Brussels, 12 May 2023

COST 061/23

DECISION

Subject:	Memorandum of Understanding for the implementation of the COST Action “Cyber-Physical systems and digital twins for the decarbonisation of energy-intensive industries” (CYPHER) CA22151

The COST Member Countries will find attached the Memorandum of Understanding for the COST Action Cyber-Physical systems and digital twins for the decarbonisation of energy-intensive industries approved by the Committee of Senior Officials through written procedure on 12 May 2023.

Funded by
the European Union

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA22151

CYBER-PHYSICAL SYSTEMS AND DIGITAL TWINS FOR THE DECARBONISATION OF ENERGY-INTENSIVE INDUSTRIES (CYPHER)

The COST Members through the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action, referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any document amending or replacing them.

The main aim and objective of the Action is to propel the collaborations between European researchers and industrial stakeholders to foster the use of cyber-physical systems and ultimately promote a safe and sustainable adoption of renewable synthetic fuels to decarbonise energy-intensive industries. This will be achieved through the specific objectives detailed in the Technical Annex.

The present MoU enters into force on the date of the approval of the COST Action by the CSO.

TECHNICAL ANNEX

OVERVIEW

Summary

Industrial production is responsible for roughly 30% of global energy use, with Energy Intensive Industries (EIIs) representing the largest share (54% of OECD's total industrial energy consumption). The current energy crisis, originated by Russia's war with Ukraine, Western sanctions against Moscow, and Russia's cut-off of pipeline gas, has made the cost of natural gas soar and ignited a cascade resulting in the increased prices of other energy sources. As a learning for the future, it is crucial to strengthen the EU's capacity to produce energy while reaching net-zero emissions by 2050. The solution lies in producing Renewable Synthetic Fuels (RSFs), including renewable hydrogen, from excess wind and solar power to decarbonise EIIs. Also, at the 26th UN Climate Change Conference of the Parties (COP26), it was unanimous that hydrogen can play a vital role in the way we bring fully decarbonised energy to our lives. However, a complete understanding of the impact of RSFs on EII systems remains unaddressed mainly due to a lack of comprehensive methods and specialised and multidisciplinary knowledge in RSFs' combustion, which can be advanced through approaches bringing together data-driven methods and physics-based modelling for accurate simulation of combustion technologies through enhanced modelling, sensing and digital twins. The main aim of CYPHER is to propel the collaborations between European researchers and industrial stakeholders to foster the use of cyber-physical systems (self-updating digital twins) and ultimately promote a safe and sustainable adoption of RSFs as a critical path for EII decarbonisation.

Areas of Expertise Relevant for the Action	**Keywords**
● Chemical engineering: Fluid flow and transfer processes ● Chemical sciences: Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions ● Mechanical engineering: Databases, data mining, data curation, computational modelling ● Mechanical engineering: Applied mechanics, thermodynamics ● Chemical engineering: Databases, data mining, data curation, computational modelling	● Data-driven modelling ● Sustainable combustion technologies ● Renewable synthetic fuels ● Soft-sensing ● Turbulent reacting flows

Specific Objectives

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

Research Coordination

- Create an interdisciplinary society of researchers, entrepreneurs, and policymakers to discover and eliminate the barriers to adopting innovative technologies to decarbonise energy-intensive industries.
- Liaise with the industrial partners from the different EIIs to understand the impact of renewable synthetic fuels on the stability of the combustion process, the associated pollutant emissions and the product quality.
- Coordinate the knowledge being created on combustion properties of RSFs and disseminate it broadly in the form of numerical models, advanced diagnostics to be applied to technological processes design and control, novel infrastructure design, etc.
- Develop methods to automatically extract the key features from data, which represents a crucial step in advancing the knowledge on RSF combustion and developing better and faster numerical simulation approaches.
- Develop reliable and affordable numerical simulation approaches using physics-based machine learning (ML) methods relying on high-fidelity data to improve the confidence of variable-fidelity simulations and explore larger design spaces in design and reduced-order model development.

- Develop self-updating digital twins to predict the impact of RSFs on EIIs systems and integrate them within cyber-physical platforms to understand, optimise, troubleshoot, and improve the design of industrial assets.

Capacity Building

- Decarbonise EIIs through a joint research agenda around digital methods, models, and cyber-physical systems, thereby fostering the EU's "digitally-enabled circular, climate-neutral and sustainable economy".
- Integrate first-principle models and ML to bring disruptive innovations in fluid mechanics and combustion science, impacting energy-intensive industries and beyond (process and food industry, air quality, etc).
- Foster the application of RSFs and digital twins in EIIs. Based on the solid implication of industrial partners, the Action will act as an incubator of new ideas and inspire entrepreneurial activity around digitalisation for industry decarbonisation.
- Facilitate scientific collaboration and knowledge exchange by organising and coordinating an open, sustainable, and multidisciplinary network using the Action website.
- Stimulate the development of a joint research agenda to facilitate the development of new research projects and participation in collective Actions under the three pillars of the Horizon Europe program (excellent science, societal challenge and European industrial competitiveness, and Innovative Europe), focusing on strong cooperation between industry and academia.
- Offer a balanced vision and expertise to European and national policy-makers by participating in the network as external advisors and by targeted communication measures.
- Identify and proactively contact new members to enlarge and strengthen the Action Network, promoting fair, diverse and gender equality membership.
- Enable dissemination of knowledge, research outputs, and opportunities to interact with and learn from other research groups.
- Mobilise and create awareness amongst Young Researchers and Innovators (YRI), including those from inclusiveness target countries (ITCs), on the problems of EIIs and existing challenges.
- Promote competitiveness of European academic and industrial partners in the digitalisation of EIIs.

TECHNICAL ANNEX

1. S&T EXCELLENCE

1.1. SOUNDNESS OF THE CHALLENGE

1.1.1. DESCRIPTION OF THE STATE OF THE ART

The recent increase in the prices of oil, natural gas and, by extension, electricity, which, combined with Europe's lack of autonomy in fossil fuels, have brought the EU face-to-face with unprecedented energy and financial crisis. REPowerEU's strategic plan aims to accelerate Europe's energy system transition towards energy security. Such events made the transition towards a green decarbonised economy even more urgent, pushing toward a massive integration of renewable energy sources to meet the EU "Fit for 55" targets.

However, this energy transition is not straightforward for the **Energy Intensive Industries (EIIs)** because of a lack of technology and prohibitive costs. EIIs are vital sectors, as underlined in the EU Green Deal, indispensable to Europe's economy, as they supply several key value chains. The decarbonisation and modernisation of EIIs is, thus, a key priority.

Industrial production is a significant energy consumer and accounts for roughly 30% of global energy use, with **EIIs** representing the largest share. EIIs encompass the manufacturing of food, beverage, pulp, and paper; basic chemicals; refining; iron and steel; nonferrous metals; and non-metallic minerals. In 2019, EIIs were collectively responsible for 22% of total EU GHG emissions, representing a clear target for a joint effort to meet the (global) net-zero emissions by 2050, as per the Paris Agreement.

World industrial energy consumption is forecasted to grow from ~242 quadrillion Btu in 2018 to about 315 quadrillion Btu in 2050, while the contribution of EIIs to this number is expected to remain at approx. 50% during that period. It is widely held that energy consumption tends to be positively associated with a higher economic growth rate. However, against this backdrop is the environmental impact of this consumption. **Consequently, the biggest challenge is maintaining economic growth while cutting down GHG emissions.** To answer this challenge, multiple technologies have been studied with the potential to reduce the carbon impact of EIIs.[i] These innovations are often complementary and enable the replacement of fossil fuels with electricity or biomass (e.g., electric glass melting, electrowinning in steel or biofuel in lime kilns), replacement of feedstock (such as geopolymers in cement or bio-based plastics) or integration of Carbon Capture and Storage (CCS) into the process design. While these technologies are beneficial by reducing CO_2 emissions, their bottlenecks prevent them from being scaled into meaningful industrial applications. For instance, the complete electrification of EIIs is currently impossible due to the need for high-temperature heat (>1300K) that requires using high-energy-density vectors[ii]. Replacement of feedstock is not scalable due to (i) sub-optimal down-cycling, (ii) low resource vs high labour costs, and (iii) traditional supply chain organisation. Finally, CCS requires additional energy demand, costs, and infrastructure to transport captured CO2.

Renewable Synthetic Fuels (RSFs), including renewable hydrogen, are enjoying reaffirmed and rapidly growing attention as a concrete solution to decarbonise EIIs[iii]. However, a complete understanding of the impact of RSFs on EII systems remains unaddressed, mainly due to a lack of comprehensive methods and specialised and multidisciplinary knowledge in RSFs' combustion to pave the way to solutions that can ensure 1) step-wise upscaling, 2) retrofitting existent plant, 3) exploit scale-reducing effects, and ability of new firms to enter EIIs with low carbon innovations.

Moreover, by 2040, all major sectors of the European economy will be deeply digitalised. Digitalisation will affect decarbonisation efforts because of its impact on energy demand, employment, competitiveness, and trade patterns and its distributional, behavioural and ethical implications. In this context, the ***digital revolution acts as a critical enabler for decarbonisation***. The network of partners in this ACTION believes that **digital transformation can unlock the solution to transform EIIs in a sustainable sector**. Specifically, the Action aims at advancing knowledge in RSFs' clean combustion through data-driven turbulent reactive flows modelling, advanced sensing, and digital twins, in agreement with the Sustainability by Design principles.

Based on this scenario, producing RSFs from excess wind and solar power is a very attractive opportunity to create energy-dense carriers with neutral carbon balance for industries where electrification is not an option due to the required high energy densities and temperature levels. Many macroeconomic models support the need for RSFs such as hydrogen and hydrogen carriers (e.g. ammonia), synthetic methane, and carbon-neutral liquid fuels as part of the Swiss knife of energy tools required to meet the energy needs in a carbon-neutral and sustainable way. To enable RSFs use in EIIs through digitalisation, experimental techniques and sensors, reactive flow models and data analytics are continuously evolving. Still, there are **essential gaps** in the state-of-the-art preventing their scalability.

1) Combustion models for RSFs

Combustion processes are characterised by vast ranges of time and length scales, transitions, bifurcations, and multiple interacting physical phenomena that are extremely complex to predict. While turbulent combustion models have become commonplace across industries, their **current predictive capabilities fail to meet the standards needed for new design and regulation**[iv], especially concerning pollutants and stability limits[v]. The latter issues are amplified when RSFs are used in unconventional operating conditions, typical of EIIs that must simultaneously meet near-zero emission and fuel flexibility requirements. Combustion models have often been classified into two categories, the flamelet-like[vi] and PDF-like approaches[vii]. Besides them, there are reactor-based[viii] and conditional-moment approaches[ix]. Data-driven methods are starting to impact the design of improved sub-grid models for large-eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) simulation closures[x].

Progress in the field of combustion science and engineering is inexorably linked to data. The key to developing better models lies in the availability of data and effective approaches able to extract the information of interest and encode it in a suitable model. **High-fidelity direct numerical simulations (DNS) of combustion systems are still limited to specific aspects of a turbulent combustion process and simple building blocks**. On the one hand, these simulations generate vast data over some dimensions (resolution in space and time). On the other hand, the data generated is very sparse in other dimensions, such as flow conditions and fuel composition, to name a few, leading to generalisation challenges. Still, **they are rich in information that could help to decode the complexity of turbulence-chemistry interactions** and guide the development of filtered and lower-fidelity modelling approaches for faster evaluations[xi], **if appropriate feature extraction algorithms were available**. Besides, **high-fidelity experimental data** are only available for laboratory-scale devices, and the amount and accuracy of measurements decrease going from small to large scales. Moreover, even with the most sophisticated diagnostic techniques, **only a limited number of variables of interest are accessible, with limited spatial and temporal resolution.** Nevertheless, experimental data remains our window into reality and the most reliable validation of computational approaches.

Over the past 50 years, many techniques have been developed to process combustion data from experiments and simulations to advance the predictive capabilities of modelling approaches[xii]. These analyses have strongly **relied on domain expertise and heuristic algorithms, leading to limited success in increasing the reliability and generalisability of turbulent combustion models**[xiii].

2) Numerical simulations

The paucity of experimental data and the chemical complexity are the main challenges in constructing and utilising detailed kinetic mechanisms and transport models for multidimensional simulations of turbulent reactive flows[xiv]. Fuel oxidation and product/pollutant formation are described by chemical kinetic mechanisms (collections of elementary reactions) consisting of hundreds of species tightly coupled in thousands of chemical reactions. Considering the impact of large kinetic mechanisms on the computational time of detailed numerical simulations (the computational time scales more than quadratically with the number of involved species), many different strategies have been developed in the last two decades to reduce the burden of numerical combustion simulations. Despite their variety, all methods fall under two main categories, i.e., rate-based and state-space. Rate-based methods aim to generate systematically reduced mechanisms (with a lowered and thus affordable size) by eliminating unimportant chemical species and reactions, before[xv] or during the simulation itself[xvi]. The use of adaptive chemistry models, coupled with on-the-fly classification to adjust the size of the chemical mechanisms to the local flow conditions[xvii], has gained interest over the last few years. State-space methods are based on the re-parameterization of the chemical state-space[xviii] with a reduced number of convenient variables: the archetypal example is the flamelet model where the local stoichiometry and the progress of reaction are used to identify a low-dimensional manifold in the composition space along which the evolution of the system is constrained. Recently, state-space methods have been further developed and combined with data-driven approaches. Modal techniques (such as the principal component analysis - PCA) were used to create reduced-order models for combustion simulations based on the solution of transport equations for the principal components[xix], in combination with non-linear regression techniques to develop a more accurate mapping between the low-dimensional manifold, the state-space and the associated chemical source terms[xx].

While several approaches have been proposed to adapt to the complexity of chemical mechanisms during a numerical simulation, **little effort has been placed in developing data-driven approaches for selecting optimal closures, differential equations (DE) solvers, tabulation and solution tolerances during a combustion simulation**. Thus, it holds a potentially crucial development to make the simulation of realistic combustion systems feasible and affordable.

3) Reduced-order models (ROMs)

In industrial applications, a fast evaluation of the system response is required (for control, optimisation, etc), thus limiting the use of time-consuming simulations. In this context, ROMs are used to approximate the underlying hidden relationship between inputs and outputs, using available observations to estimate the system response at new conditions. Black-box approaches have been widely used in combustion to create static input-output maps[xxi] and system identification[xxii] to predict macroscopic quantities such as exhaust gas emissions and temperature and to detect oscillatory patterns such as thermoacoustic instabilities, respectively. An interesting approach to generating combustion ROMs is the use of reactor network models[xxiii], which fall in the category of grey-box models, as they combine a theoretical structure, i.e., the chemical reactors, with data to generate the network. The approach can also be regarded as an example of multi-fidelity methods, being high-fidelity tools (i.e., computational fluid dynamics - CFD) used to construct the reactor network and the simplified network model used to evaluate pollutant emissions and other quantities, using detailed chemical mechanisms. These techniques benefit large and complex systems, such as industrial furnaces or gas turbines. However, their **current overall fidelity and generalizability are limited by the high-fidelity simulations required to generate the network structure**, indicating interest for data-driven approaches in this area of research.

ROMs based on modal decomposition (using PCA and other techniques) have been quite successful, in combination with non-linear regression approaches, in developing ROMs for uncertainty quantification[xxiv] as well as in designing simulation-based digital twins (DT)[xxv] of industrial systems. However, **the combined use of heterogeneous data streams for the continuous update of the DT still represents an open research area where data-driven techniques can contribute significantly towards the development of genuinely integrated cyber-physical infrastructures**.

In this field, **experimental data with different levels of fidelity are also needed** when combined with numerical results to build a DT. Such high-fidelity data from experiments are usually available only for laboratory-scale devices, and both the amount and accuracy of measurements decrease going from small to large scales. Moreover, **even with the most sophisticated diagnostic techniques, only a limited number of variables of interest are accessible, with limited spatial and temporal resolution.** Therefore, in this field, little effort has been placed into developing advanced sensing approaches for the measurements and detection of critical quantities in harsh environments on large scales or on scale-bridging experiments.

1.1.2. DESCRIPTION OF THE CHALLENGE (MAIN AIM)

The main aim of CYPHER is to propel the collaborations between European researchers and industrial stakeholders to foster the use of cyber-physical systems (self-updating digital twins) and ultimately promote a safe and sustainable adoption of RSFs as a key path for EII decarbonisation. To achieve this primary goal, the ACTION will establish an open, competent, and multidisciplinary European network of experts in chemistry, fluid dynamics, combustion, and machine learning (ML) methods to collect data, analyse and investigate clear pathways for significant integration of RSFs in EIIs. Thus, a vital element of this ACTION is to leverage and disseminate the knowledge generated around digitalisation as a critical vehicle to implement RSFs in EIIs. The ACTION includes 81.9% Higher Education & Associated Organisations, 11.2% Business enterprise, 5.2% Government/Intergovernmental Organisations except Higher Education, 0.9% Private Non-Profit, and 0.9% Standards Organisation across the network, thereby maximising the impact.

The gradual transition into a carbon-neutral future using RSFs requires technologies ensuring fuel-flexible operation, which is challenging because of the vastly different properties of hydrogen and hydrogen carriers when compared to conventional fuels such as natural gas. A particularly promising technology in this perspective is MILD combustion[xxvi] and other related concepts (flameless combustion[xxvii] and colourless distributed combustion (CDC))[xxviii], where the strong preheating and dilution of the fuel charge by the exhaust gases (by internal recirculation) leads to a combustion regime with distributed heat release that is characterised by high stability, increased fuel flexibility, and near-zero emissions. Despite these beneficial features, implementing low-emission combustion technologies at an industrial scale is still challenging. In the transition to RSFs, **it is mandatory to ensure that even with new fuels and fluctuating mixtures, energy conversion is safe, takes place without harmful emissions, and that energy efficiency and industrial production are not compromised.**

To reach this goal, significant developments are needed in combustion science, fluid mechanics and ML methods to address the research questions and technological challenges associated with the adoption of RSFs in energy-intensive industries: i) What is the impact of changing a fuel/oxidiser/burner technology on the combustion process taking place in large industrial furnaces? ii) How can stable combustion be ensured with near-zero emissions for fuel-flexible operation? iii) What will be the impact of changing fuels on the overall process efficiency and the characteristics of the developed products?

Addressing these questions will require better combustion models, faster numerical simulations and truly integrated cyber-physical platforms. The R&D challenges of each are (addressed via CYPHER):

Better models. A potential solution for improving the fidelity of combustion models, mainly when RSFs are used, is the exploitation of data from DNS and experiments to develop physics-informed ML-based models. ML-based and data-driven approaches have tremendous potential in advancing engineering and fundamental sciences. However, to date, the success of data-driven strategies in complex and highly non-linear applications has been very modest. New ML techniques, especially hybrid ML techniques with physics-based knowledge, are promising to advance our understanding of complex processes and fully exploit the information in large experimental and numerical data sets. However, caution is needed when applying ML approaches to physics-based problems such as combustion. Indeed, for typical ML applications, such as advertising, image, or speech recognition, the impact of a single ML prediction is small, and the training data are so vast that virtually all tasks may be regarded as interpolation. The situation is quite different in turbulent reacting flows due to data sparsity, heterogeneity, and uncertainty. Large data sets are available, but for very few operating conditions: the impact of each prediction is critical, and guarantees on accuracy and physical realizability must be provided, thus requiring ML algorithms that are interpretable, explainable, and generalisable.

Faster simulations. Combustion problems are computationally very expensive, and this burden limits the possibility of exploring many scenarios. The development of adaptive simulation frameworks rooted in the combination of unsupervised classification algorithms, dimensionality reduction and reduced-order models offers the opportunity of retaining the model fidelity while substantially reducing the simulation time. The main challenge in this perspective is associated with the development of adaptive simulation frameworks able to adapt the sub-grid closures, number of transported species, DE solver and tabulation, and solution tolerances, based on the local flow conditions. Another challenge is the generation of training data representative of the conditions met during the simulations. To date, constructing an appropriate data set for the optimal low-dimensional representation of a system is still an open question[xxix], not only for combustion problems.[xxx] Merging different reactor and flame archetypes into a single database for training and model development requires sampling and regularisation approaches that are not yet mastered.

Cyber-physical infrastructures. The design of complex systems is an iterative process that requires a certain number of model evaluations and exploring “what if” scenarios. As such, it cannot rely solely on high-fidelity tools, admitting that they are available for the scale of interest. A combination of approaches is needed to bridge information from high and low-fidelity models into a reduced representation of a complex asset. Data-driven strategies can lead to a step change in this field of research, allowing to address of existing challenges related to the calibration of low-fidelity models, the parameterisation of the discrepancy between high- and low-fidelity models, and the integration of heterogeneous data streams (numerical/experimental, fine/coarse-grained, etc) in the calibration and model update process. The combination of simulation and experimental data is required for large-scale combustion systems to develop digital twins that can forecast combustion evolution in real time and act as soft sensors. Unlike other assets, the extensive use of physical sensors in harsh environments such as furnaces is not feasible. Advanced laser diagnostic is not adapted for industrial combustion systems, besides being extremely expensive. Moreover, most sensors are single points and single parameters, so only a tiny portion of the system and a small set of physical/chemical parameters can be monitored.

The previous argument is crucial for the modern automation of combustion systems for the EIIs that still rely on relatively few sensors from the field and consequently on a limited amount of information and detail about single operating components. Only the principal process parameters are effectively measured to feed the control system, while the status and health of single critical components are usually established only because of scheduled maintenance inspections. Advanced, robust, plantembeddable sensors for real-time diagnostics of combustion systems are crucial elements required by innovative burner operation control and optimisation strategies. Accordingly, they are also essential for burner Digital Twin development and operation and for IoT concept integration in new and existing plants.

The development of integrated cyber-physical infrastructures will require advances in the three areas above to improve the fidelity of combustion models, explore a more significant number of scenarios thanks to the availability of faster yet reliable simulations, and integrate heterogeneous data in the development and continuous updates of digital twins replicating the behaviours of their physical counterparts.

The above challenges can only be addressed by an Action establishing a framework where key actors (researchers, entrepreneurs, innovators, policymakers, etc) from combustion, fluid dynamics and data science interact in a dynamic and focused way to tackle the listed challenges, to promote the spread of knowledge, to reach multidisciplinary actors, which will develop interdisciplinary research and create innovation while empowering and retaining young researchers to realising a broader impact.

1.2. PROGRESS BEYOND THE STATE-OF-THE-ART

1.2.1. APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE OF THE ART

The main challenges in combustion modelling are associated with the number of species involved in combustion processes, the small scales, and the non-linear turbulence-chemistry interactions. **CYPHER's approach is to develop hybrid ML methods to propel combustion science and treat some of the previously unmet challenges[xxxi], providing interpretable feature extraction techniques**, delivering generally applicable approaches to **locally adapt comprehensive chemical mechanisms of RSFs** and **sub-grid models**, designing **new closures** to parametrise the unresolved fluctuations, and **developing robust and predictive digital twins of large-scale combustion assets of EEIs**, both for **online monitoring** and **control** of combustion devices and to make informed and confident decisions on new technological developments.

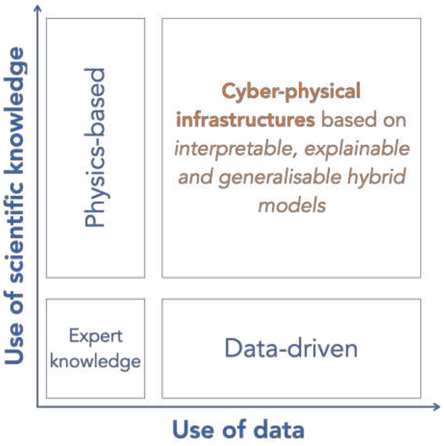


Figure 1 -CYPHER approach beyond state-of-the-art

The CYPHER COST ACTION will, furthermore, take advantage of the existing European critical mass of researchers covering the large spectrum of competencies required to decarbonise EIIs through RSFs, establish a forum for exchanging ideas, techniques, and protocols, organise workshops, training schools, and promote the mobility of researchers. CYPHER will directly benefit society and contribute the Horizon Europe's Strategic Plan (Key Strategic Orientation C): "Making Europe the first digitally-enabled circular, climate-neutral and sustainable economy through the transformation of its mobility, energy, construction and production systems" and the impact area "Climate change mitigation and adaptation", enabling the use of renewable fuels in EIIs and providing the required tools to retrofit and adapt complex industrial assets. Considering the CO2 emissions from EIIs (9.2 Gtons worldwide), the potential savings and environmental and societal benefits are enormous.

Significantly, **this COST ACTION will promote advances beyond state-of-the-art** by reducing the fragmentation of research efforts and fostering the interchange of knowledge between academics, entrepreneurs, and policymakers. Towards this aim, the Network of Proposers will proactively establish a dynamic consortium with experts from academia and industry, fostering new knowledge and research lines that create new opportunities for Young Researchers and Innovators (YRI) to tackle the future challenges in modelling industrial systems. More so, the applicants will actively recruit new members to join the network during the period of the Action. The Network will develop a website as a platform to reach new members and communicate with the current ones.

The Network of Proposers has a deep understanding of current challenges and aims at conveying efforts and knowledge to advance the state-of-the-art in the following areas:

Better models. Considering the typical size of high-fidelity combustion data sets[xxxii], the development of feature extraction approaches requiring minimal supervision is strategic to identify low-dimensional manifolds in chemically reacting systems, reveal the key features of complex non-equilibrium phenomena, and eventually gather insights into turbulent reacting flows that will help design novel and innovative modelling approaches. While several methods have been proposed for analysing combustion datasets, their application relies largely on expert knowledge and educated guesses. Unsupervised learning methods can advance our understanding of reacting flows; however, the challenge is to design algorithms able to formulate "questions" and explore new avenues, relying on assessment criteria that can help define whether an outcome is interesting for a given, intended use (e.g. stability limits, emissions, efficiency). **Feature extraction approaches will be extended to incorporate existing physical knowledge,** expressed in the form of conservation principles, via the definition of complex loss functions accounting for low-dimensional reconstruction error and physical constraints.

Feature extraction algorithms coupled to dimensionality reduction will be explored in detail since working in feature space can make the algorithm less sensitive to noise and applicable across different flow conditions[xxxiii]. **Approaches to optimise the topology of the low dimensional manifold will also be developed** [xxxiv], which is a crucial step to create accurate reduced-order models to improve the predictivity of existing state-space combustion models for turbulent combustion simulations.

Research in "topology-free" closures[xxxv], such as reactor-based models, will also be pursued. These models do not make assumptions about the structure of the flame and the potential separation of scales. They have been shown to handle well combustion regimes characterised by very intense turbulence-chemistry interactions and finite-rate chemistry effects, such as diluted combustion modes. **High-fidelity parametric DNS data will be processed using advanced feature extraction techniques and regression models (e.g. NNs, CNNs, etc) to design a new generation of filtered and lower-fidelity modelling approaches**. Priority will be given to formulations that preserve the physics of the problem (for the possibility of constraining the resulting model to known physical bounds) and residuals forms (i.e., using data-driven models only for additive or multiplicative correction terms) compared to black box approaches providing the filtered source terms of state variables directly. The use of non-linear regression approaches, such as Gaussian Process Regression (GPR), Polynomial Chaos Expansion (PCE), Neural Networks (NNs) and Convolutional NNs, appears particularly attractive for this task.

Faster simulations. Several approaches exist to adapt the complexity of chemical mechanisms prior to and during a numerical simulation, However, little effort has been placed in developing data-driven strategies for the selection of optimal generalised closures, DE solvers/tabulation and solution tolerances during a combustion simulation. **CYPHER will push research in fully adaptive models that adjust the comprehensiveness of the chemical mechanism for RSFs, the number of transported species, the turbulent combustion closure, and the numerical solvers and tolerances in Computational Fluid Dynamics (CFD) simulations of complex combustion assets**, depending on the local flow conditions. The main ingredient to make this possible is the development of approaches to process heterogenous data and identify regions with diverse needs in terms of chemistry representation, sub-grid modelling and numerical solution settings. Chemical mechanism reduction and state-space parameterisation, traditionally representing different dimensionality reduction paradigms, will be combined to maximise the computational saving while keeping the model fidelity. Projecting the thermochemical scalars into a feature space using techniques such as PCA[xxxvi] or tabulation methods can significantly reduce the computational intensity of large combustion simulations.

Cyber-physical infrastructures. The combination of simulation and experimental data is a crucial requirement for developing digital twins of complex industrial systems. Indeed, the extensive use of physical sensors in harsh environments such as furnaces is not feasible. **A multi-fidelity approach will be pursued within the network, where simulations of different fidelities (canonical reactors and reactor networks, RANS and LES simulations) are combined to generate reduced-order models for the variables of interest.** The combination of feature extraction approaches based on PCA, NNs and CNNs with non-linear regression will be investigated to map the low-dimensional features to input parameters of interest (fuel composition, operating conditions etc).

Moreover, strategies for updating the DT while in operation will be developed, using Data Assimilation (DA) techniques[xxxvii] and sparse sensing[xxxviii] to adapt the nonlinear mapping between the feature and the input parameter spaces based on available data from experiments and new simulations. **Proper advanced sensing strategies combining optical, chemical and mechanical techniques will be pursued for monitoring and control purposes of combustion in lab-scale devices.** They will be used in the context of data assimilation and fusion, where measurements of different process characteristics and dynamics are combined to generate data on physical variables that may be inaccessible to hardware sensors. Moreover, soft sensors will be implemented on facilities with different levels of complexity to verify their accuracy and robustness. In this context, low-cost sensors for monitoring in large-scale devices and proper soft-sensing strategies for control of RSF combustion will be developed to be integrated into the cyber-physical infrastructure. This approach will **deliver self-**

updating digital twins and contribute to creating integrated cyber-physical infrastructure to design, operate and optimise large combustion systems employing renewable synthetic fuels.

Progress beyond SOA identified above, requires a network with competencies bridging fundamental research in fluid mechanics, combustion science and ML methods with applications of RSFs in energy-intensive industries. This underlines the critical need for a network not only covering the different fields and disciplines of interest for the Action but ensuring the necessary transfer from academic laboratories to industrial applications. With the active participation of the glass and steel industries, CYPHER fulfils this crucial need and can become a living laboratory to drive decarbonisation in EIIs.

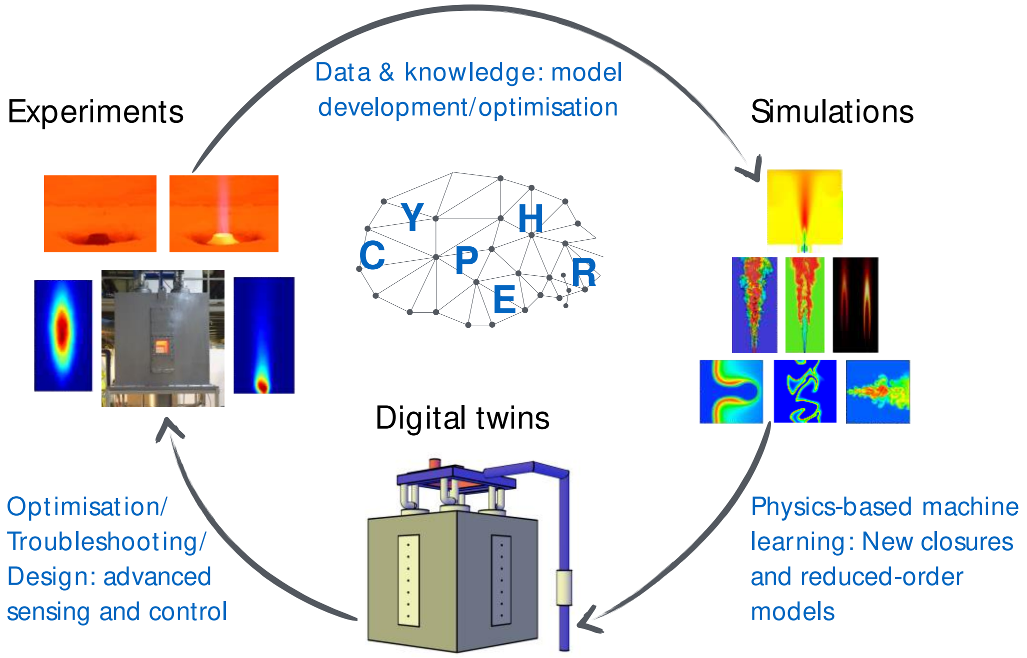


Figure 2 – CYPHER multidisciplinary approach.

1.2.2. OBJECTIVES

1.2.2.1. Research Coordination Objectives

The main objective of the CYPHER Action is to create a European-wide network of high excellence with academic, research and industrial partners capable of addressing the “grand challenge”: decarbonise EIIs through digitalisation. The achievement of this objective will keep European science and technology at the forefront of the world scene. To achieve this, the following Objectives will be pursued:

1) Create an interdisciplinary society of researchers, entrepreneurs, and policymakers to discover and eliminate the barriers to adopting innovative technologies to decarbonise EIIs.
2) Liaise with the industrial partners from the different EIIs to understand their energy needs. Collect data (operational requirements), and coordinate experiments to understand:
    a. the impact of changing a fuel/burner technology on the combustion process taking place in large industrial furnaces;
    b. how stable combustion can be ensured with near-zero emissions for fuel-flexible operation with varying fuel charges;
    c. the impact of changing fuels on the overall process efficiency and the characteristics of the developed products.
3) Coordinate the knowledge being created on combustion properties of RSFs and disseminate it broadly in the form of numerical models, advanced diagnostics to be applied to technological processes design and control, novel infrastructure design, etc.
4) Develop methods to automatically extract the key features from data, which represents a crucial step in advancing the knowledge on RSF combustion and developing better and faster numerical simulation approaches.

5) Develop reliable and affordable numerical simulation approaches using physics-based ML methods relying on high-fidelity data to improve the confidence of variable-fidelity simulations and explore larger design spaces in design and reduced-order model development.
6) Develop self-updating digital twins to predict the impact of RSFs on EIIs systems and integrate them within cyber-physical platforms to understand, optimise, troubleshoot, and improve the design of industrial assets.

1.2.2.2. Capacity-building Objectives

The main capacity-building goals of this Action are to join the excellent researchers working on combustion, fluid dynamics and data science to create synergies between academics, entrepreneurs and policymakers, thereby boosting a focused research and training agenda. The net yield of this Action is, thus, a new research community capable of responding to the challenges of EIIs through innovation and capacity building, including retention of young researchers and innovators in future lines of research stemming from CYPHER. To achieve these goals, the following objectives will be pursued:

1) Decarbonise EIIs through a joint research agenda around digital methods, models, and cyber-physical systems, thereby fostering the EU's "digitally-enabled circular, climate-neutral and sustainable economy".
2) Integrate first-principle models and ML to bring disruptive innovations in fluid mechanics and combustion science, impacting energy-intensive industries and beyond (process and food industry, air quality, etc).
3) Foster the application of RSFs and digital twins in EIIs. Based on the solid implication of industrial partners, the CYPHER Action will act as an incubator of new ideas and inspire entrepreneurial activity around digitalisation for industry decarbonisation.
4) Facilitate scientific collaboration and knowledge exchange by organising and coordinating an open, sustainable, and multidisciplinary network using the Action website.
5) Stimulate the development of a joint research agenda to facilitate the development of new research projects and participation in collective Actions under the three pillars of the Horizon Europe program (excellent science, societal challenge and European industrial competitiveness, and Innovative Europe), focusing on strong cooperation between industry and academia.
6) Offer a balanced vision and expertise to European and national policy-makers by participating in the network as external advisors and by targeted communication measures.
7) Identify and proactively contact new members to enlarge and strengthen the Action Network, promoting fair, diverse and gender equality membership.
8) Enable dissemination of knowledge and research outputs, and opportunities to interact with and learn from other research groups.
9) Mobilise and create awareness amongst Young Researchers and Innovators (YRI), including those from inclusiveness target countries (ITCs), on the problems of EIIs and existing challenges.
10) Promote competitiveness of European academic and industrial partners in the digitalisation of EIIs.

2. NETWORKING EXCELLENCE

2.1. ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1. ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

European and International efforts focus on individual aspects of EIIs decarbonisation, thereby failing to address the problem holistically as proposed in this multidisciplinary COST Action. There is no COST Action or other EU-funded initiative currently running that covers the aimed broad scope of CYPHER.

Decarbonizing EIIs can only be addressed by offering a common platform to discuss ideas, and share knowledge, to enable breakthrough scientific developments leading to new expertise, data, models, and solutions. Such ambitions are far beyond the capacity of a single group or research institution. They therefore must be based upon research collaborations resulting from the international, interdisciplinary and intersectoral interactions between academic partners (universities and research centres), industrial partners including SMEs and partners in R&D-intensive countries with those from ITCs. The CYPHER

Consortium will continue looking for new collaborations with other Near Neighbour Countries (NNCs) and International Partner Countries during the implementation of the Action. Such interactions will be fostered through the CYPHER networking activities (staff exchange through STSMs, Training Schools for PhD students and Early Career Investigators, dedicated workshops and conferences) to keep Europe at the forefront of these areas of research and technology.

The Network of Proposers is highly multidisciplinary, with many academics participating in European programmes and in scientific networks distributed throughout Europe, such as Organizations and Associations or Alliances limited to the local combustion and/or fluid-mechanics communities. The partners will benefit from the knowledge generated through an MSCA DN on generalised hybrid ML-based digital infrastructure. The knowledge created in this area can advance sensing technologies being developed through ERC or Horizon-funded programs covering other aspects related to CYPHER. Members of the network meet complementary research challenges through European and/or national funding programs aimed at developing technologies to produce renewable synthetic fuels sustainably or to combine different methods to improve hydrogen combustion technologies.

The existing networks and projects are often limited to one technology or element of the digitalisation of EIIs when RSFs are used or, when holistic, only superficially address specific problems related to CYPHER. The added value of the CYPHER Action is building a solid pan-European, interdisciplinary network with the geographical spread and critical mass required to tackle existing challenges to the digitalisation of EIIs and the utilisation of RSFs to support their decarbonisation and by coordinating the research of the existing and new projects – comprising ML, new combustion concept and advanced sensing – in which its members are experts.

CYPHER will, thus, leverage existing European initiatives in different related fields to deliver a cohesive/ unified response to EIIs decarbonisation. Access to high-performance computing facilities across the continent is made possible by several projects funded by the Horizon framework programs. CYPHER will collaborate with the consortia and associations as part of the mentioned initiatives to join forces and prevent effort duplicity. This is only possible in coordination and supporting Action such as this COST. The network will enlarge to accommodate the expertise and infrastructure to reach the final objective: strengthen Europe’s capacity to address EIIs decarbonisation challenge.

2.2. ADDED VALUE OF NETWORKING IN IMPACT

2.2.1. SECURING THE CRITICAL MASS, EXPERTISE AND GEOGRAPHICAL BALANCE WITHIN THE COST MEMBERS AND BEYOND

CYPHER is a Pan-European group represented by 33 countries: 18 ITC countries, one international partner (US) and a COST cooperating member (Israel). This inclusive network integrates European leaders in the field and includes researchers from highly to less research-intensive countries. The consortium is committed to achieving gender balance from an already fair distribution, with 60% males and 40% females, and to involve young researchers and innovators, starting with a Network composed of 48.3% YRIs. Overall, the network brings together 31 COST Full Members, promoting the representation from the north, centre, south, east, and west of Europe. This Action comprises 116 Proposers encompassing expertise in fluid dynamics, combustion modelling and experiments, data analysis, and ML. From the list of proposers, 5 are relevant industries for the co-definition to develop innovative technologies, tools and methodologies that are expected to originate a generalised digital infrastructure with application in the different EIIs. Because the success of this Action depends on applying the knowledge in the industry, it is crucial to bring the most representative actors that compose the multitude of EIIs. Thus, as part of this Network, the industrial partners vary from steel makers, energy from waste specialists, burner manufacturers, and metal processing designers.

This structure creates a critical mass of researchers devoted to investigating, advancing, and applying knowledge to solve a significant challenge of transforming the production industry to meet sustainable goals. For the continued evolution of the Action, the Network of Proposes will be open to recruiting new members and experts in the field from all regions of Europe and beyond. Most importantly, recruiting new members will promote diversity and gender equality, with prominence to new members at an early stage of their careers. The network will be organised into five Working Groups (WPs), cf. section 4.

2.2.2. INVOLVEMENT OF STAKEHOLDERS

The Network of Proposers has identified the stakeholders, who are the actors with the potential to exploit the research outcomes, connecting the scientific communities, enterprises, policymakers and society.

1) **Policymakers** are EU and national regulators that work to ensure that industrial processes follow quality and safety standards. Therefore, these will need to be convinced to approve that the outputs of the Action can be translated to industry without imposing harm. The plan to include more policymakers in the Action involves: 1) further identifying relevant policymakers; 2) reaching out to them via diverse channels (email, LinkedIn); 3) communicating and raising awareness about the Action by sharing the website link; 4) inviting them to participate in the activities part of CYPHER and take a relevant role, e.g. provide an informed opinion at meetings and workshops, offer lectures in Training schools; 5) liaising with them in relevant conferences and disseminate the new outcomes of the Action. In the end, the Action expects to have a group of policymakers engaged and supporting the translation of the innovations generated into the industry.

2) **The scientific community** are interested in using the knowledge created in the Action. These are investigators that are mainly involved in research activities. CYPHER will reach academics and researchers, independent of their background, via email and LinkedIn. These will have an interest in the knowledge created to be used and further advance the combustion, fluid dynamics and data science field, as well as with relevance to research other topics: air quality and urban planning, process industry, digital health, aviation, aerospace, etc. The plan to include the large scientific community in the Action involves: 1) further identifying relevant members actively and through networking; 2) contacting them; 3) informing them about the Action and its outcomes; 4) inviting them to participate in workshops, meetings organised by the network of Proposers, training schools and STSMs.

3) **Enterprises** are interested in translating the knowledge created into applications with impact to reduce GHG emissions. Moved by the taxes and sanctions imposed by governments around the world, EEIs are eager to adopt solutions that will help them reduce GHG emissions in a smoother convertible process. Thereby, the Network of Proposers has successfully convinced EIIs to be members of the Action. Still, the higher representation throughout the Action lifetime will be a precise measure of success, as their input is crucial to develop custom-tailored solutions. The plan to include the enterprises in the Action involves: 1) further identifying relevant ones (willing to enter the digital transformation, and which consequently will benefit most from GHG emissions reduction); 2) reaching out to them via email, LinkedIn and conferences to communicate about CYPHER; 3) inviting them to participate in Action organised meetings, workshops, training schools, and receive researchers to learn on the field about their processes (STSMs).

3. IMPACT

3.1. IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

3.1.1. SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

Scientific impact. The CYPHER COST Action will develop a unique platform encompassing a wide variety of researchers from combustion, fluid dynamics and data science and a strong representation of the different sectors that compose the EIIs. This complementary and collaborative network will have a significant scientific impact as it will advance cyber-physical Infrastructure in EIIs by generating scientific knowledge on RSF combustion, data-driven turbulent reactive flow modelling, enhanced sensing, and digital twins, defining new strategies to decarbonise EIIs. A vital element of this Action is coordinating the research efforts to address this COST challenge. Also, as part of the dissemination plan, the knowledge will be spread to the broad scientific community to advance other fields such as air quality and urban planning, process industry, digital health, aviation, aerospace, etc. Thanks to the involvement of the non-academic sector, the knowledge will have real applicability, resulting in a fast passed achievement of the EC goal of net-zero emissions by 2050, hence positioning Europe at the forefront of decarbonising EIIs. The network expects to leverage significantly the number of publications and breakthrough findings, which will be driven by the cross-fertilisation of ideas and research efforts enabled through this COST Action. Hence, the partners expect to double the number of annual publications of high-impact scientific articles stemming from the WGs 1-4 (see section 4.1) and coordinated by their leaders focused on: 1) RSF combustion experimental data; 2) RSF combustion with details on fuel mixtures, operating conditions, and target applications; 3) Strategies to develop hybrid ML-based models adapting the combustion closure to local conditions; strategies for self-updating DT using heterogeneous data sources.

Technological impact. The advances beyond state of the art through CYPHER will have repercussions across the different EIIs (food, pulp and paper, basic chemicals, refining, iron, and steel, etc), aviation, aerospace, and other industries, as well as across value chains: hydrogen, blockchain, ML, and the overall industry. More specifically, the co-definition of the research according to the market needs performed by the Network of Proposers, is aimed at supporting the development of innovative technologies, tools and methodologies that are expected to originate a generalised digital infrastructure with application in the different EIIs, thereby assisting in their transitions to sustainability and net-zero emissions, without impacting production and economic growth. The network envisions two outcomes that will impact industries: 1) hybrid ML approaches for high-fidelity predictions; 2) digital twins to control industrial systems subject to time-varying fuel charges.

CYPHER will enable the advancements of novel combustion technologies to boost decarbonisation and diversification of the energy mix in EIIs with processes that cannot be realistically electrified. Numerical simulation tools, reduced-order models and digital twins that will be made available through the Action can be exploited for the smart retrofit of industrial combustion systems to allow them to handle RSFs, enhancing efficiency without harmful emissions. Nowadays, the operation and design of combustion devices strongly rely on virtual prototyping. However, the urgent need to convert industrial heating furnaces to be fed with green fuels requires technological improvements that cannot be pursued without advanced mathematical models. CYPHER will unlock the potential of cyber-physical infrastructures in industry, providing practical tools for designing and operating sustainable combustion systems.

Socio-economic impact. The CYPHER activities follow the 'Fit for 55' package within the Green Deal, aimed at reaching the CO_2 reduction targets by 2030 to ensure the climate-neutrality. Here, renewable and low-carbon gases, i.e., biogas and biomethane, renewable and low-carbon hydrogen and synthetic fuels, can act as critical players in reaching the climate goals as electrification is not feasible in all EIIs' sectors. The security of the supply of our energy system has become an urgent priority in light of the Ukraine war. This is testified by several Joint European Actions, such as the "REPowerEU" for more affordable, secure and sustainable energy", to make the EU independent from fossil fuels well before 2030. Indeed, one of the two pillars pursues larger volumes of biomethane and renewable hydrogen production and imports. Thus, CYPHER will carry on research and make available data and tools that are crucial in meeting the goals of competitiveness in the energy field in this transition era. The EIIs that can benefit from CYPHER tools are key sectors in the EU, contributing to about 20% of the total value added of manufacturing. Their presence gives an essential competitive advantage to high-tech production.

Digital transformation is generating a fierce debate among policymakers, economists, and industry leaders about its societal impact. As digitalisation disrupts society ever more profoundly, the concern is growing about how it affects issues such as jobs, wages, inequality, health, resource efficiency and security. To better assess the impact of industry digitalisation on society, the World Economic Forum has performed a qualitative analysis resulting in the following three points:

1) **Creating a workforce for the machine age.** Digitalisation could create up to 6 million jobs worldwide between 2016 and 2025 in the logistics and electricity industries. Digital transformation will enable businesses to upskill employees and shape the next generation of talent for the machine age.
2) **Transitioning to a sustainable world.** Digital initiatives in the industries can deliver an estimated 26 billion tonnes of net avoided CO_2 emissions worldwide from 2016 to 2025. This is almost equivalent to the CO_2 emitted by all of Europe across that period. Realising and scaling this potential means overcoming hurdles relating to accepting new, circular business models, customer adoption and the environmental impact of digital technology itself.
3) **Building trust on digital economy.** Digitalisation improves workplace safety by enabling data collection and preventing equipment malfunction. Also, it alerts the operator of possible operational mistakes. Machines have replaced some of the repetitive tasks previously carried out by the human workforce. This has brought health improvements – less chronic injuries and tiredness from repetitive movements. Digitalisation has created higher safety and quality work life for human resources.

3.2. MEASURES TO MAXIMISE IMPACT

3.2.1. KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

To successfully achieve the main aim of decarbonising the EIIs by digitalisation, a coordinated effort is crucial among all Network Proposers and beyond. Due to the complexity and multidisciplinary theme involving chemistry, physics, engineering, and computer science, a collaborative platform for knowledge creation and transfer is vital. As part of the flux of knowledge, this Action will empower researchers to evolve and be recognised for their proven excellence in the form of grants and publications.

Knowledge creation. This Action aims to organise meetings to discuss new advances in the field and to coordinate the research to be implemented by the academic part of this COST to reduce replication of effort, increase focus, and accelerate the production of results. The industry will participate in the meetings to assist in the R&D co-development. STSMs will promote the mobility of researchers to foster a two-way exchange of knowledge and skills.

Transfer of knowledge. This Action aims to organise meetings among WGs, workshops, training schools and attend conferences to facilitate knowledge transfer. The primary vehicles to transfer knowledge will be scientific articles, presentations, and posters to disseminate the knowledge created and make it open and accessible to the whole community. Sharing the participants' knowledge between participating countries and beyond will enable a new generation of researchers to think about their work differently and cross-sectoral.

Career development. This Action will be crucial to empower YRIs and academics from ITC and to establish a good pool of gender-balanced and inclusive members who work as a task force to advance the field while pushing each other to achieve excellence. The network's critical mass will promote unprecedented research collaborations and access to excellent infrastructure not possible without this Action. These opportunities will be crucial for the COST members to gain competencies and enhance their career development by participating in competitive Horizon Europe programmes, receiving grants and publishing high-quality journal papers. Also, the participation of industry and policymakers provides a better overview of the market needs for focused research with higher impact, thereby boosting both individuals' and groups' growth. **The Network of Proposers aims to become the task force that will decarbonise EIIs.**

3.2.2. PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

To maximise the impact of the Action, WG5 will be dedicated to communicating, disseminating, and exploiting (CDE) the results of CYPHER to the relevant target groups. To ensure a proper CDE, the leaders of the WG1-4 will be members of the WG5. They will develop a Communication, Dissemination and Exploitation Plan in the first three months of the Action, which will be updated during the Action. CDE will have specific aims and targeted audiences as described below:

Communication Activities aim at raising awareness about the importance of applying multidisciplinary (chemistry, physics, RSF combustion, fluid dynamics, big data analytics and ML) research to develop sustainable solutions to facilitate a meaningful reduction of energy consumption by EIIs, which has positive implications for the environment, citizens, and society. Importantly, CYPHER will inform the general public about the scientific advances produced in Europe with the support of the European Cooperation in Science and Technology and the European Commission. The Action will take advantage of the CYPHER website, mailing lists, relevant associations, press releases, public talks, science campaigns, and school visits to reach the general public, scientific peers, industry high school students and policymakers about the Action, its challenge and objectives and the expected impacts.

Dissemination Activities aim to present, demonstrate, and provide access to the outcome of the Action. These will be important to the scientific community, policymakers, and industry to gain knowledge on the advances achieved and offer ways to discuss and provide input to progress further. Thus, the Action will take advantage of the meetings, workshops, and training schools organised by the Network of Proposers, the conferences and scientific articles published to disseminate the Action outcomes. The Action aims at consolidating the dissemination activities through scientific publications in open-access and renowned journals and attending several conferences per year in Europe and US. At the same time, a big data repository will be created to increase the visibility of this Action as a unique consolidated framework. Finally, the workshops and training schools will be an opportunity to recruit new members for the Action by inviting them to offer lectures and presentations, reaching a broader audience.

Exploitation Activities aim at using the outcomes of the Action to "use of results in further research and innovation activities other than those covered by the Action concerned, including, among other things, commercial exploitation such as developing, creating, manufacturing and marketing a product or process, creating and providing a service, or in standardisation activities", as per the Model Grant Agreement. Therefore, protecting intellectual property rights on new results is essential. The Network foresees that newly generated results ought to be covered by equitable and fair provisions for the management of their use, ownership, and/or protection under intellectual property rights (patent, trade secrets, licensing). Those provisions may not hinder the communication and dissemination of the COST Action results; each Action Management Committee (MC) shall take the necessary steps, be it by written agreement among the participants or otherwise, to protect these rights.

CYPHER will collect, organise, and share the results obtained at different stages of the Action with the scientific community and relevant industries to exchange know-how and best practices and advance further. The Action Network is comfortable with organising and holding online conferences and meetings. Thus, regular meetings between the different Working Groups will occur online. Still, the Action will have face-to-face events and activities as a priority to engage the whole network and promote discussions, workshops, and training events. CYPHER will, furthermore, foster open access to research outcomes, including FAIR (Findable, Accessible, Interoperable, Reusable) data handling, after assessing and/or protecting the foreground generated in the execution of the Action. The general principle will be to keep research data generated as open as possible and as close as necessary.

4. IMPLEMENTATION

4.1. COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

4.1.1. DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

CYPHER will be composed of five WGs that will work in coordination to implement the Action. Every CYPHER member will participate in at least two WGs. The number of members composing each WG may vary, depending on the effort and expertise required for the successful implementation of the WG. Also, the WGs composition will be periodically assessed by the WG participants. If specific expertise is needed, collaborations within and outside the Action will be actively sought to update the WG composition. The WGs, respective objectives and actions are:

WG1: Renewable synthetic fuels (RSF) combustion. The main goals of WG1 are to accelerate the creation of new knowledge on the combustion properties of RSFs and advanced combustion technologies operating in distributed and diluted (MILD Combustion) conditions and to generate and collect high-fidelity experimental data for the validation and continuous improvement of numerical simulation approaches. **The specific research and innovation objectives of WG1 are:** i) establish protocols to assess the feasibility of RSFs combustion in a broad range of experimental conditions, representative of different industries; ii) implement advanced sensing based on the combination of optical diagnostics and intrusive probes with ML algorithms; iii) characterise specific features and subtleties of hydrogen and hydrogen carriers focusing on kinetic and transport properties, as well as on the interaction of the latter with turbulence. *Tasks (T) and Activities (A):* ***T1.1*** *Identify a roadmap for the integration of RSFs in existing infrastructures;* ***T1.2*** *Establish guidelines for RSF's combustion experiment design and data gathering;* ***T1.3*** *Develop strategies for optimal sensor placement in experiments;* ***T1.4*** *Generate experimental datasets to be exploited by WG3 and WG4;* ***A1.1*** *Coordinate research on RSF's combustion.*

WG2: High-fidelity combustion simulations and data analytics. The main goal of WG2 is to propel knowledge of RSF combustion in distributed and diluted conditions beyond state-of-the-art using high-fidelity simulations, providing a virtual framework for lower-fidelity model development and validation. WG2 will focus on the acceleration of reacting flow solvers relying on models able to adapt to the local flow conditions. **The specific research and innovation objectives of WG2 are**: i) high-fidelity CFD models of combustion systems representative of different industries ii) develop unsupervised algorithms for the identification of coherent regions in RSFs' combustion flow fields; iii) exploit and combine dimensionality reduction paradigms to alleviate the computational intensity; iv) generate appropriate datasets for the subsequent low-fidelity model development of WG3 and multi-fidelity data integration of WG4. *Tasks (T) and Activities (A):* ***T2.1*** *Create a collaborative library of high-fidelity numerical models for RSF's combustion simulation;* ***T2.2*** *Identify, develop and implement unsupervised algorithms for state-space clustering and classification;* ***T2.3*** *Assess the validity and accuracy of adaptative strategies for the on-the-fly model choice/reduction;* ***T2.4*** *Generate variable-fidelity datasets to be exploited by WG3 and WG4;* ***A2.1*** *Organize an annual meeting on numerical methods for high-fidelity simulations of RSF's combustion, mainly oriented to the scientific community.*

WG3: Hybrid physics-based data-driven models. The main goal of WG3 is to promote the hybridization of first principles and data-driven approaches to design and calibrate physics-aware and physics-constrained models, exploiting the heterogenous data streams from WG1 and WG2. **The specific research and innovation objectives of WG3 are**: i) parametrise with higher accuracy and more efficiently sub-grid quantities of interest in the simulation of realistic combustion systems ; ii) design computationally affordable simulations of advanced combustion technologies combining state-space parametrisation and rate-based methods to explore a large number of operating conditions; iii) develop reduced-order models for specific quantities of interest in the combustion of RSFs (I.e., pollutant emissions, stability limits, efficiency). *Tasks (T) and Activities (A):* ***T3.1*** *Retrieve data from heterogeneous sources, e.g., WG1 and WG2;* ***T3.2*** *Develop methods to identify low-dimensional* *manifolds and optimise their topology;* ***T3.3*** *Design and calibrate ML-based models incorporating physics in the loss functions;* ***T3.4*** *Assess model discrepancies, interpretability, explainability and generalisability against available data;* ***A3.1*** *Organize periodic workshops on physics-based data-driven methods for RSF's combustion.*

WG4: Digital twins and cyber-physical systems. WG4 aims to propel the creation of self-updating digital twins to build cyber-physical infrastructures across different industrial segments, which can predict and control the impact of RSF on EII combustion systems, e.g., design efficiency, stability, pollutant emission, fuel flexibility, and burner efficiency. **The specific research and innovation objectives of WG4 are:** i) develop linear/non-linear techniques to map high-fidelity numerical simulations into feature spaces that preserve most of the original data information; ii) design approaches to update and continuously improve the digital twin based on newly available data from both experiments (from WG1) and simulations (from WG2 and WG3); iii) design advanced soft-sensing strategies based on the integration of digital twins and traditional measurement techniques to enhance the sensing opportunities in industrial assets. *Tasks (T) and Activities (A):* ***T4.1*** *Implement methods for multi-fidelity data fusion to combine heterogeneous information from the network into a Digital Twin of a complex system;* ***T4.2*** *Develop strategies to assimilate data from operating systems at low cost/impact;* ***T4.3*** *Develop an integrated framework for self-updating Digital Twins of large combustion systems;* ***T4.4*** *Coordinate the efforts of WG1, WG2, and WG3 towards optimal experimental/numerical design;* ***A4.1*** *Identify and reach out to enterprises who are willing to exploit solutions tailored on DTs;* ***A4.2*** *Organize a meeting on digital industrial solutions, oriented to enterprises and policymakers.*

WP5: Communication, Dissemination, Partnering with industry and policymakers. The main goal of WG5 is to promote internal communication within the Network (amongst WGs and the MC) and beyond the Network (general public, industry, policymakers, etc). **The specific outreach goals of WP5 are:** i) coordinate the design and development of the CDE plan, and ii) facilitate the fulfilment of the objectives of the CYPHER COST by creating fluent and efficient communication channels among the Action participants and the society. *Tasks (T):* ***T5.1*** *Set up and maintain a website as a dissemination and internal communication platform;* ***T5.2*** *Create a professional social media account (e.g., LinkedIn and Twitter) to keep professional stakeholders updated about the Action;* ***T5.3*** *Develop communication material (posters, abstracts, QR code for links to website info) appropriate and adjusted to the event and each group of stakeholders;* ***T5.4*** *Coordinate the publication of reviews, protocols, scientific articles, white papers, etc;* ***T5.5*** *Organise round table discussion with Network members and policymakers to clarify the aim of the* Action *and provide updates;* ***T5.6*** *Organise annual conference and identify potential new members to be invited and integrated into the* Action*;* ***T5.7*** *Coordinate the organisation of training schools (in close collaboration with WGs 1-4);* ***T5.8*** *Coordinate the organisation of STSMs.*

4.1.2. DESCRIPTION OF DELIVERABLES AND TIMEFRAME

#	Description	Type*	Diss.**	Month
D1.1	Roadmap for the integration of renewable synthetic fuels in existing energy-intensive industry infrastructures.	R	PU	M18
D1.2	Guidelines for the implementation of renewable synthetic fuels in combustion experiments and data collection.	R	PU	M18
D1.3	Report on strategies for optimal sensor placement in experiments and integration between physical and soft sensors.	R	CO	M30
D1.4	Report on renewable synthetic fuel combustion experimental data in various laboratory and industrial-like configurations.	R	CO	M48
D2.1	Report on unsupervised algorithms for the optimal local selection and simplification of modelling approaches.	R	CO	M24
D2.2	Collection of high-fidelity simulation data on renewable synthetic fuel combustion in a wide range of operating conditions.	Other	PU	M48
D3.1	Report on low-dimensional manifolds identification and topology optimisation for constructing reduced-order models.	R	CO	M18
D3.2	Position paper on hybrid physics-aware data-driven models for renewable synthetic fuel combustion.	R	PU	M48
D4.1	Report on multi-fidelity data fusion for the construction of self-updating digital twins	R	CO	M12
D4.2	Position paper on strategies to assimilate data from operating systems at low cost/impact	R	PU	M30
D4.3	Position paper on self-updating digital twins and cyber-physical infrastructures of large combustion systems	R	PU	M48

D5.1	Publication of the Action website, detailing its aim and objectives as well as the networking opportunities.	DEC	PU	M3
D5.2	Publication of the LinkedIn page to highlight and showcase the Action accomplishments, the organised events and the opportunities for networking.	DEC	PU	M3
D5.3	Report on the Action plan for communicating, disseminating, and exploiting the results of the Action.	R	PU	M6

** **R** = Document, report; **DEM** = Demonstrator, pilot, prototype, plan designs; **DEC** = Websites, patents filing, press & media actions, videos, etc.; **OTHER** = Software, technical diagram, etc. ** Dissemination Level: **PU** = Public, fully open, e.g. web; Or **CO** = Confidential, restricted under conditions set out in Model Grant Agreement*

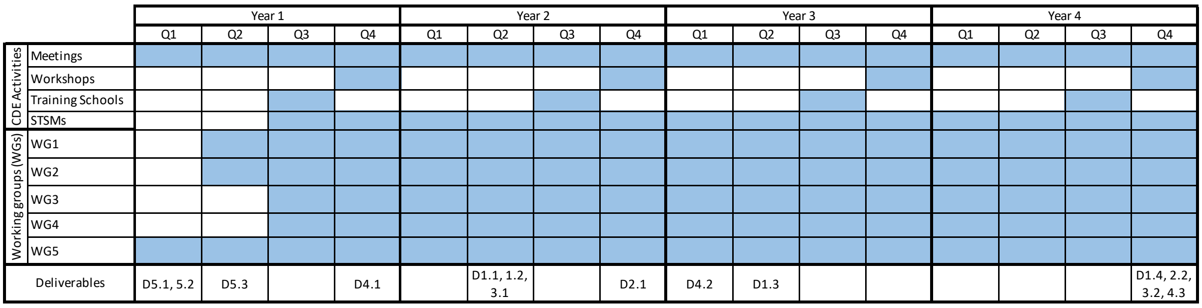
4.1.3. RISK ANALYSIS AND CONTINGENCY PLANS

The Network of Proposers has assessed and listed the possible risks and this COST Action will implement the following contingency measures:

RISK DESCRIPTION	**CONTINGENCY PLAN**
Not reaching expected inclusive and gender balanced network participation	CYPHER includes 116 members covering all areas of expertise. The intention is to expand this initial number to involve all relevant stakeholders and to balance the gender distribution further. The partners will not only prioritise the search and recruitment of female members to balance the equation but also that members come from ITCs.
Lack of cooperation among different WGs.	The MC will organise annual presential and monthly/quarterly virtual meetings to promote the interaction amongst WGs. The virtual meetings will require the participation of all members of the WGs, or at least with the main proposers.
Difficulty in achieving research objectives on time	In case of delay in achieving one or several research objectives, the WG leader will report to the MC, which will convey if it can be resolved within the Network of Proposers or requires external help/ expertise.
Unsatisfactory scientific results.	Work plan adaptation by WG leaders and MC while searching for alternative methods: consulting both CYPHER colleagues and external peers.
Low impact of communication and dissemination.	Proactive interaction with stakeholders, coordinated by the WG leaders to create measures and activities for efficient communication and dissemination.
Lack of funding to develop collaborative research programmes	Some of the initiatives arising from newly established collaborations might not find financial support to be developed. The mitigation plan requires the WG leaders to actively search for public and private agencies to which the CYPHER members might apply.

In addition to these risks, the WGs leaders will actively identify, analyse, and manage other potential risks that might hinder the implementation of CYPHER. Risk evaluations will be addressed during the WG meetings, and contingency plans to avoid or mitigate those risks will be developed during the Action. Risk analysis and contingency plans will be reported to the MC.

4.1.4. GANTT DIAGRAM



		Year 1				Year 2				Year 3				Year 4			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
CDE Activities	Meetings	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	Workshops				■				■				■				■
	Training Schools			■				■				■				■	
	STSMs			■	■	■	■	■	■	■	■	■	■	■	■	■	■
Working groups (WGs)	WG1		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	WG2		■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
	WG3			■	■	■	■	■	■	■	■	■	■	■	■	■	■
	WG4			■	■	■	■	■	■	■	■	■	■	■	■	■	■
	WG5	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
Deliverables		D5.1, 5.2	D5.3		D4.1		D1.1, 1.2, 3.1		D2.1	D4.2	D1.3						D1.4, 2.2, 3.2, 4.3

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