley index [92].

In a wider context than the modeling of RSF physics, the emergence of scientific foundation models (SFMs) and large language models (LLMs) is reshaping ML in scientific domains, including combustion. These large, pre-trained models can generalize across tasks with minimal labeled data via masked prediction, enabling zero- and few-shot learning. A striking feature of SFMs is their *emergent abilities*, unexpected capabilities like in-context learning and multi-step reasoning that improve with scale. This makes them especially promising for combustion problems, where data is often scarce, noisy, or costly to obtain [93]. Recent works in computational chemistry have explored the potential of SFMs, LLMs, and transformer-based models for analyzing reaction mechanisms [94]. Still, their use can be extended to various other tasks, including surrogate modeling for costly reactive flows, flame diagnostics, automated literature reviews, and experimental design guided by reinforcement learning. Nonetheless, their adoption in combustion raises familiar challenges, limited interpretability, potential biases, and reliability under extrapolation, which require further research and a coordinated community effort.

Concluding remarks

The recent convergence of large datasets and advances in ML is opening new opportunities for breakthroughs in modeling RSF physics. By capturing complex nonlinear relationships within data, ML techniques offer powerful tools for accelerating chemical kinetics, improving combustion modeling, and developing surrogate models for RSF systems.

However, current ML models still face major limitations in generalization, due to both the scarcity of diverse, high-quality RSF datasets and the lack of model interpretability. Progress in incorporating physical priors, gray/open-box modeling, and hybrid physics-ML frameworks is beginning to address these issues, leading to more accurate, robust, and explainable models with strong potential for RSF applications.

Nonetheless, sustained research is needed to generate diverse RSF datasets and to develop rigorous validation strategies that assess generalization performance. Broader deployment of hybrid models will also require tighter integration across fluid mechanics, chemistry, and ML communities—collaboration that will be essential to accelerate progress.

Acknowledgments

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5. The role of digital twins in decarbonizing energy-intensive industries with renewable synthetic fuels

Luc Vervisch¹, Eduard Petlenkov², Abiodun Emmanuel Onile³, Peter Gorm Larsen⁴, Raffaele Ragucci⁵, Giancarlo Sorrentino⁵ and Alessandro Parente^{6,7,8}

¹ CORIA-CNRS, INSA Rouen Normandie, Saint-Etienne-du-Rouvray, 76800, France

² Centre for Intelligent Systems, Department of Computer Systems, Tallinn University of Technology, Akadeemia tee 15A, Tallinn, 12618, Estonia

³ Department of Software Science, Tallinn University of Technology, Akadeemia tee 15A, Tallinn, 12618, Estonia

⁴ Electrical and Computer Engineering Department, Aarhus University, Denmark

⁵ Institute of Science and Technologies for Sustainable Energy and Mobility, STEMS-CNR, Naples, Italy

⁶ Aero-Thermo-Mechanics Laboratory, École Polytechnique de Bruxelles, Université Libre de Bruxelles, Brussels, Belgium

⁷ Brussels Institute for Thermal Energy (BRITE), Brussels, Belgium

⁸ WEL Research Institute, Wavre, Belgium

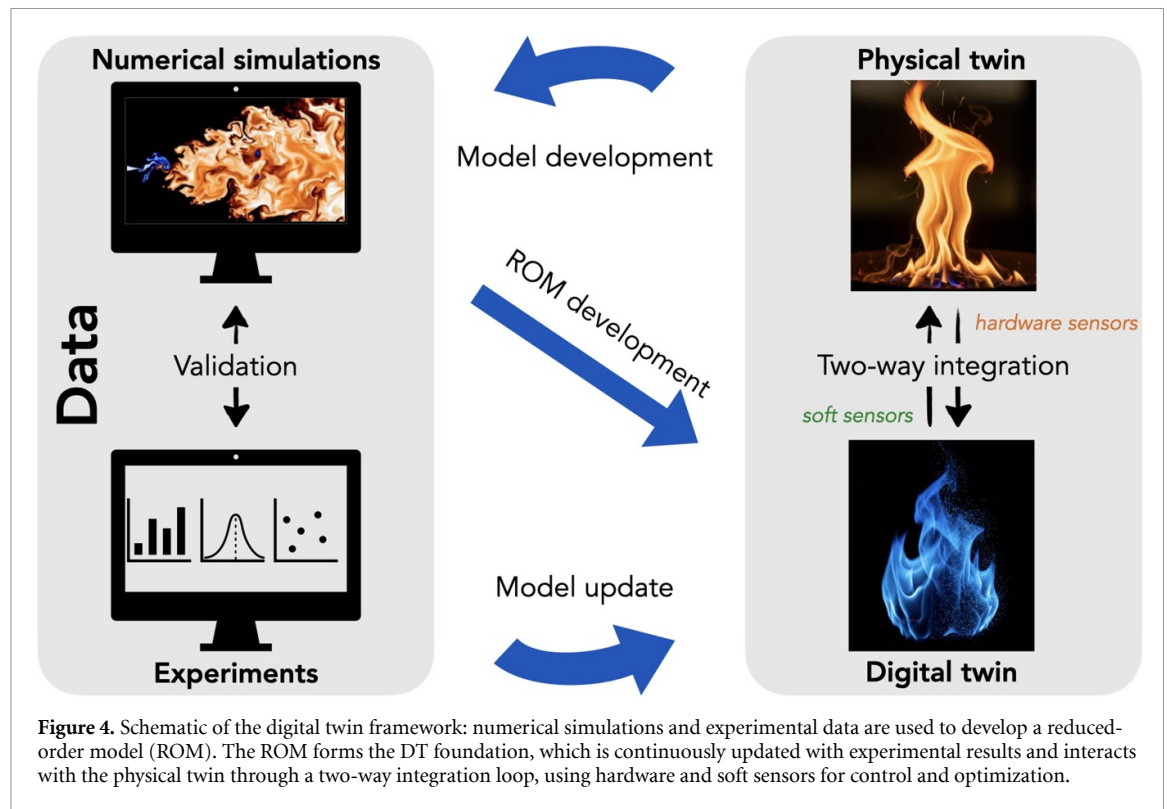
E-mail: luc.vervisch@insa-rouen.fr, eduard.petlenkov@taltech.ee, pgl@ece.au.dk, raffaele.ragucci@cnr.it, giancarlo.sorrentino@stems.cnr.it and Alessandro.Parente@ulb.be

Status

The adoption of Industry 4.0 technologies and the progression towards Industry 5.0 are critical for driving the global transition toward environmentally friendly, efficient, and intelligent solutions. In this context, digital technologies hold significant potential [95] to optimize, innovate, and accelerate the development and implementation of renewable and sustainable energy solutions [96]. This is particularly relevant to the field of combustion, which remains crucial across diverse sectors and heavily contributes to global carbon dioxide emissions. Hard-to-electrify industries requiring high-grade heat (e.g. steel, cement, and glass), transportation sectors demanding high energy density (e.g. shipping, trucking, and aviation), and chemical manufacturing require the elaboration of low-carbon solutions able to reduce their carbon footprint. The ability of digital technologies to enhance sensing capabilities in industrial equipment and to optimize, control, retrofit, and transform thermochemical conversion processes is essential for achieving sustainability goals.

Digital representations of physical systems exist on a spectrum, from static digital models with manual data exchange to digital shadows with automated unidirectional data flow, up to fully integrated DTs [97–99]. A true DT emerges when seamless, bidirectional data exchange occurs between the physical system and its digital counterpart, allowing for real-time monitoring, control, and optimization [100]. The predictive power of these digital representations is significantly enhanced by ML, which can improve the models using datasets from either physical systems or high-fidelity simulations. The integration of DT technology with ML is a crucial factor in improving the performance of advanced energy systems, especially for addressing the uncertainty of renewable energy sources. These ML models can be data-driven, relying on historical data, or physics-based, which integrate scientific knowledge to ensure adherence to physical laws, with Physics-Informed Neural Networks (PINNs) being a notable example [101, 102]. In fluid dynamics, for instance, these ML techniques are used to improve turbulence models [66–69], though ensuring the models generalize well to new conditions remains a challenge.

Some studies have explored the potential of DTs in energy systems, from planning photovoltaic deployment to forecasting grid behavior [103, 104] and to help decarbonize the shipping sector with synthetic fuels [105]. However, the widespread deployment of such technologies in combustion applications remains limited, and current examples are often closer to digital models or replicas [106]. In this context, the adoption of dimensionality reduction and non-linear regression methodologies has been key to developing real-time ROMs capable of reconstructing system responses across a wide range of operating conditions [107]. More sophisticated data assimilation approaches have been used to dynamically adapt simulation-based ROMs of different fidelity [59, 91]. To reduce the high computational cost of data generation, multi-fidelity approaches have also been introduced, which blend a limited amount of expensive high-fidelity data with numerous cheaper low-fidelity models, such as chemical reactor networks (CRNs) [85]. In this context, a pivotal aspect in realizing effective DTs for combustion systems is the development and integration of advanced sensing techniques, including both hard and soft sensors, to acquire high-quality, representative, and real-time data. Advanced sensing technologies are vital in providing real-time, distributed, and non-intrusive measurements within combustion environments,



making them suitable for industrial-scale deployment [108]. Soft sensors (virtual sensors that infer hard-to-measure process variables from available sensor data, models, and data analytics) are particularly valuable in harsh combustion environments, where installing physical sensors is limited by extreme temperatures, inaccessibility, or cost constraints. In the context of DTs, soft sensors bridge the gap between sparse, high-fidelity measurements and the need for high-resolution, multi-variable process monitoring. In a recent work, the reactors of a CRN were used as ‘soft sensors’ within a sparse sensing framework to reconstruct the full high-fidelity CFD fields, demonstrating a cost-effective method for developing DTs with extrapolation capabilities [109]. A representation of the DT framework is reported in figure 4.

This model supports a DT that interacts bidirectionally with the physical twin via hardware and soft sensors. Continuous updates enhance the fidelity of the DT for optimization and control. In summary, the fusion of advanced distributed hardware sensing, soft sensing methodologies, and data-driven analytics underpins the successful implementation of DTs for combustion systems. This approach not only improves real-time monitoring, optimization, and emission control but also enables the safe and sustainable adoption of RSFs in challenging industrial contexts.

Current and future challenges

Foundational challenges: Data and model fidelity

A central challenge in developing DTs for combustion systems lies in acquiring suitable training data and managing model uncertainty. Datasets must be comprehensive and representative, yet there is often a scarcity of industrial-scale experimental data, which necessitates ‘scale-bridging’ efforts. While numerical simulations can complement experiments, high-fidelity models are computationally expensive and difficult to generalize [61]. This leads to uncertainty, as both experimental data and model simplifications introduce errors that can propagate through the DT and affect its predictive capabilities. Consequently, robust methods for quantifying and addressing these uncertainties are crucial for building reliable models [110].

Implementation challenges: system integration and operation

Deploying a functional DT also involves significant practical difficulties beyond model creation. In combustion-dependent industrial settings, major barriers include the high upfront investments required for information technology (IT) and connectivity infrastructure, as well as the challenge of ensuring model reliability [106]. To mitigate overall costs, initiatives such as DT as a service (DTaaS) platforms are being explored [111]. Furthermore, integrating internet of things (IoT)-enabled sensing, communication, and data-driven analytics poses substantial data management and communication challenges in

energy systems [96], while the lack of standardized terminology and classification further complicates scoping and can increase development costs [103]. Finally, the collection and exchange of operational data raise privacy, security, and ethical concerns [112], which must be addressed for wider DT adoption [113].

Advances in science and technology to meet challenges

The development of DTs for large-scale combustion systems poses a significant challenge, primarily because of their complexity. These systems involve a complex interplay between chemical kinetics, turbulence, and heat transfer, and their interactions can vary significantly depending on the specific conditions [106]. This complexity makes it difficult to accurately model and predict combustion evolution in real time, which is a key requirement for effective DT implementation.

Addressing these challenges requires a multifaceted approach. Several key areas can be identified where advances are necessary: the acquisition of representative training data, data analysis and feature extraction, the development of adaptive simulation frameworks and subgrid models, the creation of ROMs, the utilization of advanced sensing and soft-sensors for two-way integration, and the implementation of DTs with lifelong learning capabilities, using data assimilation. It has been emphasized that tackling the diverse challenges requires a strong interplay between data and cyber-physical infrastructures, as well as collaborative efforts to drive innovation in energy-intensive sectors. Progress in each of these areas requires not only domain-specific expertise but also close collaboration among researchers from diverse disciplines.

Conclusion

The integration of DTs represents a transformative step towards decarbonizing the energy sector, offering a powerful framework to optimize combustion processes and facilitate the adoption of RSFs. By creating dynamic, real-time virtual replicas of physical systems, DTs provide unprecedented opportunities for enhanced monitoring, control, and predictive maintenance. However, the path to their widespread implementation is laden with significant challenges. These include the scarcity of high-quality data, the inherent uncertainty of predictive models, the high costs of development, and crucial issues surrounding connectivity, security, and ethics.

Meeting these challenges demands a concerted, multi-disciplinary effort. Future progress will depend on advancements in sensing for robust data acquisition, the development of sophisticated, generalizable AI/ML models that incorporate physical laws, and the creation of adaptive frameworks capable of lifelong learning through data assimilation. Ultimately, overcoming these hurdles will unlock the full potential of DTs, paving the way for more efficient, resilient, and sustainable energy systems and accelerating the transition to a low-carbon future.

Acknowledgments

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6. Industrial implementation of renewable synthetic fuels

Anes Kazagic¹, Alessandro Della Rocca² and Jörg Leicher³

¹ JP Elektroprivreda Bosne i Hercegovine d.d., Sarajevo, Bosnia and Herzegovina

² Tenova S.p.A., Genoa, Italy

³ Gas- und Wärme-Institut Essen e.V., Essen, Germany

E-mail: a.kazagic@epbih.ba, alessandro.dellarocca@tenova.com and joerg.leicher@gwi-essen.de

Status

The industrial implementation of RSFs holds promise for decarbonizing hard-to-abate industries such as aviation, shipping, heavy industries, manufacturing, and power generation. This section explores the current landscape of RSF project implementation and research and development (R&D) or pilot programs, categorizing them by the specific needs of different industries. While some key challenges and general barriers to practical exploitation are generally shared (e.g. production cost, availability, safety), sector-specific issues also need proper consideration. Opportunities for collaboration among stakeholders, possibly from different sectors of the economy, are likely to accelerate adoption. At the same time, a stable and clear regulatory and policymaking framework is required to reduce energy transition risks.

Current landscape

Given the substantial global energy demand and the crucial role of energy-intensive manufacturing processes, decarbonizing hard-to-abate industries is often considered one of the biggest challenges in global decarbonization efforts. Process heat applications require decarbonization, as they account for about two-thirds of total industrial energy demand, and roughly half of that is used at temperatures above 400 °C [114]. The two main pathways towards decarbonized process heat are generally considered to be electrification (with electricity from sustainable sources) and alternative fuels, often RSFs [115]. Both pathways have their specific advantages and drawbacks: in terms of energy efficiency, direct electrification is usually superior to synthetic fuels due to the efficiencies of electrolyzers, as well as because electric heating is generally more efficient than combustion-based heating, even in high-temperature applications (e.g. [116]). Fuel-based technologies, on the other hand, can usually achieve higher heat flux densities at high temperatures (resulting in smaller furnaces for a given production rate) and are easier to retrofit into existing thermal processing plants. Also, many manufacturing processes require more than just heat transfer: often, the interaction of the product with the furnace atmosphere is important for achieving the desired product quality, e.g. in the glass, metals, and ceramics industries.

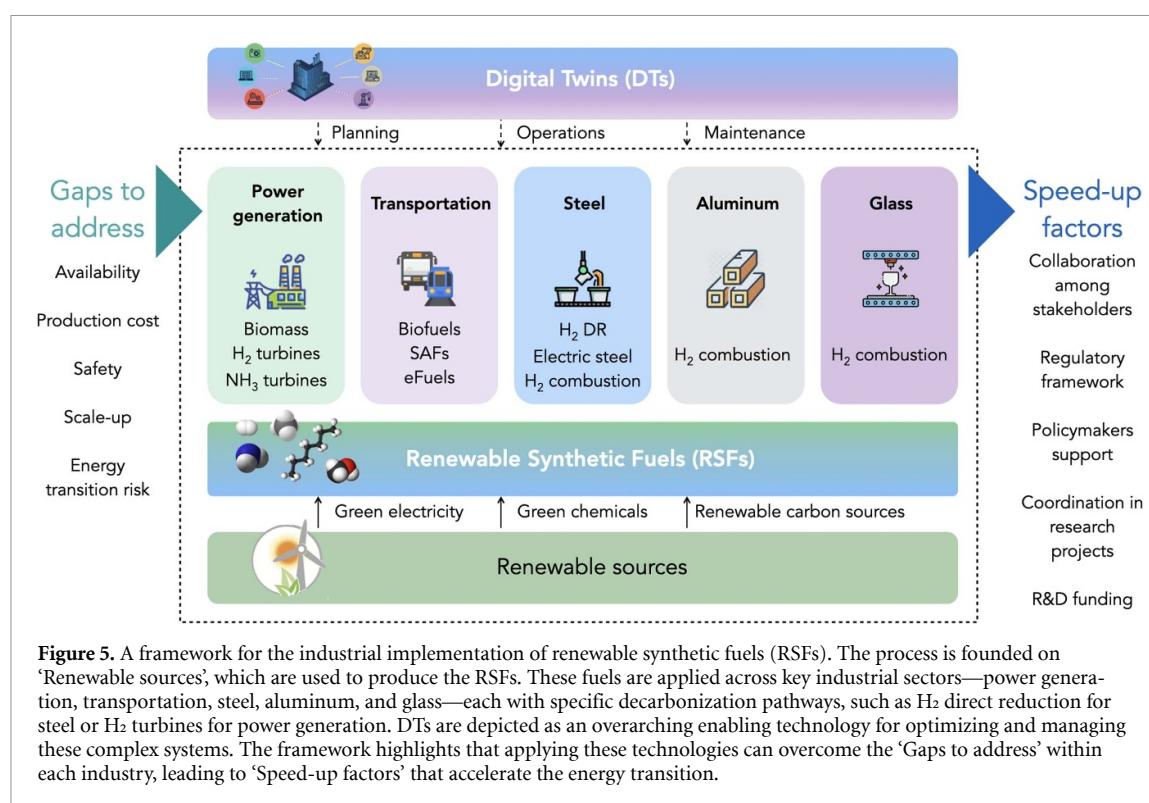
As energy system modelers focus on energy quantities and efficiencies in their analyses, they tend to predict that most process heat will be electrified (e.g. [117]). However, these high-level approaches often neglect product- and process-specific requirements, which can make synthetic fuels, particularly hydrogen, the better option overall, despite the inherent efficiency loss compared to direct electrification [115].

While the specific application of RSFs must be tailored to each industrial sector, many decarbonization strategies rely on a shared set of enabling technologies. Foundational elements such as green hydrogen, renewable carbon sources like biomass, and the basic building blocks for e-fuels are used across diverse industries. Similarly, DTs can be used to optimize processes, coordinate the use of renewable sources, and manage the risks of the energy transition (figure 5).

Several industrial projects and pilot programs are actively exploring the use of RSFs to advance decarbonization in power generation. Companies such as Siemens [118], General Electric [119], and Ansaldo Energia [120] are actively developing hydrogen-capable GT technologies. Companies such as Mitsubishi Power and MAN Energy Solutions focus on ammonia applications in power generation. Mitsubishi has been developing ammonia combustion technology for its GTs, focusing on zero-carbon operations [121]. The Allied Green Ammonia project [122] in Australia aims to produce hydrogen and ammonia on a large scale for energy and shipping.

In transportation, many research programs and pilot facilities are investigating the use of SAFs, synthetic diesel, and other e-fuels for offsetting carbon emissions:

- In collaboration with the South Australian government and aviation industry partners, Zero Petroleum is conducting a feasibility study for Plant Zero. SA. This facility aims to produce up to 10 million liters of SAF, gasoline, and diesel annually.



- The mining company Rio Tinto is initiating a biofuels pilot project by acquiring 3000 hectares in North Queensland to produce renewable diesel [123]. This initiative aims to reduce Rio Tinto's emissions, which account for 10% of its footprint in Australia, while engaging local communities and experts.
- The startup Twelve has developed technology that converts CO₂, water, and renewable electricity into synthetic fuels called e-fuels. Their first production plant in Washington is expected to commence operations next year, producing 50 000 gallons annually [124].
- ORLEN has partnered with Yokogawa to develop a DT to optimize the production of SAF. This technology enables simulation and analysis of production processes, enhancing efficiency and reducing costs [125].

The iron and steel industry has long been involved in pilot-scale applications to reduce carbon emissions since the European research program ULCOS [126] began in 2004. In recent years, the Green Deal in Europe has led to substantial public financing of full-scale direct-reduction plants or electric arc furnaces, replacing traditional coal-based blast furnaces. Collectively, European steelmakers are actively involved in around 60 projects that have the potential to reduce CO₂ emissions by 81.5 million t yr⁻¹ by 2030, according to Eurofer, the European steel association [127]. As of 2023, the European decarbonization project portfolio was set to cut emissions by 30% by 2030 and by 100% by 2050, with steelmakers shifting mostly to electric arc furnaces, though this is considered a possibility. Currently, the following projects can be regarded as the most relevant for scale and ambition:

- HYBRIT: SSAB, LKAB, and Vattenfall are making a joint effort to produce the first fossil-free steel at pilot scale using a green hydrogen-based direct reduction process. In the next phase, the process will be implemented on an industrial scale [128].
- SALCOS: Salzgitter and Tenova are building a 2.1 million t yr⁻¹ direct reduction plant based on Energiron® technology [129]. Central elements of the project are electricity from renewable sources and their use in electrolytic hydrogen production, reducing carbon emissions to 95% compared to standard steelmaking processes.
- STEGRA: The first production plan using the direct reduction process is under construction in Boden, Sweden. It is on track to produce green steel and green iron by 2026 using green hydrogen [130].

Starting in 2023, two of Europe's leading steelmakers slowed their energy transition plans, partly because the cost of green hydrogen production has not declined as quickly as expected. In their plans for green hydrogen technology, it is likely to only make a meaningful difference after 2030. Other relevant projects in terms of green steel production using green hydrogen are:

- Brazilian miner Vale and green energy park collaborated to investigate green hydrogen production in South America to produce direct-reduced iron for export to electric steelmakers [131].
- Australian miners Rio Tinto and BHP are joining forces in BlueScope Steel to develop a low-CO₂ ironmaking facility in Perth using direct reduction with natural gas-hydrogen blends [132].

Glass manufacturing is an energy-intensive process that today relies heavily on fossil fuels, mainly natural gas. GHG emissions arise not only from combustion; 25% to 30% of CO₂ emissions are process emissions, due to chemical reactions involving carbonates in the melt. The process is very sensitive, and small changes in process conditions can lead to problems with product quality. Due to the high process temperatures, pollutant emissions (primarily nitrogen oxides) are a significant concern for operators. Another aspect to consider is that the glass manufacturing process is highly integrated, with several continuous steps (melting, fining, forming, and post-forming). Melting and fining are the most energy-intensive steps. Any interruption can not only lead to a loss of production but also cause physical damage to furnaces and other equipment. Consequently, demand for continuity of energy supply is key [133]. The global glass industry explores different pathways towards decarbonization.

Fully electric glass melting furnaces have been in operation for decades. They are more energy-efficient than fuel-fired furnaces [116], but are limited in production rate (about 200 t d⁻¹), whereas gas-fired furnaces can achieve production rates up to 1200 t d⁻¹ and firing rates up to 100 MW. There are physical limitations on how much energy can be electrically transferred to the melt, at least with current furnace designs. Also, darker glass colors are difficult to produce electrically, as is the use of large amounts of cullet [116]. Furnace manufacturers are developing larger fully electric furnaces. Still, in applications like float glass production, it is expected that fuel-based solutions will continue to be used, often in hybrid furnaces. In the context of hydrogen, many fundamental questions have already been addressed in national (HyGlass [133, 134] and COSIMA [135]) and EU-funded (H2Glass [136]) projects. In terms of product quality, hydrogen combustion can lead to changes in the material samples compared to natural gas combustion [137], due to the higher water vapor content in the flue gases. While fundamental research projects have identified no major issues with hydrogen use in glass applications, industrial-scale trials have demonstrated its viability in glass manufacturing. Projects such as H2Glass [136] and the UK's Industrial Fuel Switching Program [138] confirmed that technical aspects, such as product quality and NO_x emissions, are manageable. At the same time, the primary challenges identified were primarily logistical, such as supplying sufficient hydrogen, and bureaucratic, such as permitting delays. While combustion control could be more challenging in the presence of hydrogen, this is considered solvable, potentially using DTs.

The aluminum industry is another prominent carbon emitter among the energy-intensive sectors. The carbon intensity of primary aluminum is mainly driven by indirect emissions at smelting sites, suggesting a possible relocation to geographies with direct access to green electricity infrastructure. Another route to decarbonize aluminum production is through improved recycling operations, which currently account for about 35% of global output. As in glass manufacturing, both natural gas-fired and fully electric furnaces are well established in the aluminum recycling industry, though natural gas combustion remains the preeminent form of heat generation for economic and technological reasons. While electric heating may be more energy efficient, this does not necessarily translate into lower operational costs, as natural gas is much cheaper per unit of energy than electricity. Electric furnaces tend to be smaller than their gas-fired counterparts (16 tons vs 120 tons maximum charge) [139]. Some process-specific reasons favor a combustion process. Aluminum scrap is often contaminated with organic residues from paint, glues, or lubricants, which can readily oxidize in a combustion system. At the same time, they can degrade product quality and reduce material yield in an electrically heated system. In the EU, the H2AL project [140] aims to demonstrate the applicability of hydrogen combustion for decarbonizing aluminum recycling. The project aims to retrofit an existing recycling furnace in Italy from natural gas-air combustion to hydrogen-oxygen combustion for at least 100 h with consistent, if not better, product quality, efficiency, and NO_x emission levels. Another project focus is using simulation and DT approaches to streamline the conversion process.

Challenges and barriers

The industrial implementation of RSFs faces several general challenges shared across different industries:

- *Availability and cost of green hydrogen and RSFs.* Green hydrogen, green ammonia, synthetic methane, and other e-fuels remain more expensive than conventional hydrogen production methods. The high costs are primarily due to substantial energy requirements for electrolysis and the need for large-scale renewable energy sources. In the case of intermittent sources and an energy curtailment scenario, the leveled cost of hydrogen primarily depends on the capital investment required for electrolyzer plants. A recent review [141] of cost prediction curves for green hydrogen production defines a trajectory from 5.3 €/kg in 2020 to 4.4 €/kg in 2030 and possibly down to 2.7 €/kg in 2050. Such prediction models need substantial reality checks against the future developments of world markets and policymaking.
- *Safety issues for large-scale green hydrogen storage facilities.* Green hydrogen is a fundamental building block of many RSFs' production processes and, as a chemical feedstock, requires appropriate facilities for large-scale storage. In this respect, a pressurized tank or underground storage is the main option, but it poses significant challenges for risk analysis and safety.
- *Regulatory hurdles.* The development of RSF projects often encounters complex regulatory frameworks. For instance, despite government support, Australia's green hydrogen initiatives have faced setbacks due to high construction costs and insufficient demand from buyers.
- *Lack of standardized practices.* The absence of standardized methodologies for RSF production and utilization hampers scalability and integration into existing industrial processes. This lack of standardization can lead to inefficiencies and increased costs.
- *Workforce training needs.* The transition to RSFs requires a skilled workforce handling new technologies and processes. For example, the shipping industry anticipates that by 2030, approximately 450 000 seafarers will need training to safely manage low-carbon fuels such as hydrogen and ammonia.

In addition to the general key points above, the iron and steel industry shows specific issues worth considering. Indeed, the transition from blast furnace/basic oxygen furnace (BF/BOF) to the direct reduction/electric arc furnace route (DRI/EAF) [142] using green hydrogen poses specific technical challenges. Using pure hydrogen requires a new recarburization step, as the iron produced is carbon-free; using biochar for this is a potential but complex solution [143]. Using ammonia as a hydrogen substitute, as proposed, introduces nitrogen contamination issues in both the process gas and the final steel [144]. Furthermore, carbon-free fuels in downstream reheating furnaces can increase oxidation and scale formation [145], thereby negatively affecting product quality and yield [146].

Similarly, the large-scale implementation of DTs must overcome challenges that are common among different industrial sectors:

- *Data accuracy and completeness.* The effectiveness of a DT strictly depends on the accuracy and quality of the input data. In practical industrial implementations, significant effort is required to assess the quality of the dataset and segment it to extract only the meaningful portion of the system, while omitting portions that are either not significant or corrupted by sensor-level malfunctions. Sometimes, this results in preliminary consistency checks or anomaly-detection procedures to select data sets that are accurate and complete for the DT goals.
- *Complexity and integration.* Developing and maintaining DTs in industrial environments is a complex task that requires collaboration among process, automation, AI, and data science expertise. This implies that full-scale implementation of DT is a multi-disciplinary task for which dedicated teams of internal and external experts must be assembled. Such teams need to have a lifespan on a quite broad time horizon, since maintenance operations typically span over time and are subject to interoperability constraints that allow only very limited speedup strategies. In addition, in many sectors, these DTs need to be integrated alongside existing automation systems, which are often responsible for critical operations and overall plant safety.
- *Culture and competence hurdles.* Maintaining DTs in industrial environments is a specialized activity that also requires the efforts of operations and maintenance personnel, who are normally dedicated to basic plant functions. The shift required in both internal competencies and culture across different age groups is not a secondary hurdle in industrial implementations in realistic settings.

- *High initial cost.* Due to the aforementioned factors, integrating DTs can be expensive and require substantial investment in technology and workforce. Such investment is obviously approved under the premises of a certain ROI, for which realistic use and demo cases need to be elaborated and assessed.
- *Cybersecurity risks and system resilience.* DTs rely on real-time data and connectivity and provide suggestions in operational and maintenance procedures. As such, they may be vulnerable to cyberattacks that compromise the safety and integrity of each installation. In this sense, cloud-based solutions were less acceptable to end users sensitive to such aspects or to those with limited resources and capabilities in this domain.
- *Overall life-cycle assessment (LCA) of DT solutions.* Initially, DTs have been suggested as an effective way to address sustainability issues by providing access to a fine-scale level of energy optimization, especially in hard-to-abate industries featuring energy-intensive processes. While this is correct at the conceptual level, there is still room to better assess energy demands at the very bottom of AI and ML architectures. The trade-off between energy costs from industrial processes and energy demand from data centers supporting DT technologies remains under investigation.

Additional environmental, social, and governance (ESG) topics related to DT adoption and an overview of the different applications across industries have recently been summarized, together with the challenges of AI [147].

Opportunities for collaboration

Collaboration among academia, industry, and policymakers is essential to overcome the fundamental challenges of implementing RSFs on an industrial scale. Academic institutions can partner with industry stakeholders to advance R&D, focusing on improving the efficiency, cost, and scalability of RSF and DT technologies. In addition, policymakers must create supportive regulatory environments and provide financial incentives to encourage investment; for instance, some acts offer subsidies for the construction of supply chains and set standards for low-carbon hydrogen. To facilitate broader adoption, collaborative efforts are also needed to establish standardized practices and certifications. Finally, joint initiatives can develop training programs to equip the workforce with the necessary skills, ensuring a smooth and safe transition to these new technologies.

Concluding remarks

The industrial implementation of RSFs has moved from foundational research into large-scale pilot programs. These real-world trials reveal a critical shift: the main barriers are no longer fundamental technical questions but practical hurdles such as the high cost and logistical complexity of fuel supply. Common strategies are emerging across sectors, such as the transition to hydrogen-based direct reduction in steelmaking and the use of hybrid furnaces in glass and aluminum manufacturing. Across these efforts, DTs are consistently being used to optimize and de-risk these complex conversions. Therefore, future success depends less on new scientific breakthroughs and more on focused collaboration between industry, academia, and policymakers to solve these pressing economic and logistical challenges. In this future scenario, there is space for the coexistence of RSFs with electrification solutions: the different applications have intrinsic process constraints that define the trade-offs needed for the specific decarbonization solution. In a broader perspective, electrification is a fundamental enabler for the development of RSFs, providing the backbone for a large-scale adoption.

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7. Techno-economic feasibility and social acceptance of renewable synthetic fuels

Ingrid El Helou¹, Thiago Lima Silva², George Skevis³ and Chiara Caccamo⁴

¹ Marble I, 75011 Paris 11, France

² SINTEF Industry, 7031 Trondheim, Norway

³ CLEOS, 175 64 P. Faliro, Athens, Greece

⁴ SINTEF Energy Research, 7031 Trondheim, Norway

E-mail: ingrid@marble.studio, thiago.silva@sintef.no, gskevis@cleos.gr and chiara.caccamo@sintef.no

Status

In Europe, high costs remain the main challenge for RSFs produced via electrolysis using renewable energy, due to their complex production pathways and the need for large-scale storage solutions to balance intermittent renewable energy sources. As electrolyzers continue to improve in efficiency, costs will drop but will remain thermodynamically limited by the 33 kWh kg⁻¹ H₂ required [148]. Infrastructure is another hurdle, requiring large capital expenditure and specialized transport networks and storage units, especially for hydrogen [148]. RSFs, including green hydrogen, SAFs, green ammonia, and e-methanol, have been proposed as potential decarbonization solutions for hard-to-abate sectors such as industry, aviation, and shipping, where direct electrification is insufficient (figure 6). See table 2 for a breakdown of these RSFs' key performance indicators (KPIs).

Industry is still highly dependent on fossil fuels and is responsible for ~6.5 Gt of energy-related CO₂eq emissions annually [149], with green hydrogen via electrolysis among the more mature decarbonization pathways. Hydrogen's low volumetric energy density makes transportation and storage both difficult and expensive. Today, 99% of hydrogen production still comes from fossil fuels, with over 60% produced through steam methane reforming, a process that emits 10–17 kg of CO₂eq/kg H₂ [148, 150]. The potential to achieve over 90% emissions savings from the fuel, in sectors such as steel, is highly dependent on the price of green hydrogen, which today costs up to 15 \$/kg and would need to drop to as low as 1.5 \$/kg to be competitive [150–152]. See table 2 for the KPIs of green hydrogen in industry. Green hydrogen will be most critical in industry for decarbonizing existing hydrogen uses, such as ammonia and methanol production and steelmaking, before expanding to new applications [148].

Aviation today is responsible for 2.5% of global annual CO₂ emissions [153]. In this chapter, the focus is on SAFs produced using renewable energy, via pathways such as FT or methanol-to-jet (MTJ). These fuels are drop-in options but currently contribute <0.1% to annual jet fuel consumption [153, 154]. Today, SAFs remain 3–7 times more expensive than conventional jet fuel, with higher green premiums for SAFs produced with CO₂ from direct air capture (DAC) than for point-source capture, but they provide the highest CO₂eq savings of up to 90% [153, 155]. These SAFs require large amounts of renewable energy, 80%–90% of which is needed to produce green hydrogen via electrolysis [153]. See table 2 for the KPIs associated with SAFs. In the EU, ReFuelEU Aviation requires the share of SAFs in aviation fuel supplied at EU airports to rise to 70% by 2050, including a 35% minimum share of SAFs, which would require an additional 870 TWh of renewable electricity [153]. In addition to fully synthetic power-to-liquid routes, hybrid e-biofuel pathways, often referred to as PbtL, should also be acknowledged as an emerging option for SAF production [156, 157]. By combining biomass-derived carbon with renewable hydrogen, these pathways can improve the utilization of biogenic carbon compared with conventional biomass-to-liquid routes [156]. They may also reduce system costs compared with fully synthetic e-fuels under stringent decarbonization constraints [157]. More broadly, recent transport-sector assessments confirm growing interest in bio-electrofuels as part of the portfolio of low-carbon fuels for hard-to-electrify sectors [158]. While this chapter remains centered on RSFs, the potential contribution of e-biofuels to future SAF deployment in Europe merits explicit consideration alongside pure PtL pathways.

The shipping sector is responsible for 2.4% of global CO₂ emissions today and currently operates almost exclusively on HFO, with <1% of fuel coming from renewable sources [148, 159]. E-methanol and green ammonia are considered long-term solutions to decarbonize the sector, a choice dictated by price, availability, technological development, and infrastructure readiness [160, 159]. Today, green ammonia and e-methanol remain 2–4 times more expensive than bunkering fuel on an energy basis [148, 160]. Neither fuel is a drop-in alternative for HFO and would necessitate engine modifications.

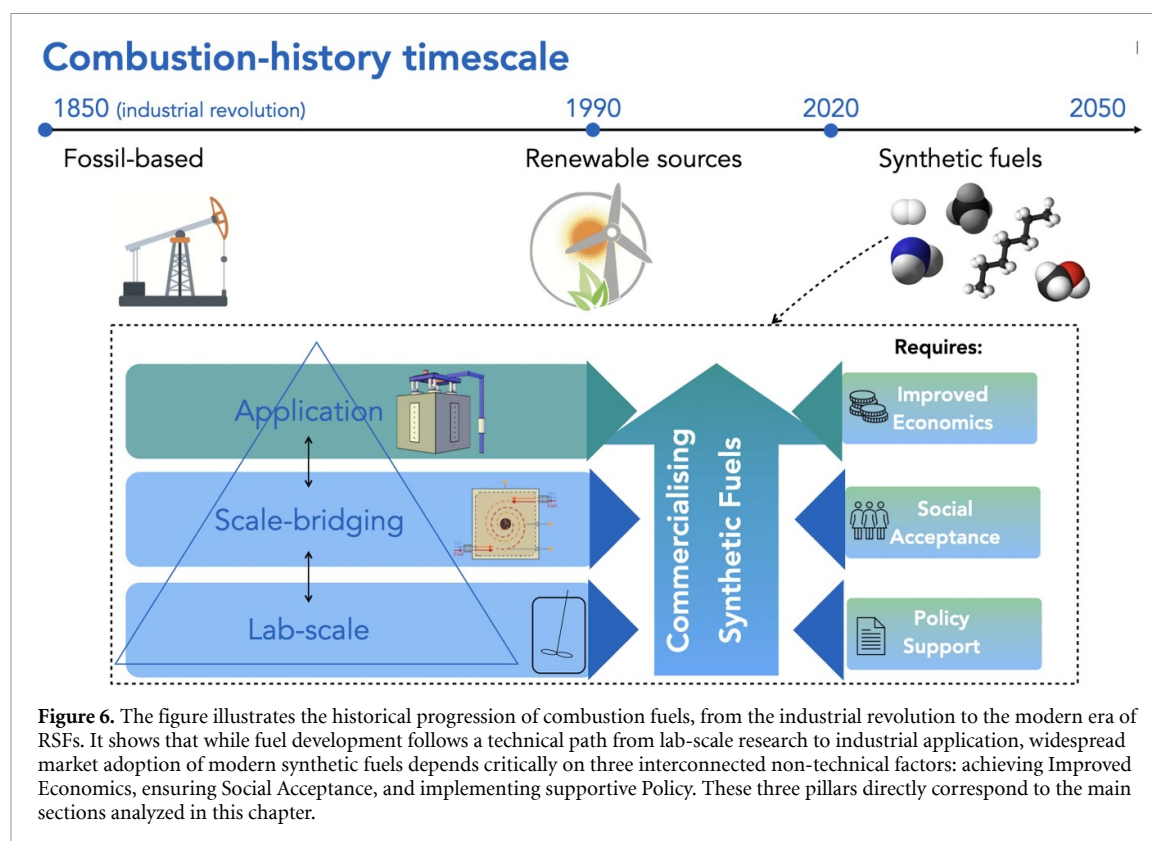


Table 2. TRL, scalability, cost competitiveness, and CO₂ savings of RSFs across industry, aviation, and shipping.

Sector	RSF	TRL	Scalability	Cost competitiveness ^a	CO ₂ savings ^a	References
Industry	Green Hydrogen	5–9	Dependent on: green electricity electrolyzers	500%–1000%	Could be >90%	[148, 150, 161]
Aviation	SAFs	5–9	Dependent on: green electricity, green hydrogen, sustainable CO ₂	300%–700%	Up to 90%	[161, 153–155]
Shipping	Green Ammonia	8	Dependent on: green electricity, green hydrogen	200%	100% ^b	[148, 161, 162]
Shipping	E-methanol	7	Dependent on: green electricity, green hydrogen, sustainable CO ₂	400%	Could be >90%	[148, 161, 163]

^a Relative to the conventional alternative.

^b This does not take into account N₂O emissions, a gas 298 times more potent than CO₂ [160].

Methanol is attractive because of its ease of handling and combustion, while ammonia poses challenges in both respects and is also toxic. However, ammonia is a zero-carbon fuel compared to methanol, but it does lead to N₂O emissions, a potent GHG [160].

As RSFs remain more expensive, requiring upfront expenditure to overcome several hurdles, financial market mechanisms such as carbon pricing, blending mandates (e.g. ReFuelEU Aviation in the EU), low carbon fuel standards (LCFS), or subsidies and private investment derisking, are necessary to help close

the commercialization gap, accelerate RSF deployment, and provide long-term visibility over the demand for these fuels [153, 154, 160, 164].

Social acceptance

The adoption of RSFs and DT technologies to help curb emissions will affect both workers and consumers across sectors, making policies that protect them and support social acceptance essential for deployment.

In aviation, in particular, the cost of decarbonization is expected to trickle down to consumers, with ticket prices projected to increase by 25%–30% by 2060 compared to today's levels [154]. These additional costs, accompanied by a wider availability of alternative modes of transport on shorter routes, could lead to a 30% drop in passenger travel kilometers, assuming constant ticket price elasticities [154]. Thus, government intervention is necessary to ensure that policies are progressively distributed and that the wealthiest 25%, responsible for >90% of aviation's emissions, bear a larger share of the cost. At the same time, low-income travelers are only marginally affected, for example, through frequent flyer levies [154, 165, 166].

Across all sectors, cyber-physical systems and DT technologies help optimize fuel consumption and maintenance, and prolong unit lifetimes. These technologies have simultaneously destroyed and created jobs over the years. Policy should focus on the social impact of digital transformation to ensure a just transition by upskilling the existing workforce, supporting the training of the next generation, or supporting the workforce's transition where upskilling is not feasible, as the industry needs to maintain a productive workforce.

Investment in workforce training is thus essential to bringing employees up to speed with novel digital technologies and fuels. In shipping in particular, training to handle new fuels both onboard ships and at the ports is essential, especially when working with ammonia, which is both toxic and hazardous [160]. Investment in the industrialization of digital technologies and RSFs is essential to ensure effective management of change, enabling the workforce to evolve as new systems are introduced.

Policy recommendations

Today, RSFs remain scarce and costly relative to fossil fuels. Therefore, policy mechanisms are essential to creating a business case for these fuels.

Cross-sectoral policy must ensure effective RSF utilization by prioritizing their deployment in hard-to-abate sectors such as aviation, shipping, and industry, over sectors such as road transport and building, where direct electrification is feasible as a decarbonization solution [153, 164]. For RSF deployment to be truly meaningful, its uptake must be coupled with the decarbonization of current hydrogen uses before deploying green hydrogen in novel sectors, such as a feedstock for shipping and aviation synthetic fuels.

Financial mechanisms are essential for the uptake of RSFs and for closing the commercialization gap with conventional fuels, as RSFs remain more expensive. Policies such as carbon pricing can help by setting a price on the CO₂ emitted from conventional fuels, either through a tax or an Emissions Trading System (ETS) [153, 154, 160, 164]. For example, the EU ETS currently implements a carbon price of ~76 EUR/tCO₂. The International Transport Forum (ITF) estimates that a carbon price of ~400 USD/tCO₂ would be needed to phase out fossil fuels completely in aviation, while Cordero-Lanzac *et al* find that a carbon tax of at least ~300 USD/tCO₂ would be needed for an e-methanol plant to reach break-even [16, 154]. Blending mandates and LCFS can only be effective when implemented with binding noncompliance penalties that ensure these policies are adhered to [153, 154, 160, 164]. These policies must be effective at stimulating RSF demand to trigger industry action and derisk investment, which is crucial for low TRL solutions to cross the valley of death, build demonstration projects, and achieve commercialization. Focusing solely on production and waiting for a second-stage policy framework to support demand can jeopardize first-stage efforts. Without demand, there is no market. And without a market, there is no investment.

In aviation, policies such as a frequent flyer levy can help ensure that the cost of decarbonization is not passed on to the lowest-income traveler. Instead, progressive taxes are introduced based on the number of flights taken per year. This shifts the cost onto wealthier, frequent travelers and higher-income countries, which are responsible for more than 70% of aviation's annual emissions [165, 167].

Concluding remarks

There is no business case for RSFs today, whether green hydrogen for industry, SAFs for aviation, or e-methanol and green ammonia for shipping. These fuels remain up to 10 times more expensive than their fossil alternatives and face additional transport, storage, handling, technological, and social hurdles

that hinder their large-scale deployment. Policy is crucial to stimulate demand for RSFs through blending mandates, bridging the cost gap with fossil fuels through carbon pricing, and ensuring these scarce resources are first used to decarbonize current uses and then prioritized for hard-to-abate sectors with no alternative decarbonization solutions. In parallel, a just transition must be ensured by shielding those most vulnerable to price volatility, as well as the workforce that needs to adapt to the digitalization of the sector and the adoption of novel fuels.

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Data availability statement

No new data were created or analysed in this study.

Author contributions

Alessandro Parente  0000-0002-7260-7026

Conceptualization (lead), Funding acquisition (lead), Methodology (lead), Supervision (lead), Visualization (lead), Writing – original draft (lead), Writing – review & editing (lead)

Giancarlo Sorrentino  0000-0002-6975-0702

Conceptualization (equal), Methodology (equal), Writing – original draft (equal), Writing – review & editing (equal)

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