EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on
Fuel Cells and Hydrogen technologies (JP FCH)

IMPLEMENTATION PLAN 2018 - 2030

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Endorsed by:

Summary of the *Joint Programme on Fuel Cells and Hydrogen technologies*

The overall objective of this Joint Programme (JP) is to align medium to long term pre-competitive research activities at EERA institutes and associated institutions to create a technical-scientific basis for further improvement of Fuel Cells and Hydrogen (FCH) technologies and to guarantee enduring cutting-edge competence in Europe in the mid-long term. Though commercialisation of FCH technologies has started all across the world, there is still a necessity to make a quantum leap in terms of lifetime and costs. To find adequate and viable solutions long-term research is highly needed. In this JP we aim to highlight the main areas where long-term research activities will help these technologies to reach breakthroughs towards larger markets, to explore the possibilities for joint European technology development, and identify and exploit the potential synergies therein in order to enhance the deployment and commercialization of fuel cells and hydrogen technologies.

The added value of JP FCH is the possibility to become of strategic importance in defining the research agenda for the next phase of fundamental and break-through research in this field. This commitment is exemplified in the present Implementation Plan (IP) for the 2018-2030 period. The aim is to use this document as a basis for the discussion of a structural framework for the support of integrated programmes on long-term research in alignment with industrial requirements for enduring commercialization of Fuel cells and Hydrogen technologies. Furthermore, thanks to and using this IP as a reference, more specific reference documents can be issued concerning very basic, breakthrough and long term research pointing out priorities, main topics, required funds.

The joint programme focuses on fuel cell and water electrolyser issues and related electrochemical aspects, in addition the Hydrogen sub programmes deal with non-electrochemical hydrogen production, hydrogen handling and hydrogen storage. The sub programmes are:

SP1 Electrolytes
The Sub-Programme Electrolytes mainly deals with developing new generations of high performance, low cost and durable electrolyte materials for low and high temperature fuel cells and electrolysers. Activities are harmonised with other SPs, and in particular with SP2 on Catalysts and Electrodes, to develop an integrated mid and long term research programme combining expertise from experimental approaches and computational modelling. Synergies are sought between research organisations for the rational use of facilities, exchange of students and researchers, exchange of materials and information.

SP2 Catalysts & Electrodes
The sub programme targets the development a new generation highly active, low cost and durable catalysts/electrodes. This is addressed by identifying requirements of each electrochemical process which defines the type of electrode to be used. By harmonising activities with other SPs, a rational support and catalyst design is achieved, combining expertise from computational models and experimental approaches. Besides, synergies are achieved by sharing facilities which are available in the EERA laboratories to address specific problems and to investigate rate determining steps for the processes involved in low, intermediate and high temperature fuel cells, electrolysers and regenerative cells.

SP3 Stack Materials and Design
The sub programme concentrates on issues that allow the cost effective manufacturing of 'robust' stacks. The latter term denoting stacks that can be rapidly thermally and load cycled and that can tolerate a defined degree of 'mistreatment' in the form of vibration, transient operation, fuel and air impurities etc. The issues encountered are very much focused on materials and novel design development and, although related to a goal of successful product engineering, specifically concern basic research in materials, materials processing, and component design.

SP4 Systems
This sub programme deals with developments made on both a system level and a component level. The system level approach includes development of innovative fuel cell system concepts,

while for the function/components level general targets will be decreased costs of components, prolonged life-time and availability of components.

SP5 Modelling, Validation and Diagnosis

The sub programme aims at reaching better understanding of the degradation mechanisms and the relationships with operating conditions. It also includes a more detailed development of mathematical descriptions of phenomena to be used in the prediction of performances and lifetime. To improve data input to the modelling and verification of models, specifications of experimental development of accelerated aging tests will be given.

SP6 Hydrogen Production and Handling

The sub programme concentrates on researching and developing cost effective and efficient non-electrochemical hydrogen production methods by improving catalysts and materials, identifying novel approaches, optimising materials processing, and developing new, break-through designs for hydrogen production systems. The SP is also involved in the development and implementation of new Codes and Standards related to the aforementioned technologies, and strengthens the cooperation between the groups involved by promoting staff and student exchanges.

SP7 Hydrogen Storage

The sub programme focuses on research, development and optimization of application integration of different technologies for hydrogen storage: a) compressed gas from low pressures up to 700 bar and more, b) liquid hydrogen, c) hydrogen carriers, i.e. solid state based hydrogen storage in metal hydrides, porous materials and irreversible hydrides. Combinations of different technologies are also considered, e.g. cryo-compressed hydrogen storage or compressed hydrogen – solid state hydrogen storage. Activities are focused on the following topics: a) materials development and characterization for tank hulls, e.g. metals, polymers, composites; b) materials for hydrogen carriers, both in solid and liquid state; c) hydrogen tank system development, including thermal management and gas control devices; d) integration of hydrogen stores with applications in the fields of hydrogen production, hydrogen transport and hydrogen use, as such as well as for conversion to electrical energy by fuel cells. Like in all SPs, SP7 is involved in the development and implementation of new Codes and Standards related to the aforementioned technologies, and strengthens the cooperation between the groups involved by promoting staff and student exchanges.

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Background

As an integral part of the effort to tackle climate change, the European Union (EU) has set ambitious goals to drastically cut the greenhouse gas (GHG) emissions towards 2050. New energy technologies play a key role in this effort, and their further development is crucial for meeting the targets of reducing GHG emissions by 20% by 2020 and >80% by 2050.

The Strategic Energy Technology (SET) Plan constitutes EU's framework and agenda for how to address these challenges including long-term energy research. Fuel Cells and Hydrogen are explicitly mentioned in the SET-plan as key technologies to reach the goals.

Fuel Cells and Hydrogen technologies have been utilised for decades, initially for space applications in the 1960s, but during the 1990s the passenger vehicle market became the main driver for technology development. Stationary fuel cell applications, providing combined heat and power (CHP), constitute another main driver, due to high efficiency and modularity.

Around the turn of the millennium several car manufacturers announced mass production of hydrogen powered Fuel Cell Electric Vehicles (FCEVs). Technological progress was slower than foreseen, as both cost and durability of the fuel cells for vehicle propulsion were still unsatisfactory. The year 2003, however, marked the start of defining the strategic research agenda, as the High Level Group (HLG) launched their Vision Report[1].

Early markets for hydrogen technologies are currently emerging, in areas such as remote telecommunication towers, fuel cells for forklifts and critical load facilities. These markets are expected to feed in to further technology development with time, and facilitate cost reduction needed to enter other and larger market segments.

The Hydrogen Europe Industry Grouping represents the European Industry Initiative (EII) in this field. In March 2008, the European research community joined forces and established the Hydrogen Europe Research Grouping (formerly N.ERGHY), currently counting close to 70 member institutions with an overall number of researcher exceeding 2000. In October 2008, the European public-private partnership entitled Fuel Cells and Hydrogen Joint Undertaking (FCH JU) was officially launched and FCH JU became autonomous in 2010.

Over the last decade, we have witnessed significant technological progress in fuel cell and hydrogen technologies. However, there is a consensus in industry and academia that significant long term research is still needed to realise the foreseen commercialisation of mobile, stationary, portable, and micro application, as for instance passenger cars and buses, micro-CHP, decentralised power plants, battery replacers, and a variety of mini and micro products ranging from mobile phone charging up to medical implants, as well as being crucial in making large-scale renewable energy storage feasible by improving the power-to-hydrogen chain in terms of efficiency and cost effectiveness, which will also be a key development in the coupling of strategic infrastructures such as the power grid, gas grid and transportation networks.

The continued need for ground-breaking research even when a technology turns into a mass market commodity is testified for by today's large number and broad range of research activities for motor vehicle engines – which, as a technology – were invented around 150 years ago and are one of the foremost drivers of the world economies. This research continuously improves the technology performance and its cost competitiveness, and takes care of all the environmental issues connected to it. The same can for example be said for food processing (a history of some ten thousands of years) or, more recently, mobile phones and smart phones, that are established technologies but still not at the end of the innovation process.

[1] Special Report: Hydrogen Energy and Fuel Cells - A Vision for Our Future (2003).
Available at: http://www.fch-ju.eu/page/documents

Value added of the JP FCH

The Joint Programme on Fuel Cells and Hydrogen (JP FCH) provides the strategic leadership in defining the agenda for the next phase of fundamental and break-through research in this field.

With the establishment of the Fuel Cells and Hydrogen platform and, subsequently, of the Joint Undertaking (FCH JU) the prioritisation of activities related to fuel cells and hydrogen technologies has been given to industrial stakeholders. The consequence is that most of the research within FCH JU is product/demonstration oriented, whereas basic or long term research is not at focus. The EERA partners strongly believe that long term research is still needed (see above), and thus we here lay out our vision of the JP FCH with the idea of assembling and focussing a critical mass of research capabilities.

The JP FCH gathers the competence, knowledge and the research infrastructures of major European research centres and Universities to substantially improve the cooperation on common strategic topics between national research institutes and universities, by collectively planning and implementing a joint research programme. The JP will be open to all European academic institutions and research organisations. We especially encourage universities to participate in the activities. We have identified electrochemical energy conversion in Fuel Cells and Electrolysers as a suitable area for starting the definition of a joint research programme. This is appended by other technologies for hydrogen production and will be further developed as the initiative matures.

Acknowledging that more than 90 % of the European R&D budgets are provided at national level, the JP FCH will aim at aligning and harmonising national activities, sharing Research Infrastructures (RI) and establishing trans-European expert groups representing the leading competence in each field of research. To speed up the realisation of the SET-plan goals the JP will also coordinate its actions with the other JPs, such as AMPEA, Energy Storage, Smart Grids, Bioenergy, and Concentrated Solar Power, with the aim to share the definition of common topics with them so that each JP will perform part of the activities, and in such a way avoid overlapping and encourage synergies.

Objectives of the JP FCH

The general objective of the JP FCH is to align medium to long term pre-competitive research activities at EERA institutes and associated institutions to create a technical-scientific basis for further improvement of Fuel Cells and Hydrogen technologies. The JP aligns and explores synergies with (i) the research grouping Hydrogen Europe Research (ii) the European public-private partnership FCH JU, and (iii) other JPs. Most of the partners involved in the present JP are also members of FCH JU.

FCH JU revised its Multi Annual Working Plan (MAWP) in 2012 and 2017, setting new very ambitious targets for 2020 and 2030. Our goal will be to contribute to the 2030 targets and beyond, accelerating the development and deployment of fuel cells and hydrogen technologies by promoting the involvement and the cooperation of national research institutions and universities. Moreover, the JP FCH has the ambition to strengthen European competitiveness enabling industry to bring fuel cell and hydrogen technologies to the market.

The JP FCH is broken down into seven sub programmes, with the following leaders and thematic objectives:

SP1 Electrolytes (Deborah Jones, CNRS – Vito Di Noto, University of Padova)
The Sub-Programme Electrolytes mainly deals with developing new generations of high performance, low cost and durable electrolyte materials for low and high temperature fuel cells and electrolysers. Activities are harmonised with other SPs, and in particular with SP2 on Catalysts and Electrodes, to develop an integrated mid and long term research programme combining expertise from experimental approaches and computational modelling. Synergies are

sought between research organisations for the rational use of facilities, exchange of students and researchers, exchange of materials and information.

SP2 Catalysts & Electrodes (Peter Holtappels, DTU – John Irvine, University St. Andrews)
This sub programme targets the development a new generation of highly active, low cost and durable catalysts/electrodes. This is addressed by identifying requirements of each electrochemical process which defines the type of electrode to be used. By harmonising activities with other SPs, a rational support and catalyst design is achieved, combining expertise from computational models and experimental approaches. Besides, synergies are achieved by sharing facilities which are available in the EERA laboratories to address specific problems and to investigate rate determining steps for the processes involved in low, intermediate and high temperature fuel cells, electrolysers and regenerative cells.

SP3 Stack Materials and Design (Nikolaos Margaritis, FZJ – Marie-Laure Fontaine, SINTEF)
This sub programme concentrates on issues that allow the cost effective manufacturing of 'robust' stacks. The latter term denoting stacks that can be rapidly thermally and load cycled and that can tolerate a defined degree of 'mistreatment' in the form of vibration, transient operation, fuel and air impurities etc. The issues encountered are very much focused on materials and novel design development and, although related to a goal of successful product engineering, specifically concern basic research in materials, materials processing, and component design.

SP4 Systems (Asif Ansar, DLR – Jari Kiviaho, VTT)
This sub programme deals with developments made on both a system level and a component level. The system level approach includes development of innovative fuel cell system concepts, while for the function/components level general targets will be decreased costs of components, prolonged life-time and availability of components.

SP5 Modelling, Validation and Diagnosis (Mathias Gérard, CEA – Martin Andersson, Lund University)
Sub programme 5 is transversal to the others. It aims at reaching better understanding of the physico-chemical process, at different scales, from the catalyst material to the system level, and also to provide numerical tools for material optimization, design optimization, architecture and control validation. The lifetime estimation and mitigation is one of key objective It also includes a more detailed development of mathematical descriptions of phenomena to be used in the prediction of performances and lifetime. Both approach, bottom-up and top-down is developed. The development of a multi-scale methodology is also a key point to the success of this sub-program. To improve data input to the modelling and verification of models, specifications of experimental development of accelerated aging tests will be given.

SP6 Hydrogen Production and Handling (Robert Steinberger-Wilckens, Univ. Birmingham – Asuncion Fernández, CSIC)
This sub programme concentrates on researching and developing cost effective and efficient non-electrochemical hydrogen production methods by improving catalysts and materials, identifying novel approaches, optimising materials processing, and developing new, break-through designs for hydrogen production systems. The SP is also involved in the development and implementation of new Codes and Standards related to the aforementioned technologies, and strengthens the cooperation between the groups involved by promoting staff and student exchanges.

SP7 Hydrogen Storage (Marcello Baricco, University of Turin – Klaus Taube, HZG)
This sub programme focuses on research, development and optimization of application integration of different technologies for hydrogen storage: a) compressed gas from low pressures up to 700 bar and more, b) liquid hydrogen, c) hydrogen carriers, i.e. solid state based hydrogen storage in metal hydrides, porous materials and irreversible hydrides. Combinations of different technologies are also considered, e.g. cryo-compressed hydrogen storage or compressed hydrogen – solid state hydrogen storage. Activities are focused on the following topics: a) materials development and characterization for tank hulls, e.g. metals, polymers, composites; b) materials for hydrogen carriers, both in solid and liquid state; c) hydrogen tank system development, including thermal management and gas control devices; d) integration of hydrogen

stores with applications in the fields of hydrogen production, hydrogen transport and hydrogen use, as such as well as for conversion to electrical energy by fuel cells.

The JP FCH Implementation Plan 2018-2030

The objectives and activities in this JP relate to long-term research. These are based on the idea of taking advantage of results that are publicly available and can be shared by the partners, and the drive to generate the maximum impact from these results by aligning future regional, national and European programmes in the field in order to promote further collaboration in structured funded frameworks.

The main points of reference in this context are the frameworks for Research & Development in Europe: **Horizon 2020** and **Horizon Europe**. Especially in this stage of deployment of the first commercially available systems, it is crucial that fundamental research activities are encouraged and guided in order to guarantee the necessary pace of development of Fuel Cells and Hydrogen technologies to keep up with the evolving market. This document serves to present a convincing and concrete action plan as regards the contribution of the EERA research community towards effective and large-scale implementation of FCH technologies by 2030 and beyond.

In the following, the research goals, action plans and priorities for the period 2018-2030 (according to the JP FCH) are broken down according to the seven sub-programmes described above. Each of these areas of competence has specific needs and priorities that need to be addressed through a systematic and concerted approach. The key items that must define each of these approaches are described in detail for each sub programme.

This Plan in its current form (version 4.0), complete with key performance indicators (KPIs) for the monitoring of progress and achievements in the research topics proposed, has received the endorsement and significant contributions from Hydrogen Europe Research, the Research Pillar of the Fuel Cells and Hydrogen Joint Undertaking.

Infrastructures and facilities

The *H2FC European Research Infrastructure*-project was granted support from the FP7 Capacity-programme. The initiative was led by Karlsruhe Institute of Technology (KIT), and incorporated 19 European research institutions, some of which are also partners in the JP FCH. *H2FC European Research Infrastructure* gathered a joint European effort for enhanced utilisation of facilities. By mapping the needs and identifying gaps, this framework formed the basis for involving more laboratories in agreement and close collaboration.
H2FC European Infrastructure generated a structured and integrated alliance based on complementary, state-of-the-art, or even beyond state-of-the-art, unique infrastructures to serve the needs of the scientific hydrogen and fuel cells community and facilitate future research:

- a single integrated virtual infrastructure to accommodate hydrogen and fuel cell communities' test and analysis facilities.
- transnational access for the hydrogen and fuel cell research communities to member state infrastructures.
- expert working groups to enhance work at the provided facilities and to seek more general coordination in the aspects of safety, performance and durability.
- central databases and libraries of safety, performance and durability data and codes http://www.h2fc.eu/files/downloads/public_deliverables/D4.4_H2FC_vers.1.1%20draft.pdf
- coordinated education and training, pertinent to the set-up, use and maintenance of hydrogen and fuel cell research, test and assessment facilities.

H2FC European Infrastructure as a funded project ended in November 2015, which forced the web-based platform to go off line. The main outcomes of the project are contained in the Deliverables and Reports that are available through the SESAM pages of the European Funding & Opportunities Portal.

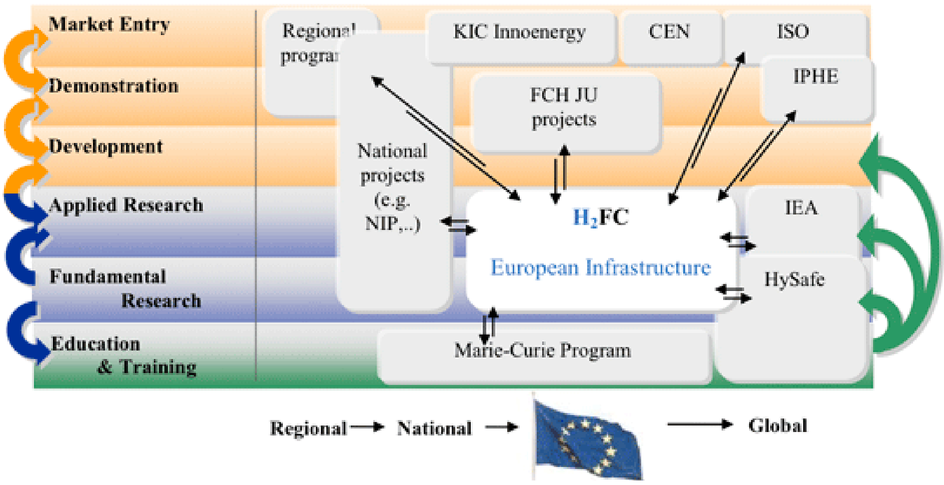

Figure: Positioning of the project H2FC European Infrastructure

The EERA JP FCH organised a joint public workshop together with *H2FC European Infrastructure* in April 2015 (at the Royal Flemish Academy of Belgium for Science and the Arts in Brussels) to present the outcomes of the former's research implementation plan and the latter's assessment of research infrastructures and bottlenecks.
Since *H2FC European Infrastructure* there have been sporadic initiatives to recuperate and build on the vast work done by the FP7 project. Lack of opportunities within H2020 to gain funding for this has paired with a major focus of the FCH community (research as well as industry) towards the Fuel Cells and Hydrogen Joint Undertaking (FCH JU, http://fch.europa.eu/), the public-private technology initiative that manages the budget for development and deployment of hydrogen and fuel cells in Europe. This platform has been particularly successful in bringing these technologies to market entry, over the course of 13 years of intensive collaboration, aligned advocacy and market focus. This has led to a highly valuable portfolio of studies, interest groups, partnerships, roadmaps, policy papers and results. However, no opportunity has materialised for generating a comprehensive, online database of research infrastructures.
Within EERA, further attempts to create a network of infrastructures were initiated, one of which gained funding within the 2016 Horizon 2020 Call on European Common Research and Innovation Agendas (BALANCE, Grant Agreement 731224) but which focuses mainly on a survey of stakeholders and research programmes across the EU Member States. Nevertheless, it appears that the EERA JP FCH would be the right environment where these databases of research infrastructures should be born and nurtured, possibly in collaboration with Hydrogen Europe Research, the research pillar of the FCH JU.
The FCH JU has recently established a platform for gathering information and data from all the funded projects (TRUST) which forms the basis for a future instrument for management of open access data.

Interface with other JPs

Five other EERA JPs have been identified with potential overlaps with this FCs&H2 JP. Clearly defined interfaces with these will be established, to avoid duplication of activities and foster complementarities and synergies. The interfaces towards these 5 JPs and management thereof are described in the Table below:

Interface with JP	Interface description	Interface Management
AMPEA	Materials development and characterization, relevant for all but SP4 of JP FCH	Interfaces have been discussed in a face-to-face meeting with the coordinators of the three first JPs mentioned above. The agreement is to exchange
Smart Grid	System aspects, BoP component development, mainly concerning power conditioning, diagnostic and	

	control, interconnection between FC system and the grid primarily relevant in SP4 of JP FCH	DoW between JP and to have, on regular basis (annual), either teleconferences or physical meetings to check the right alignment of the JPs.
Energy Storage	Hydrogen storage, Solid state storage, material development. H2 Handling (improved compression and liquefaction) H2 Safety, Codes and Standards	
Bioenergy	Hydrogen production from Biomass/Biological waste and Algae	A similar approach of interface management as the one described above will be taken for the potential overlap with these 3 JPs.
Concentrated Solar Power	Hydrogen production from solar energy, Thermolysis and Photocatalysis	
CCS	Use of FCs for CO_2 separation from flue gases	

In the definition of objectives and activities of each SP of JP FCH we have taken into account the above mentioned areas of possible overlap as far as this has been possible.

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Joint Research Programme on
Fuel Cells and Hydrogen technologies (JP FCH)

SUB-PROGRAMME 1: *Electrolytes*

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

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1. Background

Electrolytes are at the core of fuel cells and electrolysers. General requirements of electrolytes include low area resistance, high ionic conductivity (proton, hydroxide ion, oxygen ion) and mixed ionic-electronic conductivity for non-galvanic electrolysers, under target operating conditions (temperature, pressure, relative humidity), chemical, mechanical and thermal stability, processability, low cost. In addition the electrolyte must impede the direct cross-over of fuel.

Advances in polymer based systems can be achieved by increasing the temperature range of operation and accessing lower cost materials both for membranes and catalysts. Alternative systems can also capitalise on the advantages of alkaline (anion i.e. OH^- ion), conducting material. Such membranes replace the liquid alkaline electrolyte and offer advantages of reduced costs and high efficiency.

Advances in solid oxide systems will come about by the development of new materials with increased ionic conductivity at lower temperatures, thanks to basic studies on structure-related properties and on defect equilibria under strongly reducing or oxidising conditions in fuel cell or electrolysis mode. Besides investigation of new materials, the thin film electrolyte deposition is also an emerging and highly active field of research. If the electrolyte thickness is reduced, new designs for the electrode/electrolyte structure are needed including, porous electrolyte functional layers.

Furthermore bridging the temperature gap between polymer and solid electrolytes could lead to radically new fuel cell and electrolyser concepts. For the use of synfuels such as dimethylether, ethanol but also ammonia, a temperature region between 200-400 °C is highly attractive, because it should allow good materials stability, fast reaction kinetics, and controllable heat recovery for a wide variety of application, but still this gap requires specific electrolyte developments.

Over recent years considerable progress has been made in the development of electrolyte materials for high and low temperature fuel cells and electrolysers. Materials development in the field of low temperature fuel cell membranes has largely benefited from improved understanding of mechanisms leading to membrane failure, however no equivalent effort has yet been engaged for membranes used in proton exchange membrane water electrolysis, and the field of electrolysis using anion exchange membranes is in its infancy. For high temperature oxide fuel cells using ceramic electrolyte membranes, there is a need to associate theoretical and experimental approaches enabling the breakthrough development of electrolytes associating stability and high conductivity. Activities in this sub-programme should include the evaluation of current and frontier approaches, and development of novel strategies with innovation for Europe for fuel cell and electrolyte membranes. Progress is needed in the development of electrolyte membranes associating the durability requirements specific to any given application, as well as satisfying the material conductivity and membrane resistance targets.

2. Objectives

Research efforts in electrolyte development must accompany the push to increase the temperature of operation of polymer based cells, and to lower that of solid oxide cells, while providing required high stability of performance and durability compatible with the target application. Research should encompass development of durable, high performance and low cost electrolytes for polymer-based, solid oxide, and proton conducting ceramic systems required for mid to long term development of fuel cell and electrolyser technologies. Additionally, bridging the temperature gap (200-500 °C) between polymer-based and oxide-based electrolytes could lead to radically new fuel cell and electrolyser concepts. Research activities will include development of novel ionomers and polymers, and membranes using advanced and novel polymer types with nanoscale control of structure and function, novel processing methods, advanced membrane architectures. The critical need to increase thermal stability of anion exchange membranes will be addressed. Research must specifically target association of both chemical and mechanical stability of polymer electrolyte membranes to guarantee adequate lifetime and propose strategies to combat premature degradation. Activities on the development of ionomers for the catalyst layer are also required. Progress in the above can be made by addressing the following key topics:

- Fundamental understanding of transport processes in fuel cell and electrolyser membranes using experimental and computational approaches
- Improved understanding of degradation processes in electrolyte materials during operation, and approaches to mitigate degradation and loss of properties
- Elaboration of new electrolyte materials and architectures with control at the nanoscale, and thin film electrolyte deposition methods
- Electrolytes for the membrane-electrode interface
- Validation of electrolytes by incorporation in membrane electrode assemblies, resulting in robust solid electrolytes for proton exchange, anion exchange and oxide fuel cells. Considerations of scale-up, durability, cost effectiveness.

3. Description of foreseen activities

Research in the area of electrolytes targets the ion-conducting materials required for all temperature ranges, and for electrolyser and fuel cell applications. The scope of work includes, inter alia, new conducting anion conducting, solid oxide and proton conducting electrolytes, high temperature proton exchange membranes and composite membranes, improved processing methods, increased understanding of degradation mechanisms and the use thereof to develop more robust and durable electrolytes, and the validation of materials' performance and durability using accelerated ageing protocols. The development of fundamental understanding of ion and water transport processes is an integral part of SP1.

Risks and mitigation strategies

1. Validation of membranes in complete cells can be achieved using commercial electrodes but should rapidly build upon progress in SP2 for added value.
2. Critical mass in each of the technologies and temperature ranges is present in Europe and can be assembled under EERA to provide a research push.

Topic 1.1: Fundamental understanding of transport processes in fuel cell and electrolyser membranes using experimental and computational approaches

Fuel cell and electrolyser cell electrolytes are complex materials in which chemical composition, structure and morphology, surface and interfacial properties determine the overall behaviour and properties, and where the cell environment (temperature, relative humidity) plays a critical role on performance and durability. Improved understanding of ion and water transport processes in polymer and ceramic membranes is required, as well as new and improved techniques to characterise electrolyte materials and their interfaces (solid-liquid-gas).

Objectives:

- Develop computational and experimental tools and methodologies for improved description of transport and diffusion processes in ion-conducting fuel cell and electrolyser membranes, including ionic species, water, solvents, contaminants, fuel, air, oxygen.
- Develop computational and experimental tools and methodologies for an improved understanding of microstructure of ion-conducting fuel cell and electrolyser membranes and its impact on properties
- Develop temporally and spatially resolved techniques for the characterization of fuel cell and electrolyser electrolytes

Expected Outcomes:

- Improved description of membrane microstructure and its impact on membrane properties
- Improved understanding of the impact of membrane composition and structure on undesired crossover (contaminants, fuel)
- Greater use of central synchrotron and neutron source facilities by the EERA FCH community for investigation of electrolytes

- Improved knowledge base in fundamental understanding of transport phenomena in proton, anion, oxygen ion conducting electrolytes

Topic 1.2: Improved understanding of degradation processes in electrolyte materials during operation, and approaches to mitigate degradation and loss of properties

Motivation:
Electrolyte degradation leads to catastrophic cell failure and must be mitigated through better understanding of the phenomena leading to membrane thinning/cracking/perforation, the interrelation between chemical and mechanical instability, and the implementation of specific strategies to offset known degradation mechanisms. This area is dependent on the generation of fundamental understanding, the use of which in implementation of mitigation strategies has huge technological impact.

Objectives:
- Identify the origins of premature membrane failure in fuel cells and electrolysis cells, and develop improved understanding of chemical degradation pathways in polymer membrane materials in acidic and alkaline fuel cells and electrolysis cells. This understanding should be derived from investigations of membrane materials both ex situ and in situ, and with consideration of the various interactions between cell components
- Improve understanding of the interrelation between chemical and mechanical instability in fuel cell and electrolysis membranes
- Develop diagnostic tools to predict the occurrence of membrane catastrophic failure
- Develop characterization techniques and methodologies allowing detailed chemical structural and morphological level understanding of degradation phenomena
- Develop robust accelerated ageing methodologies adapted for high/low temperature acidic/alkaline polymer membranes, solid oxide cells, electrolysis cells for general use within the EERA community, FCH-JU and beyond
- Develop tools and methodologies to investigate the fate of radical scavenger and peroxide decomposition catalysts incorporated in fuel cell membranes, or at the interface with the electrode
- Develop low-cost and scaleable materials-based strategies for robust electrolyte membranes
- Develop numerical modeling and simulation tools in support of the above

Expected Outcomes:
- Series of technology-specific protocols to accelerate ageing/reduce lifetime of fuel cell and electrolysis cell membranes
- Identification of operation regimes critical for individual fuel cell/electrolyser technologies
- New characterization and diagnostic tools and methodologies
- Increased understanding of degradation pathways and their operation condition dependence
- Knowledge-based strategies for stabilization of fuel cell and electrolyser membranes
- Improved models for degradation pathways

Topic 1.3: Elaboration of new electrolyte materials and architectures with control at the nanoscale, and thin film electrolyte deposition methods

Motivation:
New polymer, ionomer, proton and anion conductors, new proton conducting and oxide ion conducting ceramics are required for improved performance/durability and to extend the achievable temperature range of operation upwards (for "low" temperature fuel cells/electrolysers) and downwards (for "high" temperature fuel cells/electrolysers). The temperature region 200-450 °C is an opportunity to combine the advantages of polymer and ceramic technologies and requires research for a viable solid electrolyte. Europe has a strong expert research base and industrial groups that can integrate new findings into product portfolios.

Objectives:

- Develop new types of anion and proton conducting polymer materials to enable their operating temperature ranges to be extended upwards, and satisfying applications-led proton conductivity requirements over a broad temperature range
- Widen understanding to enable development of oxide ion and proton ceramic electrolytes extending the range of fuel cell/electrolyser operation temperature downwards
- Develop radically new approaches to proton conducting materials filling the temperature "gap" 200-450 °C, with consideration of associated processing methods
- Assess new electrolyte membrane (polymer, ceramic) chemistries, designs and architectures providing smarter, adaptive materials-based solutions to performance loss over time
- Develop experimental and modeling tools and methodologies for the detailed characterization of membranes and ceramic electrolytes, in situ and operando
- Develop new processing and methods for thin film electrolyte deposition
- Validate new membranes in complete cells against accepted benchmark materials
- Propose and implement novel means to limit fuel crossover in direct-liquid fuel cells

Expected Outcomes:

- Radically new membrane materials offering a step-change improvement in target properties
- Membrane materials demonstrating promise that they align with industry long-term objectives for automotive and stationary fuel cells, and electrolysers
- Thin, mechanically robust and chemically stable membranes providing high conductivity at low relative humidity, over a broad temperature range
- Highly conducting and long-term stable proton ceramic electrolytes 400-600 °C
- Novel selective membranes for crossover-free direct alcohol fuel cells
- New electrolyte materials for applications in the range 200-450 °C.

Topic 1.4: Electrolytes for the membrane-electrode interface

Motivation:

Little is known and understood about the specific properties required of the binder used in the electrode, and at the interface between membrane and electrode, of PEMFC and PEM electrolysers. Generally the same ionomer is used as in the membrane, while different properties are required (conductivity, oxygen permeability, mechanical properties etc.) Furthermore, research on development of hydrocarbon based binders for proton exchange membrane cells is in its infancy, PFSA ionomers being generally used to bind hydrocarbon membranes to electrodes. In the field of anion exchange membranes, research on electrolytes for the membrane-electrode interface is even less advanced. Mixed ionic/electronic conductors provide an opportunity that has been insufficiently explored for PEMFC.

Objectives:

- Prepare a report on the international state of the art, on-going funded investigations, opportunities
- Fundamental study of the three phase boundary
- Develop improved understanding of the properties required for a functional efficient ionomer in polymer membrane cells, including by computational methods
- Develop characterization techniques, rheology and permeability tools, and experimental protocols for electrolyte binder, and AFM methods for ionomer morphology characterisation
- Improve understanding of ageing and degradation phenomena undergone by polymer binders during cell operation
- Investigate preparative and processing routes to new binders for proton and anion exchange membranes
- Develop catalyst inks incorporating new ionomer materials and processing methods for their implementation in electrodes
- Develop methods for the characterization of ionomer distribution in a catalyst layer
- Benchmark complete cells incorporating new binders against current products in order to validate the new approaches

- Investigate mixed ionic-electronic conductors for use at the interface of cells incorporating a polymer membrane
- Develop numerical tools for micro-structure optimization. Virtual electrode structuration by simulation

Expected Outcomes:
- New generations of hydrocarbon binders adapted for anion exchange and functionalised polyaromatic hydrocarbon electrolysis and fuel cells
- Improved PFSA binders with adapted properties
- Improved understanding of the possible benefits in the use of mixed ionic electronic conductors in low temperature cells
- Novel processing methods for binder dispersions
- Improved understanding of the degradation/ageing effects specific to the electrolyte at the membrane/electrode interface, and mitigation strategies

Topic 1.5: Validation of electrolytes by incorporation in membrane electrode assemblies, resulting in robust solid electrolytes for proton exchange, anion exchange and oxide fuel cells

Motivation:
Integration of new membrane (polymer, ceramic) materials into Europe's fuel cell industry requires that they be validated under practical and realistic operation conditions and compared with state of the art reference MEAs and cells; this is essential to ensure the credibility of the results. This validation should include performance and durability considerations. Assessment is also required of the feasibility of industrial scale-up and should include a preliminary evaluation of costs.
This topic includes considerations of scale-up, manufacture, durability, cost effectiveness.

Objectives:
- Link with SP2 Catalysts and Electrodes for optimal added-value
- Investigate the electrical performance of complete cells (ceramic) and MEAs (polymer membrane) operating in fuel cell or electrolysis mode, and perform parametric studies to determine influence of cell operation variables on cell performance, and comparison with reference cells measured under the same conditions
- Apply internationally recognised accelerated stress tests, including those that may be developed in Topic 2, to assess the durability of new electrolyte materials compared with the state of the art
- Develop and apply diagnostic tools to complete cells operating with new electrolytes, to assess state of health
- Perform preliminary assessment of costs and compare with incumbent approaches
- Carry out preliminary study of the feasibility of scale-up, including considerations of the scaleability of the synthesis approach and processing steps, and toxicity, in particular with regard to chemicals and solvents used in the preparation of electrolyte materials, during processing, and for elaboration of membranes.

Expected Outcomes:
- Proof-of-concept for new electrolytes in ceramic cells and MEAs
- Transferable results for scale-up and prototyping

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

<u>Topic 1.1: Fundamental understanding of transport processes in fuel cell and electrolyser membranes</u>

<u>Rationale</u>: Improved understanding of ion and water transport processes in polymer and ceramic membranes. New and improved techniques to characterise electrolyte materials and their interfaces.

Specific Challenges	Expected outcome	KPIs	Technoogies suited	Possible Project Title	Priority	Budget M€
Develop computational and experimental tools and methodologies for improved description of transport and diffusion processes in ion-conducting fuel cell and electrolyser membranes, including ionic species, water, solvents, contaminants, fuel, air, oxygen.	Improved fundamental understanding of transport processes in fuel cell and electrolyser membranes using experimental and computational approaches, improved description of membrane microstructure and impact on properties	Spatial resolution of the characterization of the transport processes: nanometric (5-200 nm); temporal resolution of the characterization of the transport processes: seconds (experimental measurements)*	Low-temperature FC & Electrolyser technologies	Understanding of ion transport in composite systems comprising polymeric matrices and inorganic nanostructures**	1	7
				Broadband electrical spectroscopy (BES), MRI, synchrotron and neutron scattering techniques applied to temporal and spatial investigation of chemical and transport proporties of polymer-based systems	2	5
Develop computational and experimental tools and (spatially and temporally resolved) methodologies for an improved understanding of microstructure of ion-conducting fuel cell and electrolyser membranes	Greater use of central synchrotron and neutron source facilities by the EERA FC H2 community for investigation of electrolytes		All FC & Electrolyser technologies	Understanding of ion transport in multiphasic oxide conductors	1	7
				Broadband electrical spectroscopy (BES), MRI, synchrotron and neutron scattering techniques applied to temporal and spatial investigation of chemical and transport	2	5

and its impact on properties				proporties of oxide-based/ceramic systems]		

* Here it is necessary to use techniques achieving a spatial resolution that is good enough to detect the events associated to ion transport (e.g., in polymeric systems, the alterations in the mesoscale domain structure, whose characteristic size falls in the reported range). The transients affecting the operation of FCs/ELs typically fall in the seconds scale (unless triggered by external disturbances in the electric load; however, this is an engineering issue that falls outside the scope of this document), hence this it the timescale that is to be elucidated. Computational studies can achieve a much higher time resolution; however, computational results must be validated experimentally.

** Inorganic systems with more complex features than simple "fillers". These are "inorganic nanostructures" (e.g., functionalized zeolites or 2D materials).

<u>Topic 1.2: Improved understanding of degradation processes in electrolyte materials, mitigation</u>

<u>Rationale</u>: Electrolyte degradation leads to catastrophic cell failure and must be mitigated through better understanding of the phenomena leading to membrane thinning/cracking/perforation, the interrelation between chemical and mechanical instability, and the implementation of specific strategies to offset known degradation mechanisms

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Identify the origins of premature membrane failure in fuel cells and electrolysis cells, and improved understanding of chemical degradation pathways in polymer membranes, from investigations of materials ex situ and in situ, and with consideration of the various interactions between cell components. Improve understanding of the interrelation between chemical and mechanical instability	Improved understanding of degradation processes in electrolyte materials during operation ; knowledge-based strategies to mitigate degradation and loss of properties	Spatial resolution of the characterization of the transport processes: nanometric (5-200 nm); temporal resolution of the characterization of the transport processes: seconds (experimental measurements) Accelerated ageing must require no more than 1/10th of the time of regular ageing.	Proton-conducting LT fuel cells and electrolysis cells	Degradation study of proton conducting ceramic based electrolyte materials (in particular in high pressure electrolysis mode): both over long time and in cycling	1	7

Diagnostic tools to predict the occurrence of membrane catastrophic failure. Robust accelerated ageing methodologies adapted for high/low temperature acidic/alkaline polymer membranes, solid oxide cells, electrolysis cells for general use within the EERA community, FCH-JU and beyond.			All cells	Development of in situ diagnostic tool sensors for monitoring of membrane degradation	1	11
Characterization techniques and methodologies allowing detailed chemical, structural and morphological level understanding of degradation phenomena.			All cells	Broadband electrical spectroscopy (BES), MRI, synchrotron and neutron scattering techniques applied to temporal and spatial investigation of chemical and transport upon accelerated ageing	2	11
Tools and methodologies to investigate the fate of radical scavenger and peroxide decomposition catalysts incorporated in fuel cell membranes, or at the interface with the electrode			All cells	Development of in situ diagnostic tool sensors for monitoring of electrolyte degradation	1	11

Low-cost and scaleable materials-based strategies for robust electrolyte membranes			Low-temperature cells	Development of improved chemical and mechanical stabilisation routes for polymer membrane; Validation in MEAs using AST and benchmarking against SoA	1	6

Topic 1.3: New membrane materials and thin film electrolyte deposition methods

Rationale: New polymer, ionomer, proton and anion conductors, new proton conducting and oxide ion conducting ceramics are required for improved performance/durability and to extend the achievable temperature range of operation. The temperature region 200-450 °C is an opportunity to combine the advantages of polymer and ceramic technologies and requires research for a viable solid electrolyte. Europe has a strong expert research base and industrial groups that can integrate new findings into product portfolios.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
New types of anion and proton conducting polymer materials to enable their operating temperature ranges to be extended upwards	Elaboration of radically new electrolyte materials and architectures with control at the nanoscale and offering a step-change improvement in properties, and extending the temperature range of operation.	Area-specific resistance in operating conditions: 0.025 Ω cm2. Maximum crossover of fuels and oxidizers: 2 mA/cm2.	AEM, AFC	Develop stable alkaline exchange membrane for water electrolysers and fuel cells	1	14
Widen understanding to enable development of oxide ion and proton ceramic electrolytes extending the range of fuel cell/electrolyser operation temperature downwards			Intermediate T FC	Develop nanoporous oxide thin films materials as new proton conducting electrolyte for intermediate temperature	1	7
Proton conducting materials for 200-450 °C, with consideration of associated processing methods			all HT FC and electrolysers	Investigate possibility of additive manufacturing to produce high surface area electrolyte	2	4
			all FC and EC	Proton conducting materials for 200-450 °C range	2	3

New electrolyte membrane chemistries, designs and architectures providing smarter, adaptive materials-based solutions to performance loss over time			LT FC and EC	New electrolyte membrane chemistries, designs and architectures providing smarter, adaptive materials-based solutions to performance loss over time, including scale-up considerations	1	7
New processing and methods for thin film electrolyte deposition			All FC and EC	Up-scaling of physical vapor deposition technique for thin electrolyte films	1	7
Low-cost and scaleable materials-based strategies for robust electrolyte membranes			Low-temperature cells			

Topic 1.4: Electrolytes for the membrane-electrode interface

Rationale: "Little is known and understood about the specific properties required of the binder used in the electrode, and at the interface between membrane and electrode. Generally the same ionomer is used as in the membrane, while different properties are required (conductivity, oxygen permeability, mechanical properties etc.) Furthermore, research on development of hydrocarbon based binders for proton exchange membrane cells is in its infancy. In the field of anion exchange membranes, research on electrolytes for the membrane-electrode interface is even less advanced. Mixed ionic/electronic conductors provide an opportunity that has been insufficiently explored for PEMFC.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Fundamental study of the three phase boundary	Tailored electrolytes for the membrane-electrode interface, novel processing methods for binder dispersions,	The adoption of the innovative binders must give rise to single-cell devices of the appropriate type whose performance and durability	Low-temperature fuel cells and electrolysers	Improved ionomers for the membrane electrode interface : properties, preparation, processing routes, characterisation techniques and	1	5
Improved understanding of the properties required for a functional efficient ionomer						

<table>
<tr><td>Characterization techniques, rheology and permeability tools, and experimental protocols for electrolyte binder, and AFM methods for ionomer morphology characterisation</td><td rowspan="7">improved understanding of degradation effects specific to the electrolyte at the interface</td><td rowspan="7">are higher by at least 25% in comparison with single-cell devices mounting “conventional” state-of-the-art binders.*</td><td rowspan="7"></td><td rowspan="2">tools</td><td rowspan="2"></td><td rowspan="2"></td></tr>
<tr><td>Preparative and processing routes to new binders for proton and anion exchange membranes</td></tr>
<tr><td>Understanding of degradation phenomena undergone by polymer binders during cell operation</td><td rowspan="5">Catalyst inks incorporating new ionomer materials, investigation of degradation phenomena of polymer binders during cell operation</td><td rowspan="5">2</td><td rowspan="5">5</td></tr>
<tr><td>Catalyst inks incorporating new ionomer materials and processing methods for implementation</td></tr>
<tr><td>Methods for the characterization of ionomer distribution in a catalyst layer</td></tr>
<tr><td>Benchmark cells incorporating new binders against current products to validate the new approaches.</td></tr>
<tr><td>Investigate mixed ionic-electronic conductors for use at the interface of cells incorporating a polymer membrane</td></tr>
</table>

* It would be advisable that the performance and durability targets of the innovative binders taken on their own are at least the same as those for the electrolytic membranes; at the three-phase boundaries, the environmental conditions are harsher and degradation may be promoted by the electrolcatalysts themselves. It is likely to be difficult to determine whether a given binder is acceptable or not with studies carried out only on the binder on its own. The only really practical approach is to use the “new” binder in the fabrication of a single-cell device, and make sure that such device exhibits an improved performance and durability in comparison with “reference” state-of-the-art systems. Since here we consider several types of different devices, improvement is expressed in relative, percentage terms. Actually, the most relevant figure is not pure performance, but durability. It could possibly be sufficient if the single-cell device built with the new binder exhibits an improved durability in comparison with reference systems, on the condition that performance is not degraded in comparison with the state of the art.

Topic 1.5: Validation of electrolytes in MEAs under practical operation conditions with benchmarking of performance and durability, including cost-effectiveness

Rationale: Integration of new membrane (polymer, ceramic) materials into Europe's fuel cell industry requires that they be validated under practical and realistic operation conditions and compared with state of the art reference MEAs and cells; this is essential to ensure the credibility of the results. This validation should include performance and durability considerations. Assessment is also required of the feasibility of industrial scale-up and should include a preliminary evaluation of costs. This topic includes considerations of scale-up, manufacture, durability, cost effectiveness.
This Topic is closely affiliated to the Validation Topics in SP2 and SP5, and should be implemented synergically.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Investigate the electrical performance of complete cells (ceramic) and MEAs (polymer membrane), and parametric studies to determine influence of operation variables on performance	"Validation of electrolytes by incorporation in membrane electrode assemblies, resulting in robust solid electrolytes for proton exchange, anion exchange and oxide fuel cells. Proof-of concept for new electrolytes and transferable results for scale-up and prototyping.	The adoption of the innovative electrolytes must give rise to single-cell devices of the appropriate type whose performance and durability are higher by at least 25% in comparison with single-cell devices mounting “conventional” state-of-the-art binders.	All	Long time performance of novel materials	1	5
Apply internationally recognised accelerated stress tests, including those that may be developed in Topic 2, to assess the durability of new electrolyte materials compared with the state of the art				Validation of novel electrolytes from topics 1.2 and 1.3 under appropriate ASTs (as integral part of those projects)	1	5
Develop and apply diagnostic tools to complete cells to assess state of health				Establishment of open access database for fuel cells and electrolysers long term test data: available for providing and exchanging dataset	1	5
Perform preliminary assessment of costs and compare with incumbent approaches						

Preliminary study of the feasibility of scale-up, including scaleability of the synthesis approach and processing steps, and toxicity, in particular with regard to chemicals and solvents used in the preparation of electrolyte materials, during processing, and for elaboration of membranes.				Scaling up of technology combined with techno-economics : include possibility for reuse of materials	2	3

Topic	Main Outcome	Nr. projects	Budget (M€)
1.1	Fundamental understanding of transport processes in proton, anion and oxide ion conductors and their relation to electrolyte membrane microstructure	4	24
1.2	Improved understanding of electrolyte membrane degradation phenomena and approaches to mitigate degradation and loss of properties	5	46
1.3	Next-generation membrane materials: beyond the limits of current electrolytes through knowledge-based research	6	42
1.4	Improved electrolytes for the membrane-electrode interface	2	10
1.5	Validation of electrolytes in MEAs under practical operation conditions with benchmarking of performance and durability, including cost-effectiveness.	4	18
Total		**21**	**140**

5. Contact Point for the sub-programme on Electrolytes

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EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on
Fuel Cells and Hydrogen technologies (JP FCH)

<u>SUB-PROGRAMME 2: *Catalyst and Electrodes*</u>

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

Contact persons:

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1. Background

Fuel cells (FCs) and electrolysers (ECs) are electrochemical devices in which performance is much related to the electrode materials, in particular the catalysts, which determine the efficiency for energy and hydrogen production, respectively. Much effort has been invested in reducing noble metal catalyst loading and maximizing electrochemical utilization by e.g. using different support materials and improving the coating procedure. In addition, significant improvement in the catalyst activity (at the anode and/or cathode) has been achieved when tuning electro-catalyst by using e.g. multi-component catalyst surface, where one of the components (metal or non-metal) might act as co-catalyst.

However, todays fuel cell and electrolyser systems still suffer from far too high costs, insufficient lifetime and dynamic operation capability, which can only be partly addressed at the system level. Materials used in low (viz. 80 – 200 °C) and high temperature (viz. 600 – 900 °C) electrochemical cells up to now still do not allow to fully utilize the advantages of electrochemical cells. For instance, the catalysts frequently used in low temperature fuel cells and electrolysis cells are very expensive, especially if they are based on noble metals. To reduce cost without sacrificing efficiency and improve long term stability new materials are still needed in order to make electrochemical cells a competitive technology for electricity supply and hydrogen or other synthetic energy carrier production in the future.

The materials research devoted to the catalyst and electrodes should span from optimization of single materials properties or specific fabrication processes to the development of new types of materials to allow for new type of cells. Examples for the later are e.g. Unitized Regenerative Fuel Cells (URFCs), which alternatively generate, store and re-use energy (being hydrogen as energy vector), as well as so called intermediate temperature (IT) cells, making a temperature range between 200 – 600 °C accessible, which could lead to simplified systems, use of cheaper materials as cell components and in the whole system concept. In this regard, a new frontier of research for intermediate temperature solid oxide fuel cells concerns with the direct oxidation of bio-fuels (e.g. bioethanol, glycerol), alcohols and hydrocarbons. Of relevant interest for portable and assisted power units, applications are the electro-catalysts for direct methanol and ethanol fuel cells. Equally relevant is the development and integration of electrocatalysts and electrodes for micro-fuel cells devices (without polymeric membrane) based upon laminar flow concepts.

2. Objectives

Progress in the area of catalysts and electrodes can be made by addressing the following key topics:

- Fundamental understanding of FC&EC electrochemical processes (including oxygen reduction and fuel oxidation reactions, water oxidation and reduction) and degradation mechanisms.
- Determination of material properties and their inter-relationship for fuel cell and electrolysis operation, like the active surface area
- Computational assisted design of tailor-made electrodes, catalyst and supports. Modeling of electrode reactions and material transport.
- Development, adaptation and optimization of material synthesis processes to achieve tailor-made catalyst (electrodes, catalysts and supports) properties.
- Electrode engineering to integrate and optimize electrodes (catalysts and supports) into cell architectures.
- Investigation of new electrochemical processes involving alternative fuels (alcohols, biofuels, low molecular weight hydrocarbons).

These Topics form an integrated development loop of course considering particular operation modes (fuel cells/electrolysis) and conditions (temperature) and can be considered an iterative process. Based on already identified problems or gaps, new materials will be suggested and promising candidates synthesized. The development of relevant fabrication processes and the proof of concept on technically relevant scale are the subsequent steps in this cycle, which then can in principle start again with the in depth characterization of the new type of catalyst/electrode.

However, considering significant scientific overlap and to open up for more synergies between the various electrochemical cells, research topics are in the following described according to the key topics described above and spanning over low / high and intermediate temperature systems for both fuel cells and electrolysis cells.

3. Description of foreseen activities

The research in the area of catalysts and electrodes mainly targets development of a new generation highly active, low cost and durable catalysts and electrodes for fuel cells and electrolysis cells. The proposed materials research spans from fundamental understanding to design and fabrication strategies, which should be tightly linked together. In order to achieve this challenge it is necessary to establish a concomitant work that links the expertise of each SP participant for achieving improved catalysts and electrodes.

Risk and Mitigation strategies:

1. Electrode/catalyst development is very sensitive area regarding IPR, and thus exchange of information and personal can be a problem that hinders progress in this sub-program. IPR agreements should help to overcome this.
2. Integration of new materials (concepts) into cells may be challenging and require unforeseen additional competences beyond the partner's in that SP. In case of bottlenecks active search for additional partners or associates is considered to mitigate this problem.

Topic 2.1: Fundamental understanding of FC & EC electrochemical processes and materials

Electrodes/electrocatalysts in fuel cells and electrolyser cells are usually multifunctional materials in a complex environment (catalysts, supports, porous structures, gas-solid-liquid interfaces), which to date are not yet fully understood. While catalytic activity of non-noble metal catalysts is an issue for low temperature systems, the electrode processes at elevated temperatures are still not well understood. New analytical techniques are needed to better characterise materials and interfaces, and thus be able to correlate materials chemistry, morphology and functionality.

Objectives:

- Gain a better comprehension of the relationship between catalyst/electrode chemical nature and its activity (specific targets identified) under relevant and clearly defined operating conditions. This addresses single materials (e.g. catalysts core-shell structures) but also materials combinations (e.g. catalyst support interactions at various temperatures and atmospheres) and especially interfaces (electrode–electrolyte interface). This understanding should lead to:
- Identify performance limiting steps and lifetime limiting processes, and how they correlate with structural parameters, chemical and electronic properties of materials and interfaces.
- Optimize catalyst and electrode properties for the electrochemical reaction considered, i.e. oxygen reduction, fuel oxidation, and water oxidation and reduction.

Expected Outcomes:

- New characterization techniques allowing in-situ or in-operando investigation of catalyst surfaces and interfaces (incl. local polarization phenomena) to follow chemical, electronic and structural properties during operation.
- Identification of critical operation regimes for the individual fuel cell and electrolysis technologies.
- Quantitative models for electrode degradation.
- Strategies to accelerate long-term testing depending on individual fuel cell and electrolysis technologies.
- Normalized tests to assess the electrocatalyst/electrode performance.

- Knowledge-based design/quest for more active, selective and stable catalysts and material combinations for electrodes.

Topic 2.2: Design of tailor-made electrodes, catalyst and supports

Current electrode materials for PEMFCs and SOFCs seemed to be agreed on to be noble metals and Ni-cermets/rare earth perovskites, respectively. Even though developed up to high performance and several thousands of hours stability, costs and life time targets are not yet reached with state-of-the-art (SoA) electrode materials. Especially for low temperature fuel cells cost targets cannot be met with current noble metal based catalysts even at reduced loading. Here new, cheaper materials have to be searched for including new catalyst designs (e.g. nano, core-shell structures, non-precious metal catalysts (*NPMC*s), functionalized carbons, three-dimensional - hierarchically structured - porous carbons, etc.). Another strategy is optimizing the utilization of noble metal catalysts by integration in advanced electrode structures with favoured transport and turnover rates. For established alkaline electrolysis, load cycling remains an issue and new concepts based on gas diffusion electrodes are considered advantageous in this respect. New types of electrolysis cells based on new electrolyte materials (e.g. anion conducting membranes) are in an early development state and do need the development of new, adapted electrodes. The same holds for intermediate temperature cells, both fuel cells and electrolysis cells, (e.g. on proton conducting electrolytes) for which suitable electrode materials are still missing. Whereas proton electrolyte membrane water electrolysers require efficient supported mixed noble metal oxides anodes with good activity and stability to operate at high current density in a wide operating potential window (up to 1.8-2 V RHE).

Objectives:

- Develop and implement a systematic approach to design new materials for fuel cells and electrolysis cells (e.g. using computational materials design/DFT calculations/high throughput screening). This can be used further to tune catalyst and support properties (structure/reactivity/stability) to be adapted to specific electrochemical process and applied operation conditions.
- Assess of new catalyst designs and electrode architectures.
- Alternative support materials to improve stability and catalyst utilization with respect to carbon based.
- Develop electrode materials for new/advanced electrochemical cells.

Expected Outcomes:

- Suggestions for NPMCs (at least one alternative to Pt-based catalysts should be identified) for low-temperature FCs and ECs.
- New electrode structures with improved noble metal utilization
- Systematic computer assisted approach models describing different catalyst and support compositions and architectures.
- New electrodes for intermediate temperature cells (200 – 600 °C).
- Long-term stable and robust electrodes for ceramic based fuel cells.
- Bifunctional electrodes for unitized regenerative fuel cells.
- Novel anode electrocatalysts for the direct utilization of hydrocarbons at intermediate temperatures fuel cells.
- Reduced noble metal loading anode electrocatalysts for the direct oxidation of methanol/ethanol at low temperature.

Topic 2.3: Adapting catalyst synthesis for tailoring catalyst properties

New catalyst designs and electrode materials might require also new manufacturing processes to supply the materials on a technically relevant scale and competitive costs. Advanced fabrication includes for instance the synthesis of supported OER electrocatalysts with low noble metal content and of nano-structured catalyst for alkaline membrane electrolysers, as well as core shell type structures in low temperature cells. Electrodes in high temperature cells are today activated by a so-called impregnation process (like a wash coat for automotive exhaust catalysts), which is sometime hard to be controlled. Recent research addresses alternative methods to form nano sized catalysts in porous ceramic cells, the so called exsolution process, which is not yet fully explored to date. Thin-film techniques are also often discussed in the frame of electrode designs. Such and most likely other new processes need to be developed further to be sufficiently controlled for up-scaling.

Objectives:

- Explore and develop new fabrication processes for tailor-made electro catalysts and electrode materials. This will take either already existing routes up to a technically relevant level or include the search for alternative fabrication techniques in cases where no known principle can be applied for.
- Include appropriate quality assurance throughout the process. The fabrication processes should preferably by environmentally friendly, low-cost, fast and with low energy usage.

Expected Outcomes:

- Development of novel inorganic and organic electro catalysts based on e.g.: (a) Wet Chemistry (WC); (b) Sono-electrochemistry (SE); (c) Flame Spray Pyrolysis (FSP); (d) Physical Vapour Deposition (PVD).
- Synthesis of supported ORR and OER electro-catalysts with low noble metal content.
- Nano-structured catalysts for proton conduction and alkaline membrane electrolysis.

Topic 2.4: Materials integration, electrode design and fabrication

The performance of functional materials does not only depend on the materials properties alone, but also on the effective integration of the materials into a suitable structure. This is of particular importance if multi functionality has to be maintained as for electrodes: electrochemical activity, mass transport ability, electronic conductivity and mechanical integrity. In particular, this topic is relevant for micro-fuel cells based upon lateral flow. At the end a working electrode for either fuel cell or electrolysis cell has to pass a proof of concept including the demonstration of its manufacturability.

Objectives:

- Realize and characterise advanced electro-catalysts and electrodes by developing and optimizing their processing method. This includes the optimisation of manufacturing parameters (e.g. ink composition, three-dimensional electrodes).
- Develop new manufacturing techniques. The performance of the cells needs to be evaluated by investigating as much as functional aspects as possible (e.g. electrocatalytic activity, fuel efficiency, transport (water / gas, conductivity) on a technically relevant scale.

Expected Outcomes:

- Proof of concept for new electro-catalysts and electrodes
- Proof of concept for nano structured electrode designs (catalyst dispersion, thin film architectures, nano-composites)
- Proof of concept of new fabrication processes
- Optimize preparation methods for electrode inks
- Optimize solvent-free preparation technique for electrodes
- Optimize deposition techniques
- Development of methods of quality assurance

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

<u>Topic 2.1: Fundamental understanding of FC & EC electrochemical processes and materials</u>

<u>Rationale</u>: Electrodes usually multifunctional materials in a complex environment. New analytical techniques are needed to better characterise materials and interfaces. Better understanding is required of the correlation materials chemistry, morphology and functionality.

<table>
<tr><th>Specific Challenges</th><th>Expected outcome</th><th>KPIs</th><th>Technologies suited</th><th>Possible Project Title</th><th>Priority</th><th>Budget M€</th></tr>
<tr><td rowspan="2">Gain a better comprehension of the relationship between material chemical nature and its activity under relevant and clearly defined operating conditions.</td><td rowspan="2">New characterization techniques allowing in-situ or in-operando investigation.</td><td rowspan="5">ASR < 0.1 Ohm cm2

Efficiency: >95% for fuel and >90% for oxygen electrode reaction

(correspon ding to <5% and 10% electrode overpotenti al loss, respectivel y)

Catalysts/e lectrode durability 40 000 hs</td><td rowspan="5">All cell technologies</td><td>Bridging modelling and characterization correlated with Topic 2.2.</td><td>1</td><td>8</td></tr>
<tr><td>Segmented bipolar plates for local investigation</td><td>1</td><td>8</td></tr>
<tr><td rowspan="2">Identify performance limiting steps and lifetime limiting processes.</td><td rowspan="2">Identification of critical operation regimes for the individual fuel cell and electrolysis technologies.</td><td>catalyst surface structure under real operation conditions</td><td>1</td><td>8</td></tr>
<tr><td>Materials stability Oxygen electrodes large voltage span at high T</td><td>2</td><td>4</td></tr>
<tr><td>Optimize catalyst and electrode properties for the electrochemical reaction considered.</td><td>Normalized tests to assess the electrocatalyst/el ectrode performance.</td><td>Correlate materials properties to cell / stack perfromanceas already existing for Pt active surface area for non Pt catalyst -- to better utilise materials benchmarking catalysts/electro des</td><td>1</td><td>8</td></tr>
</table>

<u>Topic 2.2: Design and development strategies for electrodes, catalyst and supports</u>

<u>Rationale</u>: Performance, stability, costs and life time targets are not yet reached with SoA electrode materials. Cheaper materials have to be searched for including new catalyst.

Optimizing the utilization of noble metal catalysts by integration in advanced electrode structures. New types of electrolysis cells based on new electrolyte materials (e.g. anion conducting membranes) are in an early development state and do need the development of new, adapted electrodes.

<table>
<tr><th>Specific Challenges</th><th>Expected outcome</th><th>KPIs</th><th>Technologies suited</th><th>Possible Project Title</th><th>Priority</th><th>Budget M€</th></tr>
<tr><td rowspan="2">Develop and implement a systematic approach to design new materials.</td><td>Suggestions for non-precious metal catalysts (NPMCs) for low-temperature FCs and ECs.</td><td rowspan="7">ASR <0.1 Ohm. cm^2

(1 A/cm^2 @100mV overporten tial)

1 €/(kW&e lectrode) raw materials costs

PEM: Pt loading < 0.1 mg/cm^2</td><td rowspan="3">Low-T FC, PEM EC, AEC</td><td>Multifunctional electrocatalysts with integrated charge transfer and catalytic activity for C-containing fuels</td><td>1</td><td>6</td></tr>
<tr><td>Systematic computer assisted approach models describing different catalyst and support compositions and architectures.</td><td>Improved chemical stability PEM EC/Micro fluidic, portable fuel cells/Direct Methanol/ethan ol fuel cells with improved activity/perform ance</td><td>1</td><td>6</td></tr>
<tr><td rowspan="2">Assess new catalyst designs and electrode architectures.</td><td>New electrode structures with improved noble metal utilization.</td><td>Electrode layer composition /multiphase electrodes, structured electrodes dedicated to dry conditions</td><td>1</td><td>12</td></tr>
<tr><td>Bifunctional electrodes for unitized regenerative fuel cells.</td><td>SOC mainly, PEM for niches</td><td>Corrosion resistant high temperature electrodes</td><td>2</td><td>9</td></tr>
<tr><td rowspan="2">Develop electrode materials for new/advanced electrochemical cells.</td><td>New electrodes for intermediate temperature cells (200 – 600 °C).</td><td>Opens to intermediat e T</td><td>HT Corrosion stability related to newly identified electrolytes"</td><td>3</td><td>6</td></tr>
<tr><td>Long-term stable and robust electrodes for ceramic based fuel & electrolysis cells.</td><td>SOFC/SOEC</td><td>Stabilization and control of nano scaled elelctro catalysts, oxide ceramic elelctrodes and supports</td><td>1</td><td>12</td></tr>
<tr><td>Alternative support materials to improve stability and catalyst</td><td>Novel anode electrocatalysts for the direct utilization of hydrocarbons at IT-fuel cells.</td><td>Low-T and intermediate T</td><td>New formulations for electrocatalytic C-C bondbreaking</td><td>2</td><td>9</td></tr>
</table>

utilization with respect to carbon based.	Reduced noble metal loading anode electrocatalysts for the direct oxidation of methanol/ethanol at low temperature.				3	5

Topic 2.3: Adapting catalyst synthesis for tailoring catalyst properties

Rationale: New manufacturing processes to supply the materials on a technically relevant scale and competitive costs. Advanced fabrication includes for instance low noble metal content and of nano-structured catalyst. Address alternative methods to form nano-sized catalysts in porous ceramic cells e.g. exsolution process. Thin-film techniques are also often discussed in the frame of electrode designs.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Develop new fabrication processes for tailor-made catalysts and electrode materials. Include appropriate quality assurance throughout the process. The fabrication processes should preferably by environmentally friendly, low-cost, fast and with low energy usage.	Development of novel inorganic and organic electro catalysts based on e.g.:(a) Wet Chemistry (WC);(b) Sono-electrochemistry (SE); (c) Flame Spray Pyrolysis (FSP); (d) Physical Vapour Deposition (PVD).	ASR < 0.2 Ohm cm^2 Production costs excluding raw materials 1 Euro/(kW& electrocatalyts layer) At which scale (volume production) <10 Euro/kg	Mainly high-temperature cells But also applicable to all Low T fuel & electrolysis cells	Multifunctional electrodes materials for direct conversion and synthesis of hydrogen carriers (NH4, MeOH, ect.) Using non toxic, non critical raw materials as electrocatalysts	1	12
	Synthesis of supported ORR and OER electro-catalysts with low noble metal content.		Low T fuel & electrolysis cells	Synthesis and characterization of Pt type, but non precious metal electro catalysts	1	10
	Nano-structured catalysts for proton conduction and alkaline membrane electrolysis.		AEC	Corrosion resistant electrodes in alkaline media Mixed proton and elelctronically conducting electrodes	2	10

Topic 2.4: Materials integration, electrode fabrication and manufacturing

Rationale: Effective integration of the materials into a suitable structure. Multi functionality has to be maintained: electrochemical activity, mass transport ability, electronic conductivity and mechanical integrity. A working electrode for either fuel cell or electrolysis cell has to pass a proof of concept including the demonstration of its manufacturability..

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€

Realize and characterise advanced electrodes by developing and optimizing their processing method. This includes the optimisation of manufacturing parameters (e.g. ink composition, three-dimensional electrodes)..	Proof of concept for new electro-catalysts and electrodes.	ASR <0.3 Ohm.cm2 Current density >0.3 A/cm^2 at 0.9 V full cell Electrode efficiency @ 0.5 A/cm^2 or 0.4 W/cm^2: >90% for fuel and >80% for oxygen electrode reaction (corresponding to <10% and 20% electrode overpotential loss, respectively) 2 Euro/(kW and electrode) Catalysts/electrode durability 40 000 hs Reproducibility: Neartime 95% productivity Rejection 5% Longterm: 6 sigma productivity 9.99999% 0.000001% rejection Cell costs <10 Euro/kW	ALL	Integration and demonstration of advanced electrodes into technically sized cells	1	15
	Proof of concept for nano structured electrode designs.			Prototyping of nano structured electrode concepts based on minimized use of electro catalysts	2	12
Develop new manufacturing techniques. The performance of the cells needs to be evaluated by investigating as much as functional aspects as possible.	Proof of concept of new fabrication processes. Optimize preparation methods for electrode inks. Optimize solvent-free preparation technique for electrodes. Optimize deposition techniques			Development of nano structured electrodes by upscalable, environmentally friendly and automation ready fabrication technologies (incl industry 4.0) Protocols for durability and accelerated stress tests. Evaluation of test bench and cell configurations	3	23

Topic	Main Outcome	Nr. projects	Budget (M€)
2.1	Fundamental understanding of FC & EC electrochemical processes and materials	5	36
2.2	Design of tailor-made electrodes, catalyst and supports	8	65
2.3	Adapting catalyst synthesis for tailoring catalyst properties	3	32
2.4	Materials integration, electrode design and fabrication	3	52
Total		**19**	**185**

5. Contact Point for the sub-programme on 'Catalyst and Electrodes'

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EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on
Fuel Cells and Hydrogen technologies (JP FCH)

SUB-PROGRAMME 3: *Stack Materials and Design*

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

Contact persons:

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Introduction

The Sub Programme will concentrate on issues that allow the cost effective manufacturing of 'robust' stacks. The latter term denoting stacks that can be rapidly thermally and load cycled and that can tolerate a defined degree of 'mistreatment' in the form of vibration, transient operation, fuel and air impurities etc. The issues encountered are very much focused on materials and novel design development and, although related to a goal of successful product engineering, specifically concern basic research in materials, materials processing, and component design.

The topics addressed are

- interconnects and bipolar plates
- contacting and gas distribution
- sealing
- optimizing proved componends
- novel designs for stacks and stack modules, including the interfaces between stack (modules) and system Balance of Plant

Over the initial five year period of the programme substantial improvements are expected in the topics listed in order to enable industry to employ these results in pre-series developments. Progress will be mapped during annual workshops and reviews in order to fine-tune and readjust the programme, if necessary.

The activities are not only centred around research but also encompass student and staff exchange in order to strengthen the networking between the groups involved.

The sub-programme encompasses around 15 person-years from 13 institutions across Europe.

1. Background

The performance and reliability of fuel cells and electrolysers depends on the materials used for MEA's (low temperature fuel cells) and cells (SOFC and MCFC). The robustness and lifetime depends also on properties of the stack assembly, including interconnects, sealants, gas manifolds, contacting and other elements. Therefore the choice of materials for manufacturing stacks is not less vital than the careful design and fabrication of cells / MEA's.
On the other hand, many effects in stack assembly are not properly understood, especially all issues related to thermal and humidity cycling. Corrosion protection – both with respect to contacting, oxidation and cell contamination – will always remain an essential topic in the presence of the highly oxidising and highly reducing atmospheres encountered in a fuel cell, paired with high water vapour content or even liquid water in the case of low-temperature fuel cells. In Solid Oxide Fuel Cells and Solid Oxide Electrolysers (SOFC & SOE), the question of stable sealants with high strength remains a problem to receive more (and systematic) attention.
The above mentioned issues become increasingly important in harsh working conditions like those encountered in vehicles applications or in the case of reversible fuel cell/electrolyser system that must be developed to store renewable electricity.

2. Objectives

This Sub Programme will concentrate on the development of stacks able to withstand rapid and frequent thermal and load cycles, that can tolerate mechanical vibrations, transient operation, fuel and air pollutants and other kinds of difficult operating conditions. The sub-programme uses resources from basic research to improve materials and identify new materials, optimise materials processing, and develop new, break-through designs for fuel cell stacks and modules.

Additionally, the programme aims at strengthening the cooperation between the groups involved by promoting staff and student exchanges.

3. Description of foreseen activities

Justification of Programme

The programme described here concentrates on the more basic research topics attached to the commercialisation of fuel cells and electrolysers. Insofar it is fully complementary to the FCH JU programme and most national programmes, since these concentrate on technology demonstration and market entry. As far as the field of stacks, stack materials and design go, the topics presented address the main problems seen at the stack level today, both for low and high temperature technologies.

The projects will be performed using existing funding and programmes whose results are publicly available. Using additional funding, the scope and intensity of the task work could be considerably intensified.

The main risk encountered in this sub-programme is the failure to find any materials and materials combination that improve the current situation towards better performing, more durable and robust stacks or to find materials and component combinations that result in improvements not only in one field but combine into an overall improvement of properties. This risk can be considered as rather low since a large number of options still exist to improve fuel cell and electrolyser performance and robustness and that have already shown reasonable first results. Nevertheless, the workshop series and annual meetings will offer a platform via which the progress and deliverables of the various activities can be reviewed and – if necessary – redirected.

Topic 3.1: Interconnects and Bipolar Plates

Sub-Topic 3.1.1: Cost effective manufacturing of interconnects

Interconnect and bipolar plate materials for fuel cells and electrolysers are subjected to corrosive attack under rather severe conditions of, for instance, high water or oxygen content etc. Therefore the materials applied today are expensive. Additionally, the forming of gas channels (flow fields) is involved and costly under industrial manufacturing conditions. Work will therefore concentrate on the issues of

- thinner stainless steel plates with new low cost, corrosion resistant materials variants,
- new mass-manufacturing compatible procedures (stamping, cutting, coating etc.) reducing machining requirements

Objectives:

Reducing costs by applying either new as well as more effective industrial manufacturing techniques. Alternatives would be the employment of cheaper materials for interconnects and flow fields.,

Expected Outcomes:

implement cost effective industrial manufacturing techniques for interconnects and bipolar plates.

Sub-Topic 3.1.2: Corrosion resistant materials

Due to the corrosive environment the interconnects and bipolar plates are operated in, specific requirements apply to the materials that make them costly. The problem can also be solved by coating the steel plates. The coating also may take on an additional function in the case of SOFC/SOE where the coating also has to prevent chromium hydroxide evaporation from the interconnect. For low-temperature fuel cells the development of coatings for metallic bipolar plates, e.g. nitride coatings based on chromium, titanium, vanadium, aluminium, zirconium and mixtures thereof is a high priority for technology improvement.

The tasks include

- low cost IC/BPP materials
- new coatings and coating application technologies (ALD, PVD/CVD, galvanic, thermal spray, nano-coatings, reactive coatings, ceramic materials with high electrical conductivity etc.)
- metal plate operation under H_2/O_2 operating conditions

Objectives:
Test corrosion resistant coatings on interconnects and bipolar plates. If the coating in the case of SOFC would be good, more cost effective steel (lower Chromium content in the metal) could be engaged. True for bipolar plates also, a good coating could lead to using cheaper metals.

Expected Outcomes:
One of the major difficulties of running the stack is the corrosive environment, which leads to short durability One goal is to achieve a physical lifetime of 40.000 to 100.000 hours for SOFC and more than 20.000 hours for LTFC.

Topic 3.2: Contacting and Gas Distribution

The single cells in a fuel cell stack are connected to interconnect/bipolar plate by a gas diffusion layer (GDL) (low temperature fuel cells) or ceramic contact materials (e.g. air side of high temperature fuel cells or electrolysers). Contacting and gas distribution are vital elements in reducing overall stack internal resistance and electrode overpotentials.

Sub-Topic 3.2.1: Gas diffusion layers

In low temperature fuel cells, pressure drop across the flow fields and the electrodes can be high depending on the specific stack design (e.g. interdigitated flow fields) and the optimization of the interface flow field / GDL. GDL development must therefore target low resistance to gas flow whilst assuring high mechanical stability and good electrical contacting. These properties are mainly determined by the micro porous layer (MPL), a component still lacking fundamental understanding. The development tasks concern

- high electric conductivity
- high gas permeation and water rejection
- stable hydrophobicity
- mechanical integrity and mechanical protection of MEA

For electrolysers completely new materials for contacting and gas distribution are needed. Carbon materials are not stable and the state of the art titanium contacting elements suffer from high contact resistances. The main focus of the work concerns the stability and long –term conductivity.

Objectives:
Lowering the resistance for gas flow in bipolar plates by modelling optimized structures and identifying new coatings that increase the contacting (soft layer, for example). Testing new and alternative materials for electrolysers.

Expected Outcomes:
Optimize the flow fields and find new materials that fulfil the requirement for conductivity and low resistance to gas flow with simultaneously high mechanical stability. Electrolysers demand materials that guarantee low resistance and high stability for a long term operation. At the beginning 3000 h, at the end up to 10.000 h.

Sub-Topic 3.2.2: Ceramic contact materials

In high temperature fuel cells/SOE, the mechanically long-term stable contacting of the air electrode to interconnect is of high importance to reduce the area specific resistance (ASR) of the single repeating units (SRUs). Contact deterioration by sintering or mechanical fracture can lead to progressive degradation since the current flow paths are continuously reduced and local current density increases steadily to finally form 'hot spots'. The research tasks include

- high electric conductivity
- high mechanical integrity
- low sintering properties

Objectives:

Find sintering conditions to lower the sintering activity in operation at high temperatures and concurrently taking into account, that the material has to be soft enough to make a good overall contact.

Expected Outcomes:
Better electrical contact, no sintering of contact layer in operating mode.

Topic 3.3: Sealing

Sealing materials for low and high temperature fuel cells and electrolysers are a critical issue since they have to remain chemically stable under oxidising and reducing conditions, in atmospheres with high water content and under varying thermal stress.

Sub-Topic 3.3.1: Novel sealing materials and concepts

It is desirable that single stack repeating units can be removed to repair or replace failing units. This requires novel materials and seal design concepts, especially for high temperature fuel cells and electrolysers. Seals that can be screen-printed and have a superior stability are also necessary for low-temperature fuel cells. The often used silicone based materials are known to be responsible for MEA contamination and are not adequate for HT polymer fuel cells at 160-200 °C. Furthermore, due to mechanical stress on the membrane, sub-gaskets for MEA protection are necessary that can be assembled rapidly and should be removable to enable MEA exchange. Ideally, a seal suitable for use in a wide temperature range (-40°C up to 180°C) is required. Tasks to cover include:

- multi-layer glass sealants,
- hybrid ceramic-metallic seals,
- compressive and removable seals,
- improved seals for operation between 80 and 120°C
- sealants for 400°C operating temperature (polymers).

Objectives:
Test alternative glasses or suitable materials for sealants, which allow the use within the temperature ranges. The development of concepts, which allow to exchange either one or more stack repeating units (SRU. Test alternative methods to fabricate suitable sealing’s either for stacks within the process of manufacture as well as for repairing a stack.

Expected Outcomes:
Find an alternative material for LTFC´s that could be used in a wide temperature range. Identify materials that are as well stable in operation as suitable for replacing ga defect SRU or a sub stack without destroying the entire stack. Find methods to repair a stack like laser welding of glasses.

Sub-Topic 3.3.2: Reinforced glass ceramic materials

Glass ceramics are used for high temperature fuel cells and electrolysers. Though glass is not the strongest material it delivers chemical stability and good bonding to steel interconnects. Work is necessary in finding glass ceramics with higher strength or designing metal brazes with electrically insulating layers. Possible solutions include:

- glass ceramic materials with higher strength,
- glass ceramic materials with self-healing properties,
- glass ceramic materials with reinforcing components,
- metallic sealants and brazes combined with electrically insulating layers

Objectives:
Find glass materials with better strength, like compounds. Find isolators with self-healing properties. Could those material properties be combined in one material or in a composition of materials?

Expected Outcomes:

Optimization of glass materials for self-healing processes. Find materials with high strength and properties as an isolator. At first we solve those problems separately. Eventually we look for a combined solution.

Topic 3.4: Novel Designs (Stacks)

Fuel cell and electrolyser stacks today are still expensive to manufacture and require costly materials and/or components. At the same time the requirement to thermally and electrically cycle the stacks induces thermal and mechanical stress to the stacks which again makes countermeasures necessary that increase the complexity of designs and manufacturing steps. Simplified designs with improved thermo-mechanical properties are therefore necessary.

Sub-Topic 3.4.1: New stack designs:

New designs are required that can sustain repeated thermal cycling (including load and redox cycles, where applicable) and at the same time are cheap and simple to manufacture. This task therefore interacts closely with Tasks 1.1 and 3.1 in looking at:

- flexible stacks with thermo-mechanical elasticity,
- stacks with defined contacting pressure,
- lightweight stacks,
- miniaturised stacks,
- removable SRU/repairable stacks

Objectives:
Multiple different tasks exist in the course of this sub-topic. It's impossible to combine all of them. Consequentially we have to establish different work groups on either specific task to achieve an ideal outcome.

Expected Outcomes:
The knowledge that was collected from all the stack tests in the past should lead to modelling new stacks that achieve one or s of the above listened tasks.

Sub-Topic 3.4.2: New flow-field designs

As a sub-set of tasks 4.1, the fuel gas (or steam) distribution across the cells has to be optimised to cause low pressure drops and at the same time ensuring homogenous distribution of fuel gases, especially in the case of syn-gases. Goals of this task are:

- lower pressure losses
- better gas distribution (especially for syn-fuels)
- CFD modelling
-

Objectives:
Testing models of improved gas channels and testing modified gas channels that are adapted to the syn-gas.

Expected Outcomes:
This sub-topic has to be seen in close context with SP 5 Modelling. The experience of the stack tests has to flow in modelling. The outcome of those new models have to be tested. This topic is strongly connected to SP5.

Sub-Topic 3.4.3 Novel Stack-Sensors

In-situ, locally resolved electrochemical impedance spectroscopy sensors with reduced frequency range and low cost electronics are required for online diagnosis and early detection of malfunctions. Integrated into the stack manufacturing process, such sensors can be cost-effective. A control system based on online diagnostics has the potential for significant durability improvement of the stack. For electrolysers and fuel cells the integration of miniaturized gas sensors lead are used for an early detection of gas cross-over. Segmented bipolar plates for investigation of temperature and current distribution in three dimensions (2 D active area + cell location) during technical use in systems improve the understanding of the relevant stack interactions and lead to design improvements.

Objectives:
Build interconnects and bipolar plates for integrating sensors for temperature and different gases.

Expected Outcomes:
Building such interconnects and bipolar plates cause an increases of the stacks costs. But it is necessary due to exploring the sources of possible failures at operation.Consequentually we have to distinguish which sensor is required for operating in an industrial manufactured stack and which is not.

Topic 3.5: Novel Designs (Modules & Interface Stack – BoP)

In the same way stack manufacturing has to be simplified by more elaborate designs, the interface between system (balance of plant components, BoP) and stack has to be streamlined. The less components a fuel cell or electrolyser system has, the cheaper it inherently becomes and the less options it has to fail. The work task closely interacts with the SP Systems and complements the work done there from the point of view of the fuel cell stack.

Sub-Topic 3.5.1: Integrated designs

Stack and parts of the BoP can be integrated into 'sub-modules' in order to reduce thermal losses and facilitate system integration.

Objectives:
Combine parts of the system into one part. Test this combination of reliability and cost effectivity.

Expected Outcomes:
If the combination of parts of the BoP into the stack is possible without complicating manufacturing and repairing it would be possible to optimize the system.

Sub-Topic 3.5.2: Module designs:

System 'sub-modules' can be combined into larger units (modules) to build up systems with higher power (up to and beyond 1 MW_{el}). This task is closely linked to Task 4.1 and will result in optimisation of the trade-off between single cell size, stack architecture and number of stacks or modules in a system. The task comprises activities towards:

- stack 'towers',
- multi-stack/element sub-modules for large systems (> 1 MW),
- removable sub-units/repairable modules.

Objectives:
Build stacks as sub-modules and test the application in BoPs.

Expected Outcomes:
Stack sub-units could be an excellent solution for several reasons. A small sub-stack could be a helpful and reasonably priced solution to repair a system. Bigger sub-stacks could be combined to large systems. Test different sizes of sub-stacks. Achieve results, which suggest the ideal size and combination for its technical and commercial application.

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

Topic 3.1: Interconnects and Bipolar Plates

Rationale: Components that suffer corrosive attack under rather severe conditions, requiring materials operating in specific requirements that make them costly. Applied coating may take on additional functions, protecting and connecting. Interconnects with few simple manufacturing steps using low costs steels, or novel manufacturing methods are necessary to reduce significantly the costs. New flow fields and MEA designs are needed that improve homogeneity of current response over the active area, and increase the limiting mass flow rates (water, gas), in PEMFC.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Reducing costs by applying either new manufacturing technology (metal/ceramic 3D printing, etc..) as well as more effective industrial manufacturing techniques	Implementation of cost effective industrial manufacturing techniques for interconnects and bipolar plates	PM: Lifetime 40000hrs Cost target 3 $/kW Electrical conductivity >100 S/cm SOFC: Lifetime IC > 100000 hrs Cost target IC: 300 €/kW to reach stack cost target of 1000 €/kW Cost target Cr-barrier coating: 50 €/kW	ALL	Develop new 3D manufacturing process of non corroding ceramic interconnect for high temperature FC and electrolyser	1	5
			SOC	Development of material for 3D-printing of IC	2	4
			SOC	Development IC-design suitable for 3D-manufacturing	2	8
Employment of cheaper materials for interconnects and flow fields (HT and LT), more cost effective steel (lower Chromium content in the metal) for HTFC			SOC	Development of low cost coating techniques for Cr-evaporation barrier layers on interconnects	2	5
				Novel IC-Materials for lower operating temperatures	2	4
Good coating could for LTFC bipolar plates that lead to using cheaper metals			Low-T and intermediate T	Bipolar plates with non noble metal coatings for PEMEC	1	6
Improve cell stability and increase performance at high current	Achieve a physical lifetime of 40.000 to 100.000 hours for SOFC and		Solid oxide, proton-conducting cells	Develop interconnects for tubular cells for FC and electrolysers	1	6

density.	for LTFC more than 20.000 hours and for LT electrolysis more than 40.000 hours			In situ characterisation methods for performance and stability of bipolar plates for FC and EC	2	6

Topic 3.2: Contacting and Gas Distribution

Rationale: Contacting and gas distribution are vital elements in reducing overall stack internal resistance and electrode overpotentials (LT, HT FC and electrolysers (SOE)) in order to reduce the area specific resistance (ASR) and contact deterioration by sintering or mechanical fracture /delamination, which can lead to progressive degradation (SOFC and SOE and reversible).

<table>
<tr><th>Specific Challenges</th><th>Expected outcome</th><th>KPIs</th><th>Technologies suited</th><th>Possible Project Title</th><th>Priority</th><th>Budget M€</th></tr>
<tr><td rowspan="2">Lowering the resistance for gas flow in bipolar plates by modelling optimized structures and identifying new coatings that increase the contacting (soft layer, for example). Testing new and alternative materials for electrolysers.</td><td rowspan="5">Optimize the flow fields and find new materials that fulfil the requirement for conductivity and low resistance to gas flow with simultaneously high mechanical stability. Electrolysers demand materials that guarantee low resistance and high stability for a long term operation, ultimately up to 40.000h.

Better electrical contact, no sintering of contact layer in operating mode.

Establish root causes of power decrease by thermal cycling</td><td rowspan="5">For MEA incl GDL & sealing 14 $/kW</td><td>PEMEC</td><td>Microporous layers for PEMEC with low resistance and high stability</td><td>1</td><td>5</td></tr>
<tr><td rowspan="3">SOC</td><td>Investigation of contact loss causes during thermal cycling</td><td>1</td><td>7</td></tr>
<tr><td rowspan="2">Find sintering conditions to lower the sintering activity in operation at high temperatures but the material has to be soft enough to make a good overall contact.</td><td>Modelling and simulation of contact behaviour between cell and interconnect in stack</td><td>1</td><td>3</td></tr>
<tr><td>Development of a novel cathode flexible contact layer</td><td>2</td><td>4</td></tr>
<tr><td>New manufacturing technology (metal/ceramic 3D printing, etc..)</td><td>SOC</td><td>Additive manufacturing for improved contact and reduced area specific resistance</td><td>2</td><td>3</td></tr>
</table>

Topic 3.3: Stack sealing

Rationale: Sealing materials for LT and HT fuel cells and SOE have to remain chemically stable under oxidising and reducing conditions in atmospheres with high water content and under varying thermal stress. Glass is not the strongest material though it delivers chemical stability and good bonding to steel interconnects. Work is necessary in finding glass ceramics with higher strength or designing metal brazes with electrically isolating layers. Contact deterioration by sintering or mechanical fracture can lead to progressive degradation (SOFC and SOE).

Specific Challenges	Expected outcome	KPIs	Technol-ogies suited	Possible Project Title	Priority	Budget Million €
Test alternative glasses or suitable materials for sealants, which allow the use within the temperature ranges.	Eventually a combined solution that addresses all challenges successfully	SOFC Sealing life time >200 thermal cycles	SOC, PCFC, PCEC	Develop alternative materials with solid state reactive sintering method (ceramic seal)	2	5
			SOEC	Investigation of the effects of electrolysis mode operation on SOC-Stack sealants	1	1
Alternative methods to fabricate suitable sealings.			SOC, PCFC, PCEC	Develop automatic manufacturing for casting and/or shaping near net shape made seals	1	5
			PEM	Develop low cost integrated production processes for sealing applications on bipolar plates or MEA	1	5
			SOC	Development of modular based glass-ceramic sealant with a toolbox of additives for properties individualisation	2	2
			SOC	Investigation of additive manufacturing techniques for precisely shaped, durable and low cost sealings	1	3
Find glass materials/compounds with better strength. Find isolators with self-healing properties	Optimization of glass materials for self-healing processes.		SOC	Development of sealing materials to increase robustness of SOC-Stacks allowing > 200 thermal cycles	1	4
Develop models and screening protocols for seal evaluation/ageing	Selection oportunities and possibilities for sealing materials			Test and characterisation of different glass-ceramic sealant materials	1	3
				Development of a characterisation method for glass-ceramic sealants at operating conditions	1	3
	Material data for modelling and simulation activities and projects			Modelling and simulation of thermal stresses in stacks during thermal cycling	1	3

Topic 3.4: Novel designs – Sensors

Rationale: In-situ, locally online diagnosis and early detection of malfunctions is needed: integrated into the stack manufacturing process, such sensors can be cost-effective. A control system based on online diagnostics has the potential for significant durability improvement of the stack. For electrolysers and fuel cells the integration of miniaturized gas sensors are needed for an early detection of gas cross-over. Segmented bipolar plates for investigation of temperature and current distribution in three dimensions (2 D active area + cell location) during technical use in systems can improve the understanding of the relevant stack interactions and lead to design improvements.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Build interconnects and bipolar plates for integrating sensors for temperature and different gases. Implement the micro-sensors directly in connection devices (plastronic)	Identification of the sources of possible failures at operation, also for industrially manufactured stack. Remaining useful lifetime prognostics ability. Increased lifetime of the FC stack and system, higher efficiency, reduced cost, higher compactness.	No specific sensor for diagnostics on the market Estimation of RUL with no more than 5% error	SOC, PCFC, PCEC	Develop fuel utilization sensor (based on pO2 difference and/or humidity sensor)	3	4
			SOC, PEM	Embedded sensors	2	5
Integrate the diagnostics algorithms and hardware requirements (sensors, …) directly in the existing BOP components (e.g. the DC power converter)			SOC, PEM	Embedded diagnostic/prognostic abilities	1	5

Topic 3.5: Novel designs: stack to BoP

Rationale: Stack manufacturing has to be simplified by more elaborate designs, the interface between system balance of plant components (BoP) and stack has to be streamlined. Stack and parts of the BoP can be integrated into 'sub-modules' in order to reduce thermal losses and facilitate system integration. Considering the same primary cooling circuit for the stack and its ancillaries could be an efficient way for simplifying the BoP and reducing the costs. Improved design for high pressure operation is required as well as improved design for internal reforming operation, all leading to increasing the power density of the system.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Combine parts of the system into one part (simplify), increasing reliability and	Combination of parts of the BoP into the stack without complicating manufacturing and	1 single cooling circuit within the system	SOC, PCFC, PCEC	Better fuel recovery by incorporating oxygen transport membranes	1	9

cost-effectiveness	repairing of the system. Higher integration for a simplified system leading to reduced costs Some applications may require changing the stack configuration. For instance small portable applications.	PEM stack cost 20€/kW system cost down to 2,7 Meuros/(t/d) for SOEC/PCEC	Low-temperature FC/EC	optimization of BoP for reducing parasitic losses for low temperature systems	1	5
New stack designs: planar stacks, air breathing cells (PEMFC).			SOC, PCFC, PCEC	Develop novel design of electrolyser for pressurized hydrogen production with improved stability and lower cost (for instance, with tubular geometry, sealless etc)	1	5
			SOC, PCEC	Develop novel design of electrolyser for pressurized hydrogen production with improved stability and lower cost (for instance, with tubular geometry, sealless etc)	1	5
			PEMFC	New concept for light and efficient portable power generation, based on hydrogen and fuel cell	1	1
Direct hybridization of FC single cells with supercap cells	Hybridized system, no power electronics leading to higher efficiency, higher power density	Reach power density of 10 kW/kg	PEMFC	Concept of a stack made of PEM cell + super-capa deeply integrated	1	4
				Direct hybridization PEM-FC / Scap	1	3

Topic	Main Outcome	Nr. projects	Budget (M€)
3.1	Interconnects and Bipolar Plates	8	44
3.2	Contacting and Gas Distribution	5	22
3.3	Sealing	10	34
3.4	Novel Designs (Stacks)	3	14
3.5	Novel Designs (Modules & Interface Stack – BoP)	7	32
Total		**33**	**146**

5.Contact Point for the sub-programme on 'Stack Materials and Design'

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EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on Fuel Cells and Hydrogen technologies (JP FCH)

SUB-PROGRAMME 4: *Systems*

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

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1. Background

Fuel cells and hydrogen have a potential for reducing emissions of greenhouse gases and air pollutants, facilitating the increased use of renewable energy sources, raising overall efficiencies of conversion. Thus a sustainable energy system becomes possible with zero or minimal contribution to global climate. Long lifetime of fuel cell systems under permanent operation is a challenge for the durability of all components, including both fuel cell stacks and system components.

All these characteristics promote the development of sustainable energy systems which have a minimal effect on the global climate change. In order to achieve wide-spread utilization of fuel cell (FC) systems in energy conversion, their lifetime under continuous operation must be prolonged. This poses a challenge both to the fuel cell stacks as well as the other components of FC systems. An operating lifetime of at least 40 000 hours in the case of small-scale systems and even more for large-scale systems is required. At the same time, the investment cost related to the deployment of FC systems has to be decreased as much as possible in order to enable fuel cells' breakthrough on the commercial energy markets.

While much effort and resources are devoted to cell and stack degradation issues, less attention has been paid to the balance of plant, or components and subsystems required for an operational system. Cathode side subsystem components such as heat exchangers, burners and blowers can be significant factors in decreasing the electric efficiency of the whole system. Relatively high mass flows and corresponding pressure drops together with non-optimal components, sub-system solutions and the overall system layout can decrease the total electrical efficiency by many percentage points, and may drop the cost-effectiveness of the whole system below the limit of commercial profitability. Fuel management, and especially non-utilized fuel recirculation, is essential for achieving high electric efficiency.

Once the general criteria for the optimal design of individual fuel cell system components are fulfilled (optimal efficiency of all components, their reliability and easy availability on the market and at a reasonable cost, their integration into an energy management system), there are some key issues that must be solved strictly within the final application framework. In particular, while size, weight and noise concerns might not be essential for a stationary application, they are to be taken into account when the system is designed for a vehicle, together with satisfactory dynamic behaviour of the system and its correct electric integration in the vehicle power train. For stationary applications, the inherent voltage, power and efficiency degradation of the fuel cell requires development of application specific optimization and control strategies e.g. to achieve a constant power output at high efficiency over the entire lifetime of the fuel cell system.

All the mentioned development targets can be the main barrier preventing commercialization of the final fuel cell system.

2. Objectives

Improvements can be made on two levels: (1) the system level and (2) the component level. On the system level several approaches can be taken:

- Improve the systems' efficiency
- Decrease the number of system components by developing innovative fuel cell system concepts
- Design systems with new functionalities, for example for the coproduction of hydrogen and electricity or systems for combined, cooling heating and power production.
- Design novel concepts for the integration of FC systems with other power generation systems (Battery, GT, conventional)
- Improve systems' operational reliability and performance by introducing advanced control and diagnosis techniques ("intelligent systems")

On the function and components level, the general targets could be to (1) decrease the component price, (2) prolong the component life-time and (3) improve the availability of component. Specific work could be done within the following critical areas:

- Thermal management (new materials and designs for heat exchanger and insulation and thermo-mechanical integration of components)
- Power conditioning and grid connection
- Fuel cell systems integrated with electrochemical energy storage like batteries and super-capacitors
- Control systems (sensors and diagnosis tools)
- Fuel supply system (processing, gas and water recirculation, humidification, equipment and materials)
- Air supply system (pressure and dynamic requirements)
- Tackling BoP (Balance of Plant) component aging effects and parasitic power consumption

These system and component improvement contains both low and high temperature fuel cell technologies.

3. Description of foreseen activities

Main goal is the optimization of balance of plant single components and sub system integration, required for an operational system to overcome the main barriers preventing commercialization of fuel cell systems. Creation of value change from research organization to BOP component manufacturer and further to system integrator is important topic. Research activities in this sub-program are related to basic research and composed with the challenge of new ideas, concept and design of process.

Risks & Mitigation strategies
EERA should have an active role in promoting these development topics and the role could be for example:

- Pronounced collaboration between institutes active in this area. Input for the research needs could also come from companies

- Creation of value exchange between research organization and BOP component manufacturers as well as system integrators, especially concerning the deployment of research results in businesses

All kind of research and development contains usually significant risks due to the several uncertainties entailing the nature of research work and this sub-programme is not an exception. Despite being so, the main risks of this particular sub-programme are in finding active enough participants who are really willing to participate and share the results with all of the EERA community. The second major risk is in finding common topics between low-temperature and high-temperature fuel cells. Third major risk is the nature of the work; in system development the nature of work will easily be product oriented instead of being basic or fundamental, or even applied research.

How to avoid these risks? No ready answer can be given but open dialogue between possible partners when defining the content of the work tasks will solve many problems and help avoiding the risks from turning real.

This Sub-programme can be divided into five different topics:

Topic 4.1: Material development

BOP component can be source for impurities which decrease the lifetime of the stacks. Concurrently, the components e.g. heat exchangers, piping and other structures at high temperature must withstand the entire lifetime of the system without failures. In particular, the cost and lifetime of the catalysts used for fuel processing and oxidation of unspent fuel is one key factor defining the final costs and the required service intervals for the systems. Therefore, specific work could be done with the following topics:

- Corrosion resistant materials for BOP component
- New coating technologies
- Catalysts development for fuel processing and after burners

Rationale:
As far as BOP materials are concerned to face corrosion problems it is important to develop improved and cheaper corrosion resistant materials and/or to develop new coating technologies. Another important issue is linked to the fuel processing and to the after burners: more performing and more durable, robust and cheaper catalysts will be investigated.

Objectives:
The objective of this topic is to develop cheap and new kind of materials which can have long lifetime in fuel cell conditions. Other option is to develop coating materials which protect component well against aging phenomena.

Expected Outcomes:
Improved corrosion resistance of interconnect materials and BoP components, improved lifetime and performance of reformer and afterburner catalysts

Topic 4.2: Component/function development

While much effort and resources are devoted to cell and stack issues, less attention has been paid to the BOP, or the components and sub-systems required for an operational system. Several BoP functional units need improvement, thus research activities will concern fuel clean-up, heat management, failure detection methods, air supply, humidification, water management, power conditioning with the aim of having in general more robust more reliable, more compact, better performing and cheaper components and/or architecture than before.

- Innovative fuel cleaning technologies
- New concept for heat exchangers (materials and innovative lay-outs)
- Evaluation of performance of different air supply devices integrated in a fuel cell system (flow rate-pressure curves, power consumption and dynamic response).
- Humidification methodologies and water recirculation
- Characterization of performance and efficiency of power electronic converters in different operating conditions
- Recirculation of non-utilized fuel and fuel cell reaction products (steam/water) for increased efficiency and water-independent operation for fuel processing
- Integration of component and different functionalities

Rationale:
It is also the case that to date R&D in the areas of BOP and Systems has been limited during the past years. It has been estimated that BOP for example can make-up between 50% and 70% of the value of a fuel cell unit. Furthermore, the failure of BOP components and the inadequate level of understanding of the systems have been major contributory factors to the poor performance of fuel cell units in demonstration projects. Components and sub-systems such as fuel processing, heat and thermal management, humidification, fluid supply and management and power conditioning etc. are as fundamental to successful commercialisation of fuel cell systems as the cell and stack

Objectives:

The objective of this topic is to develop tailored BOP components which can be implementable into a real fuel cell system to fulfil performance, lifetime and cost targets for different applications.

Expected outcomes:
High temperature heat exchangers with low pressure drop (quantity depends on system size, temperature range depends on stack characteristics), long lasting and easy to manufacture.

Topic 4.3: New system concepts

Process flow schemes, thermodynamic optimization, and development and testing of integrated systems form the core of the activities of this topic. The topic covers all different application areas like stationary and transportation.

- Development and demonstration of new fuel cell system concepts shall include development of process flow schemes and thermodynamic optimization, identification and/or development of suitable subsystems development and testing of integrated systems.
- Development and deployment of Multi-fuel FC/Innovative Batteries Hybrid Systems 100 W → 100 kW, regardless of final application
- Fuel cell system integrated with gas turbine (pressurized systems)
- Energy storage systems which include fuel cell systems
- Dynamic modeling of match between components during transient operation
- System scale-up up to MW-scale

Rationale:
Current fuel cell systems are too expensive and their lifetime is too short with respect to commercial feasibility of the systems. New innovations are needed and their feasibility tested by proof-of-concept prototypes to enable a commercial breakthroughs.

Objectives:
The objective of this topic is to create new and innovative system concepts which are cheaper, more efficient and have longer lifetime than the current system solutions.

Expected outcome:
Integration of BOP components e.g. reformer, afterburner or heat exchangers into stack module build-up, providing a compact design with high level of thermal integration and lower costs.

Topic 4.4: Sensors and diagnostic tools for FCs

Diagnostics is the main theme of this topic and, as consequence, sensor development (gas quality monitoring, temperature and flow rate measurement) and set-up of methods for monitoring the state of stacks and BOP components will be among the research activities. Sensors may also include so-called soft sensors, i.e. computational estimates of the monitored variables.

- Sensor development for fuel gas quality, temperature and flow rate measurement
- Methods for monitoring current state and performance of stacks and BOP components
- Methods for early detection of component failure (preventive maintenance) e.g. fuel/air leakages from the stack
- Monitoring FC system with the least sensors

Rationale:
There are potential novel tools that could be utilized in fuel cell environment, but the usability of these methods in the high-temperature fuel cell environment is not yet verified, and their usability, accuracy, and potential cost needs to be evaluated.

Objectives:

The objective of this topic is to find reliable and cheap sensors as well as diagnostic tools to monitor the state of the fuel system and its components, especially the fuel cell stack so to guarantee maximal system lifetime.

Expected outcome:
Affordable and reliable online measurement or estimation technique for temperature and voltage distribution in a SOFC stack.

Topic 4.5: System control

Although the research and development in the area of system diagnosis and control is progressing, the field is still unexplored in many practical cases. The activities should be focused on the development of the management strategies of fuel cell systems in order to optimise their overall efficiency or the final added value to customer. This topic covers all different applications, including stationary and transportation applications.

- Develop management strategies to control fuel cell system in an optimal manner with respect to overall efficiency, lifetime or some other given criterion.
- Dynamic modelling of complete systems including their automatic controls
- Control strategies and implemented techniques for the management of fuel cell stack performance degradation over the lifetime of the system

Rationale:
The first-hand aims of this topic are to improve the reliability and operational predictability of commercial fuel cell systems, and thereby to bring down their life cycle cost. To this end, system controls including different kind of monitoring tools and algorithms should be developed to help reaching the practical maximum lifetime of the fuel cell system under normal system degradation and in the case of component malfunction. Secondarily, the aim is to optimize the chosen operational characteristic (e.g. efficiency, produced energy over lifetime, power quality) of the system within given boundaries.

Objectives:
Lengthen the system lifetime, enable reliable autonomous operation of FC systems and improve the predictability of system operation under both healthy and faulty system state by developing efficient system control. Improve fuel cell systems' operational output.

Expected Outcomes:
To develop optimal operating strategies of fuel cell systems in different applications.

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

Topic 4.1: Material development for system components (other than stack)

Rationale: Improved life time of systems and stacks by improving the supply and circulation of suitable species with low level of impurtities coming from flow management systems, reformers and other components of BoP

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies Suited**	**Possible Project Title**	**Priority**	**Budget M€**
Corrosion resistant materials	Better materials for BOP components	Corrosion rate in alkaline or acidic media of BoP parts comparable or less than interconnects < 0.1 µA/cm²	All FC & Electrolyser technologies	Cost effective alloys for the balance of plant components exhibiting high corrosion resistance	1	3
	Longer lifetime	Cost per kg of materials in the range < 5000 € / MT		New materials for high temperature BoP	1	3
	Lower cost of ownership	Commulative Cr evaporation from BOP parts < 0.0002 kg/m² for 1000 hrs				
		Oxidation mass gain < 0.2 mg / 1000 hours at operation temperatures for SOC				
New coating technologies	Improved lifetime and performance of components	Coated parts lifetime more than 40 000 hours		Coatings for high temperature heat exchangers	1	3,5
		Coating costs < 700 €/m² Influence of coating on funtional properties of the parts of less than 10%		Coatings and linings for corrosion resistance in alkaline and acidic media in BoP	1	3,5

Catalysts development for fuel processing and burners	Improved materials with longer life time, sulfur and impurities tolerance and lower cost	Life time of catalyst > 40 000 hours (acceptable degradation - 10% from initial performance in stable conditions)		New catalyst materials/support for partial oxidation and AT reforming	2	2
				Advanced materials for steam reforming	2	1,5
				Direct CO2 reforming materials	3	1,5

Topic 4.2: Component/function development

Rationale: Better efficiency, life time and cost-to-performance ratio can be attained. Reduction in both CAPEX and OPEX of systems

Specific Challenges	Expected outcome	KPIs	Technologies suited	Project Title	Priority	Budget Million €
Integration of component and functionalities	Tailored BOP component to fulfil performance, lifetime and cost targets and optimised control systems for those component	BOP cost below 400 €/kW	All FC & electrolyser technologies	Combined reformer and heat exchanger - integrated in SOC stacks	2	5
New component for fuel processing, heat management and power conditioning		System foot print reduced by at least 15%		Development of selective membranes and other fuel off-gas purification units to attain heat, power and hydrogen	1	6
Recirculation of non-utilised fuel and reaction products (water balance)		System efficiency gain by at least 3% and system cost decrease 5%		Development of recirculation blowers for anode off-gas for steam reforming	1	4

Topic 4.3: New system concepts

Rationale: Increase the applicability of systems by synergies for multi-systems. Partial-loading capability and response time can be improved while keeping relatively high efficiency. CAPEX of multisystem can be higher which is countered by values brought by lower OPEX.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Project Title	Priority	Budget M€
Demonstration of new fuel cell concepts (Hybrid, energy storage)	System with higher versatility, flexibility, larger operations	System elect efficiency > 70%	SOFC + Gas Turbine	Highly flexible combined heat, power and hydrogen systems	1	4,5
		System		Combined	1	4,5

	window and better part loading capability not attainable by stand-alone systems. System control allow SOFC system to run following electricity grid and energy demands	response time < 1 ms for Battery and FC coupled system	PEM FC + Batteries SOFC + Batteries	SOFC and gas turbine system to attain highest efficiency power plant		
		At least 2 functionality improved vs stand-alone systems and other are comparable	rSOC+Heat storage	SOC coupled with heat storage to maximize the round trip efficiency of storage	2	3
			rSOC + LOCH PEMFC + LOCH	SOC + batteries with LOHC as storage for automotive and aeronautic applications	2	3

<u>Topic 4.4: Sensors and diagnostic tools for FCs and electrolysers</u>

<u>Rationale:</u> In-operando diagnostics and sensors can pre-indicate upcoming failure event or alert at the event of a failure event indicating which kind of failure occurred. Moreover, system reliability and operation window can be increased

Specific Challenges	Expected outcome	KPIs	Technologies suited	Project Title	Priority	Budget M€
Proper sensors for fuel, temperature and flow rate measurement	Reliable online method for estimating state of the systems including important individual components	No KPIs directly set as sensors are to be adapted and not developed. guiding KPIs are: lifetime demands for the sensors > 40 000 hours cost targets 10 €/sensor	All FC & electrolyser technologies	High Temperature SOC System with integrated sensors for remote sensing, fault detection and controlling	2	5
Methods for monitoring state and the performance of stacks and BOP components with the least sensors				Low temperature FC and electrolyser systems with integrated sensors for remote sensing, fault detection and controlling	1	5
Methods for early detection of component failure						

<u>Topic 4.5: System control</u>

<u>Rationale:</u> Dynamic system operation and optimal system operating window can be defined

Specific Challenges	Expected outcome	KPIs	Technologies Suited	Project Title	Priority	Budget M€

Implemented simple and cheap techniques for sensing stack performance over the system lifetime	Intelligent fuel cell system with optimal operating strategies in different applications. SOFC system control communicate with the grid system control and be part of whole electricity grid system.	System efficiency gain > 5% System error / failure probability < 0.01%	All fuel cell & electrolyser technologies	Script based automation of system control and operation	1	7
Management strategies to control system in optimal manner		System operating flexibility under partial loading of 40%		Neural network and artificial intelligent based controls for fault tolerant system	2	7

Topic	Main Outcome	Nr. projects	Budget (M€)
4.1	Material development for system components	7	18
4.2	Component/function development	3	15
4.3	New system concepts	4	15
4.4	Sensors and diagnostic tools for FCs and electrolysers	2	10
4.5	System control	2	14
Total		**18**	**72**

6. Contact Point for the sub-programme 4 on Systems

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EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on Fuel Cells and Hydrogen technologies (JP FCH)

<u>SUB-PROGRAMME 5: *Modelling, validation and diagnostics*</u>

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

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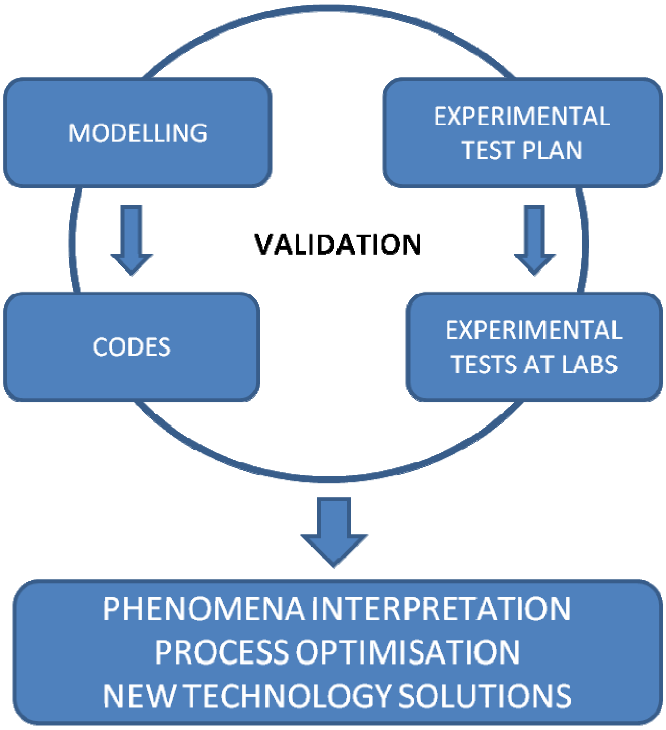
1. Background

In any engineering problem predictive simulation can help to plan new technological solutions and optimise operating conditions, while real-time simulation is a good tool for plant control. In addition, the simulation of specifically designed component/system performance is necessary to explain and classify experimental results and can be a very cost-effective method of saving on expensive experiments.
These benefits are particularly applicable for the evolving maturity and complexity of electrochemical- and fuel-cell systems for the development of competitive products. In particular, mathematical modelling, which is the basis of any simulation activity, is a key factor for the improvement of the the durability and efficiency as well as to decrease the cost and time of development of electrochemical cells (EC) and fuel cells (FC), both operating at low temperature fuel cells and high temperature. It is important to define, initially, the area of interest of the model: at the level of component layer (e.g. only modelling of flow channels, the single electrode or the electrolyte-electrode-assembly), at the unit cell level (including the channels, the electrodes and the electrolyte membrane) or on a higher level where individual cells are gathered in a stack. Also at the plant level the integration of detailed models for EC and FC with simplified packets simulating the standard components is fundamental to correctly describe all interactions, from micro-scale phenomena to global plant design.
Mathematical modelling will provide a better comprehension of parameters impacting the FC/EC performance (parameter sensitivity study, water management) and of the degradation mechanism affecting the different components of the FC/EC (loss or decrease of the porous layers hydrophobicity; corrosion of the catalyst carbon-support; dissolution and redistribution of the catalyst; thermal, mechanical and chemical degradation).
Due to strong coupling between different physicochemical and thermo-mechanical phenomena, detailed interpretation of experimental observations can be difficult, and analysis through modelling becomes crucial to elucidate system degradation and failure mechanisms, and to help improve both electrochemical performance and durability of these technologies. Moreover, the understanding of degradation and failure mechanisms, and simplified modelling of their behaviour with time could strongly help the development of algorithms for the control of complete systems that will take into account the major degradation phenomena. This would strongly enhance the reliability and durability of the system as a whole.

Within the framework of the **Modelling, Validation and Diagnostics** sub-programme (SP) it is planned to develop the modelling activities based on the following objectives:

- evaluating the contribution of different mechanisms on the global performance, determining those that are most relevant
- modelling of interconnected mechanisms at different scales
- better understanding of the relationships between operating conditions (e.g. type of current cycle, relative humidity, temperature, pressure), the components' structural and chemical properties, and long-term cell durability
- better understanding of FC/EC degradation mechanisms (catalyst dissolution, microstructural coarsening, support corrosion, ionomer degradation, material diffusion), water management, thermo-mechanical stresses and their impact on FC behaviour in real application conditions
- choosing the flow configuration in the bipolar plates (BP)
- predicting overall performance and lifetime
- inclusion of degradation and failure mechanism into system control algorithms

Numerical modelling must be completed by experimental tests that provide input for the model (e.g. determination of physical properties of materials by tomography and 3D reconstruction of the structure, catalyst size distribution, hydrophobicity, electrokinetic parameters) and for model validation (e.g. visualization of liquid water by tomography or by optical methods, local impedance spectroscopy measurements, polarization curve, local temperature measurements). Only by correct experimental validation can detailed simulation effectively accelerate and optimize the achievement of next-generation fuel cell and electrochemical cell systems.



Efficient utilization of fuel cells (FC) and electrolysis cells (EC) requires an in-depth knowledge of each individual component of a given system and degradation mechanism influencing the lifetime. In this context, modelling becomes crucial to elucidate system degradation and failure mechanisms, and to help improve both electrochemical performance and durability. In that respect, several initiatives, both national and European, are taking place, regarding the development of efficient models and their coupling to dedicated experimental measurements of individual processes, by using *in-situ* and *ex-situ* experimental techniques.
The first important step is to clearly define the area of interest of the model: at component level (e.g. catalysts, membrane, gas diffusion layer (GDL), electrodes), at single cell level (membrane-electrode-assembly (MEA) or single repeating unit (SRU), including the channels) and/or at higher level where individual fuel cells form a stack.
Mathematical models could provide a deeper understanding of individual parameters impacting the FC and EC performance and durability: e.g. loss or decrease of porous layers hydrophobicity, corrosion of the catalyst carbon-support, dissolution and redistribution of the catalyst, material diffusion, Ni coarsening, ceramic destabilisation, interface delamination, and more generally any thermal, mechanical and chemical degradation mechanisms. Once validated, these models can avoid long-lasting experiments and supply useful trends. In this sense, a suitable model should describe the impact of a given degradation mechanism on instantaneous performance (predicting FC transient behaviour, such as cell potential degradation), or lead to the specification of correct inlet gas mixtures to avoid carbon precipitation or Ni re-oxidation, or the specification of allowable thermal transients that avoid cell failure.
Numerical modelling must be coupled to targeted experimental tests in order to provide inputs for model validation (e.g. determination of physical properties of materials by tomography and 3D structure reconstruction, catalyst size distribution, hydrophobicity of carbon support, electrokinetic parameters) and validation (e.g. visualization of liquid water by tomography or by optical methods, local impedance spectroscopy measurements, polarization curves, local temperature measurements). Dedicated *ex-situ* and *in-situ* experiments have to be carried out to supply specific information (eg. physical properties) to support the modelling process.

Within sub-programme 5 of the Joint Programme on Fuel cells and Hydrogen it is planned to establish the state of the art of all these initiatives, to organise a round robin campaign between these models, allowing harmonization of modelling and diagnostic techniques and identifying topics that still deserve more basic research activities.
This EERA initiative will benefit from strong interfaces with the FCH2 JU and national programmes.

2. Objectives

The main scientific objectives of this initiative will be the following:

- better understanding of: degradation mechanisms (catalyst dissolution, support corrosion, ionomer degradation, Ni coarsening, thermal and material diffusion, ceramic destabilisation, interface delamination), effects of inlet fuel mixture composition, water management (water and multiphase transfer phenomena, thermo-mechanical stresses and their impact on the FC & EC behaviour in real application conditions;
- better understanding of the relationships between operating conditions (e.g. type of current cycle, relative humidity, temperature, pressure), structural and chemical properties of components, and long-term cell durability;
- further development of existing kinetic models (e.g. better describing the oxygen reduction reaction (ORR), catalyst oxidation and support corrosion, multiple reaction mechanisms, internal reforming, poisoning effects, etc.) based on parameters dependent on the catalyst chemical and structural properties and operating conditions (determination of the reaction mechanisms and evaluation of the kinetic parameters to be transferred to macroscale models);
- mathematical description of phenomena such as: chemical ionomer degradation, reactants crossover, mixed-potential effects, catalyst re-crystallisation, biphasic water transfer phenomena in pore and ionomer phases, interface mechanical toughness, microstructure evolution, thermomechanical stresses, accumulated damages (memory effects), etc.;
- development of virtual fuel cell, with optimization design (including material)
- modelling at different scales of interconnected mechanisms
- support towards the experimental development of accelerated aging tests
- recommendation for the flow configuration in the BP
- prediction of complete system performances and lifetime
- inclusion of degradation and failure mechanisms into system control algorithms
- development and adaption of existing models and interoperability software to improve standardized and interoperable software solutions.
-

3. Description of foreseen activities

For the 2014-2020 period, the scientific objectives mentioned above (better understanding of degradation mechanisms under different operating conditions, development of kinetic models and of mathematical descriptions of chemical and physical phenomena, prediction of overall performances and lifetime) are planned to be met following a systematic approach, subdividing the numerous and heterogeneous challenges according to levels of aggregation. Thus, the different scales of modelling will be implemented at the corresponding system levels (cell component, unit cell, stack, complete system), but maintaining an organic approach that will facilitate the multiscale integration of the different models. In addition, an important topic will be to complement experimental and numerical research by the joint development and optimization of advanced characterization tools.

Justification of Programme
The sub-programme described here focuses on five basic research topics wherein it is aimed to harmonize and concentrate efforts of the European FC modelling community, as well as a cross-cutting topic where close interaction is necessary with experimental research. The work tasks will initially make use of results that are publicly available and can be shared by the partners. Contributions to this activity will stem from regional, national or European programmes. As additional funding will be necessary in the future in order to intensify research activities on the most critical topics and crystallize real results, the programme will aim at identifying these, as well as the best candidates for further dedicated collaboration in the framework of funded initiatives.

Risks and mitigation strategies
Several risks can be associated with this activity:

1) Financial risk: since there is no financial support, the partners can only share results which have been obtained from other national or regional programmes of which the results are available in the public domain;
2) Intellectual Property Rights (IPR): since several partners develop in-house algorithms, problems could arise in terms of IPR in case of collaboration;
3) Exchange of data issued by different experiments/models: the mixing of data coming from different sources and used in multiscale modelling approaches could give rise to uncontrolled propagations of errors and uncertainties. The open data management plan could be used to extend on software and codes (executable mode of open source)

A closer cooperation among the partners should be established by harmonizing national and regional programmes, thereby providing a stimulus for closer cooperation. A clear agreement will have to take place between partners in order to avoid IPR problems on the sharing of algorithms, methods, results. For the third risk, the propagation of errors through the use of data of different origins, a clear mitigation strategy will have to be established between partners, case by case. For instance, shared data will have to be accompanied by uncertainty analyses, error bars, accuracy estimations, clear description of the data sources.

Topic 5.1: Cell component level

Modelling the individual physical processes at the cell component level is the first step that can lead to a better understanding of the different FC and EC technologies, and the improvement of their performances and life time. It is also the basis of models at the stack and at the system levels in order to determine the most relevant mechanisms at each scale.
The main difficulty is related to the scales encountered in a single cell which go from the elementary material particles (for example catalyst nano-particles, crystal lattice morphology, nano-pores and micro-pores for ionic transport and gas diffusion), to the geometric area of the active layer which is in the order of 100 or even 10000 cm².
Three kinds of models must be developed:

- The first one must be able to simulate the behaviour of the FC and EC component in usual conditions, and must be able to adapt to new materials according to cell (manufacturer) specifications,
- The second one must be able to take into account the main mechanisms that influence component life time in order to improve it by means of material and cell design optimization or by means of the development of new materials as proposed in SP 1 and 2 of this joint programme.
- The third one must be able to take into account the increasing electrode complexity with increasing cell area, as non uniformities can be already significant at the single cell scale and affect data interpretation.

All three start with the identification of the individual processes taking place in each component within the cell.
To this effect, the following sub-topics are defined, where thermal fluid dynamics are dealt with in sub-topic 1.1, mechanical and degradation aspects are analysed in sub-topics 1.2 and 1.3, and where physical and chemical kinetics are integrated with transport phenomena in gases, porous media and electrolyte as well as chemical and electrochemical reactions (sub-topic 1.4). For each, the studies must be conducted in steady state and in transient regime in order to be implemented in cell models. It must be taken into account that the models should be rendered sufficiently simple in order to go from the component to the system scales.

Expected outcomes:
For each component (bipolar plates, diffusive and catalyst layers), list all the parameters involved in gases, charges, water and heat transport:

- Define their range of values relatively to the state of art, propose values to be reached in order to obtain better performances,
- Study the influence of material properties variation especially as caused by or leading to degradations,

Mapping of operating conditions which promote materials degradations.

Develop multiscale mathematical approaches able to combine kinetics and thermodynamics at molecular level with dynamical system effects, and mathematical descriptions able to treat correctly biphasic phenomena and the influence of electric fields.
Propose relevant models simplifications in order to include them in stack and system models.

Foreseen challenges:

- Defining intrinsic parameters allowing the same models to be used for various materials in order to improve predictions on fuel cell performance and life time.
- To elaborate robust mathematical descriptions and development of new models for catalyst/functional layer evolution and model up-scaling (from nano scale to the macroscopic scale)
- Development of new models for components operation and evolution, and model up-scaling (from the atomistic scale to the macroscopic scale)

The challenges are also related to the scales going from the channel cross section dimensions (in the order of 1mm) to the total channel length (in the order of 1 m) and the corresponding simulation tools (including computational fluid dynamics (CFD)). HPC (High performance Computer) using cluster should be used to solve reference simulations. The use of open-source code should be privileged.

Sub-Topic 5.1.1: Flow channels

Objectives:

- To study the influence of the gas channels' geometry (cross section and flow field design, influence of the gas diffusion properties of the electrode) and surface properties (including surface degradation) on gases and liquid water transport and distribution, and on the pressure drop,
- To study the influence of the design of the heat removal system and of the material thermal properties on the temperature field over the bipolar plate surface.

These two parts highly interact.

- To exploit the limits of commercial CFD packages and to overcome lacks by the implementation of specific sub-routines.
- To develop, with existing CFD open-source code, new packages for fuel cell physics and design

Sub-Topic 5.1.2: Electrode supports and gas diffusion layers

Objectives:

- To study the transport mechanisms of heat, gases and water, the coupling between them, and the mechanical deformation of materials due to their compression inside the FCs and ECs.
- To study the effective transport properties of these porous media, starting from the pore level to the whole medium level and their relation with the structure (porosity and tortuosity for example) and composition of the medium (% of PTFE for example) and with the mechanical deformation.

Special attention must be paid to the properties of the MPL and their influences on the cell performances.

Sub-Topic 5.1.3: Electrolyte layer

Objectives:

- To develop new numerical tools (based on real images of the micro-structure) allowing to study the transport mechanisms from the smaller scale to the macroscale in order to define the optimal materials structure
- To develop virtual 3D electrolyte layer with optimization tools
- To study the mechanisms responsible for the unwanted transport of reagents and products across the electrolyte membrane (crossover of water, other polar solvents, contaminants, fuel or air)
- To study the operating conditions leading to electrolyte degradation (membrane dry-out, matrix coarsening, phase changes)

- To study the chemical, thermal and mechanical stresses imposed on the electrolyte material under FC/EC operation and the theoretical description of the corresponding degradation phenomena.

The following topics should be studied in relation with topic 1.3:

- Development of a mathematical description of reactants crossover and mixed-potential effects, metal catalyst re-crystallization or dissolution in the electrolyte and elemental interdiffusion between electrode and electrolyte
- Water and heat transfer phenomena in the membrane-electrodes assembly (MEA)
- To elaborate robust mathematical descriptions of these phenomena and study the corresponding up-scaling methods.

Sub-Topic 5.1.3: Catalyst / functional layer

Objectives:

- To study the structure and the effective physical properties of the catalyst layer in order to improve its performances
- To develop kinetic models able to take care of complex systems and able to predict realistic data: oxygen reduction reaction, catalyst (re-)oxidation, carbon support corrosion, multiple reaction mechanisms, CH4 internal reforming, etc. These predictions should be based on parameters dependent on the catalyst chemical and structural properties (for the determination of the reaction mechanisms and evaluation of the kinetic parameters to be used in macroscale models)
- To develop tools able to simulate experimentally observable time-evolution of electrochemical processes and characterization methods under realistic operating conditions (e.g. time-evolution of polarisation curves, impedance measurements, current interrupt response, cyclic and linear voltammetry, etc.) as a function of initial material compositions and structures (e.g. initial catalyst loadings and volumetric distributions within the electrodes, etc.)
- To study the time evolution of the performances of the active layer and the evolution of the structure and of the corresponding parameters, and include them in the macroscale model.

Topic 5.2: Unit Cell level

Starting from the results obtained in the frame of topic 1, the objectives of this part are to develop new and more robust models for cells able to combine kinetics and thermodynamics at molecular level with dynamical system effects, with the aim of integrating these with the models developed at adjacent scales (cell component and stack level).
In the frame of coupling models, the correlation must be investigated between different mechanisms (e.g. microstructure evolution, transport, electrochemistry) and the adequate coupling of the respective models in order to reliably predict FC/EC performance and lifetime (durability) as a function of overall system operating conditions. It should be noticed that much effort and care should be applied to this topic in order to estimate the propagation of errors arising from the coupling of several databases (transport data coming from one model, electrochemical data from a different model, etc.). A detailed discussion about the approximations used in the elaboration of each database is thus necessary for each developed scheme.

Expected outcomes:
Multiscale mathematical approaches able to combine kinetics and thermodynamics at molecular level with dynamical system effects. Also mathematical descriptions able to treat correctly all the phenomena involved in FC/EC operation, taking into account the specific cell structure by means of time integration of the specific kinetics model and considering the gas feeding system, geometry characteristics and so on.
Models should lead to being able to predict lifetime of a given system, but also to be able to guide system operators in maintaining the best operating conditions to increase such lifetime.

Foreseen challenges:

Different technologies will have strongly different cell characteristics and will be of difficult generalisation: the level of detail has to be calibrated in order to obtain reliable results, but avoiding too specific analyses. Repeatability of simulation and experimental results obtained during round robin tests is also an important challenge to overcome. This can then lead to a standardised methodology to identify the parameters necessary for the model with the minimum number of tests.

Sub-Topic 5.2.1: Single cell models

Objectives:

- To study all the components and all the physical mechanisms by taking into account the interface resistances (heat, mass and electrical),
- To simulate polarization curves and water and heat transport,
- To simulate impedance spectra, voltammetry, start-up and shut down, voltage variations in transient regime, etc.
- To map all the main chemical-physical parameters (temperature, pressure, composition, flow rates, polarisation, current density)

Special attention must be paid to the challenging task which aims at including in the models the mechanism of component degradation, the evolution of the cell performances with time and the corresponding characterization tools.

The objective is to be able to link through a multiscale approach different phenomena and to be able for example to study the competition between standard reactions and degradation, pollution reactions induced by macroscale conditions. In this case the influence of such conditions on performance and lifetime could be directly and accurately predicted.

Sub-Topic 5.2.2: Gaskets/sealants/bipolar plates (non-active cell components)

Non-active cell components have influence on the cell design, behaviour under operation and life time. Models for these components are scarce.

Objectives:

- To study and model all the interfacial mechanisms and processes between the non-active cell components and the core cell (anode-electrolyte-cathode), looking at chemical, thermal and mechanical interactions, electrical conductivity and gas tightness,
- To study the preparation of a modular-based approach that will allow to connect the unit cell models into stack models.

Sub-Topic 5.2.3: Experimental validation

Dedicated experiments need to be carried out in order to supply specific data for feeding the various models. Such analyses should include specific electrochemical experiments, half-cells, symmetrical cells. For instance, experiments like visualization of liquid water by tomography or other optical methods, locally resolved current and impedance spectroscopy measurements (using segmented cells), polarization curve, locally resolved temperature and pressure measurements can be used to validate modelling approaches. Some additional ex-situ experiments should also be necessary, in order to measure thermal contact resistance, mechanical stress and deformations, i.e. all the complementary parameters influencing the cell electrochemical behaviour.

Objectives:

- To develop measurement tools complete with data deconvolution and analysis procedures, which aid full-range characterization of the cell components under realistic operating conditions
- Develop validation campaigns for the assessment of model validity and robustness

Topic 5.3: Stack level

Starting from the results obtained in the frame of topic 2, the objectives of this part are to develop new models for stacks. This study must be realized in relation with SP 3 (Stack materials and design) of this program.

The main objectives are to develop models that can be used to:

- Test new stack designs and find optimal parameters, geometry and configurations of bipolar plates (gas channels and the embedded cooling circuit), clamping plates, end plates, current collectors
- Reduce the time needed for stack design which can be used in the frame of SP 3
- Develop models allowing to test the influence of auxiliaries on the stack performances (especially in transient regime) and to study the interactions of the stack with other electrical devices (hybrid systems).

These topics concern modelling and simulation tools development in steady state and transient regimes.

Expected outcomes:
Methods and rules to improve thermal and water management and the overall stack performance; simplified thermal components in terms of design, manufacturing and maintenance; robust and accurate simulation tools that can reduce the time needed for stack design;
Advanced knowledge and tools for the modelling of these devices on the FC/EC stack performances.
Scale effect and the relevant parameters

Foreseen challenges:
Implementation of specific sub-routines to overcome the lack of commercial CFD packages. To implement complete models taking into account thermal and fluid dynamics and electrochemical behaviour of the FC/EC stack.
Numerical implementation of coupling thermal and mechanical models able to simulate accurately mechanical stress in each cell of a stack. New electrical design considering the current collectors number and locations in the stack.

Sub-Topic 5.3.1: Thermal and fluid management

The scope of this topic is aimed at understanding how the fuel cell stack design influences the thermal and water management and includes improvements of actual design methods. Much of this Sub-Topic will involve the modelling of transversal heat transfer and distribution (and material migration in cells that use liquid electrolytes), and the design of bipolar plates and gas manifolds. It is realised in relation with topics 1 and 2.

Objectives:

- To develop the CFD tools and to define methods and rules to improve thermal and water management by acting on the cell/bipolar plate/gas manifold/stack geometry. Development with open-source code should be the norm.
- Co-optimization of fluid design by 3D simulation with the entire design and different layers. Use of HPC simulations.
- To map the temperature distribution along the stack, velocity of the fluids and pressure drop in the flow channels and in the components of the FC/EC.

Sub-Topic 5.3.2: Clamping and electrical architecture

This topic aims at the development of simplified clamping plates in terms of design, manufacturing and maintenance of the stacks, as well as the optimization of current collection for improved performance.

Objectives:

- The tightening plates have a strong influence on the stack behaviour. A Thermo-mechanical model of these plates must be developed in order to improve stress uniformity in each cell in the stack, reducing the weight of the stack while considering cell sizes from 1 cm^2 to several hundred cm^2, and one to several hundred cells in the stack.

- The current collectors are currently located between the tightening plates and the terminal plates of the stack. The objective is to improve knowledge in the electrical and mechanical properties and their evolution with time considering number and location in the stack, materials, configuration, etc.
- To investigate innovative electrical architectures and connections that can be used to improve performance.

Sub-Topic 5.3.3: Stack models for simulations at the system level

These subjects must be studied in relation with SP 4 (systems)

Objectives:
- Stack models for simulation at the system level allowing to test the influence of the auxiliaries characteristics on the stack performances (especially in transient regime) in particular on the fuel cell degradation, as also the effect of gas impurities and of vibrations
- Stack models to study the interactions of the stack with other electrical devices (hybrid systems).
- The use of the system as a diagnosis tool (e.g. through multivariate regression of system data) in order to reduce the number of sensors (and thus reduce the system cost)

Topic 5.4: System modelling and control

The system is composed of the FC/EC stack with the fuel processing sub-system (for fuel cell without the fuel supplier system), the fluids sub-system, the cooling/heating sub-system and the electrical converter/supplier. The operating conditions controlled by the system have direct influences on the local operation conditions into the cell and therefore a strong influence on the FC/EC durability. Moreover the different operating modes of the system, as nominal operation, idle operation, power cycles and start/stop operations, induce different degradation mechanisms. The interactions between the system inlet conditions, the stack and the cell surface must be understood in order to minimize adverse local conditions at the active layer and heterogeneities at the different scales (stack level, cell level, active layer, catalyst).
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The main problem remains currently related to the incompatibility between the size of the system and an appropriate level of modelling. In fact, most high-level theoretical approaches are too time-consuming to be applied to such problems. Much effort has to be put in to develop models able to produce correct data and correct physical descriptions maintaining high degrees of aggregation that allow for a simplification of the calculation process.
The model development should include State Of Health (SOH) indicators and adaptive procedures.

Expected Outcomes:
Development of
- Validated physical FC/EC system models at different operating range conditions and applications, with degradation mechanisms and validation,
- SOH indicators as a function of the application and Algorithms for online identification
- Energy management strategies with SOH constraints
- Predictive commands for the improvement of the FC/EC durability and adaptive commands for the improvement of efficiency, both as a function of the SOH
- Simulation tools to optimize cost, performance and durability as a function of the application and constraints
- Development of MiL (Model in the Loop) open platform, to accelerate new architecture design and control

A usable tool for the monitoring of the SOH of FC and EC systems and control of conditions to optimize the trade-off between performance, flexibility, reliability and lifetime: definition of a SOH indicators function of the application, algorithms of SOH online identification, energy management strategies with SOH constraints.

Foreseen challenges:

- improvement of the FCs/ECs durability by a predictive command and efficiency by an adaptive command function of the SOH
- develop a simulation tool to optimize cost, performance and durability as a function of the application and constraints
- organize round Robin tests of the models at the systems level.

Sub-Topic 5.4.1: Development of dynamic models of complete systems with degradation laws

Objectives:
This topic aims to develop and validate physical system models with incorporated degradation mechanisms and to introduce mathematical correlations on degradation. The following activities should be undertaken:

- To develop a validated physical system model and use it to assess design point, part load and dynamic performance of the system for different application: prediction of the system behaviour and enhancement of the control strategy using the models,
- To validate stack models by different set of data obtained in different laboratories at different operating conditions (round robin modelling tests)
- To introduce reversible and irreversible degradation mechanisms to the models.

The system can be modelled by a static or a dynamic physical approach. It is also necessary to direct the multiscale, coupled models towards a single tool for the prediction of system behaviour and enhancement of the control strategy. To this effect, the simulation has to be set up taking into account that the better solution is to couple the accurateness of detailed models for FC stacks with the flexibility of simplified models simulating the behaviour and the interactions of standard components. In this way, the modelling approach conforms to different simulation aims from micro-phenomena investigation to global plant design.

Sub-Topic 5.4.2: Development of State of Health (SOH) indicators of FC/EC systems

The State of Health (SOH) indicator of a FC/EC system is dedicated to provide a diagnostic parameter and is not yet well defined. These models development must be considered simultaneously with the sensors development and the optimization of their location into the system in order to reach the best system reliability without excessive cost.

Objectives:
This topic aims to define and develop a reliable and flexible SOH indicator. The different diagnostic methods to measure the SOH can be described and the identification of an online algorithm developed. The following activities should be undertaken:

- The SOH indicator must be defined as a function of the different online identification parameters available at different stages and applications (for transport or stationary applications,)
- Different algorithms must be developed to identify the SOH function of the physical measurements.
- Energy management strategies with SOH constraints must be developed

Sub-Topic 5.4.3: development of innovative architectures and predictive commands for FC/EC systems

The command of the different ancillaries of the system must be predictive in order to minimize adverse local conditions at the cell level and to minimize reversible and irreversible degradation mechanisms. Moreover, to reduce the systems cost, some new sub-system architecture and ancillaries can be studied.

Objectives:
This topic aims to develop a predictive command of the systems in order to optimize both efficiency and durability. The following activities should be undertaken:

- develop and validate dynamic models for the various sub-system components (compressors, valves, exchangers, pumps, humidifiers etc.) in order to test by simulation the commanding protocols

- develop SOH observer commands to minimize the reversible and irreversible degradations
- develop innovative architectures for the system to minimize the cost of the system (FCS without electrical converter for example)
- test by fast prototyping the different commands developed. Use of a MiL platform

Topic 5.5: Development of characterization tools

The operating conditions are very heterogeneous over the whole surface of the unit cell and are not very well known. These operating conditions strongly modify the degradation mechanisms and their coupling, and as a consequence the degradation rate. The local operating conditions depend, apart from current density and material morphology, very much on kinetic parameters such as for example internal reforming and water transport phenomena, which are still under debate.
As complement and in order to provide reliable data for model validation and for performance prediction a big effort will be dedicated to the development of reliable characterization tools. In particular the activities will concern: *ex-situ* and *in-situ* cell tests for the characterization of individual phenomena, accelerated aging experiments and post-mortem analysis of the aged components and dedicated advanced optical and spectroscopic techniques (such as e.g. photoemission and X-ray absorption spectroscopy (XPS, XAS), tomography, quasi-elastic neutron scattering, neutron diffraction) to analyze the relation between material structure and operating and degradation conditions.
As far as *in-situ* characterization is concerned the possibility to couple synchrotron or neutron techniques, and to develop NMR methods to operating FCs/ECs will be further explored. Since these are pioneering activities, much more R&D is needed to further develop the techniques. The complexity of the topic and especially of the equipment and the data analysis implies that joint infrastructure development and sharing as can be done in EERA will be most effective.
The development of characterization tools must be conducted at the same time as the development of models. At the component level, the *expected outcome* is to obtain the relevant and intrinsic parameters to be implemented in the models in order to simulate the cell and stack behaviours that need to be incorporated at the different levels to improve the FC/EC performances as a whole. The related *foreseen challenges* concern the repeatability of experimental results that can be reached during round robin tests.

Expected Outcomes:
Reduction of the intrusiveness and improvement of the time resolution of the existing methods and further optimization of advanced 3D reconstruction techniques to fruitfully characterize the microstructure of cell components in terms of catalyst distribution, porous network, etc.
Advanced *ex-situ* measurement procedures, analysis techniques and devices for the quantification of individual degradation phenomena. The overall objective is to develop reliable methods and equipment to quantify these phenomena.
To be able to assess the degradation of the unit cell or a cell component and quantify its influence on the performance of the electrode making use of accelerated tests.
Develop new and improved techniques and methods to monitor degradation mechanisms in real time with high time and spatial resolution during fuel cell operation.

Foreseen challenges:
The challenges concern the development of new experimental methods allowing the measurements of internal parameters without modifying the cell behaviour. They also concern the repeatability of experimental results that can be reached during round robin tests.

Sub-Topic 5.5.1: Characterization tools and Experimental validation

Special attention must be paid to the development of characterization tools allowing to highlight the transport phenomena within the cell components (in addition to the materials structure and properties). **These tools should be studied and developed in relationship with the corresponding component SP.**

Objectives:

- To develop measurement tools complete with data deconvolution and analysis procedures, which aid full-range characterization of the cell components under realistic operating conditions
- To assess and optimize the repeatability and interchangeability of experimental results and validation test rigs
- To develop validation campaigns for the assessment of model validity and robustness.

Sub-Topic 5.5.2: Development of *ex-situ* cell tests for the characterization of individual phenomena and microstructure

Objectives:
Concerning individual transport phenomena, the overall objective is to develop reliable methods and equipments to quantify them. This is strongly related to topic 1 in this sub-program and to the sub-programs 1 to 4 of the FCs&H2 joint program.

New 3D reconstruction of components, cells and stack from microscale structures to full stack size, using transmission electron microscopy (TEM) tomography, large X-ray and neutron scattering and a new tomography technique named XUM (X-ray microscopy) must be developed or optimized. They will be fruitful to characterize the microstructure of cell components in terms of catalyst distribution, porous network, etc.
The following task must be undertaken: optimize 3D reconstruction tools so that they are non-invasive and completely non-destructive, increase resolution of 3D reconstruction techniques to the sub-micron scale, improve the time resolution of tomography methods and use them during ex-situ or even in-situ experiments.

Sub-Topic 5.5.3: Development of accelerated aging experiments and post-mortem analysis of the aged components

To reduce the time of development of FCs/ECs, especially in assessing the feasibility of new cell materials and manufacturing techniques, it is crucial to develop accelerated aging experiments that replicate long-term degradation phenomena (the most critical for reliable FC/EC operation, and subsequently their commercial appeal). This is extremely difficult due to the complexity and highly coupled nature of the various degradation mechanisms and operating conditions, so that it is almost impossible to isolate (and accelerate) a single phenomenon without altering the representativeness of the experiment. In the development of such accelerated testing procedures, it is crucial to compare the outcomes at material level, i.e. the post-test morphology and distribution of cell material elements after regular long-term and accelerated testing.
Scanning electron microscopy (SEM) and transmission electron microscopy (TEM) are indispensable tools for analyzing the cell components’ microstructure and its evolution after fuel cell operation. In particular, electron microscopy analyses clearly show the catalyst distribution in the electrodes and their evolution after operation, as well as the qualitative changes in microstructure morphology.
Moreover, owing to the huge improvement of the new generation of transmission electron microscopes (Cs corrected TEM equipped with chemical spectroscopy techniques– EDX and EELS) it is now possible to have chemistry information at the atomic scale. Consequently, for example, it is today possible to acquire elemental maps at the atomic of each component of bi-metallic nanoparticles. These new powerful possibilities are indispensable to have a better knowledge of catalyst electrochemical properties, elemental interdiffusion and to follow their chemical/structural evolution during operation.

Objectives:
- To prepare, carry out and evaluate testing procedures that accelerate particular degradation phenomena
- To determine the chemical and morphological structure of the active cell components before and after ageing.

Sub-Topic 5.4: Development of *in-situ* characterization techniques

The ultimate way to assess and control degradation in FCs and ECs is to monitor these various processes *in-situ* (in the functioning cell environment), or even *in-operando* (during regular operation), without influencing significantly the operating conditions.
This is still a challenging task due the geometry and sometimes the operating conditions. Mainly, the objective is to replicate accurately the pressure, temperature, mechanical stress conditions, etc. *in-operando* at the laboratory scale.

Objectives:

- To improve time and spatial resolution of existing techniques. For this, specific single cells must be developed in order to be able to perform experiments in operating conditions completely representative of the applications.
- Further development and optimization of advanced techniques using X-Ray and neutron sources, for which a joint and aligned effort sharing key infrastructure facilities will be crucial. Develop NMR method for studying water transport in operating cells,
- Develop instrumented cells (including segmented cells) allowing the measurements of internal parameters and temperature, pressure, current, relative humidity, electrical potentials,… fields

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

Topic 5.1: Cell component modelling: flow channel, Electrode support and GDL, electrolyte layer, catalyst

Rationale: Modelling the individual physical processes at the cell component level of the different FC and EC technologies to improve performances and life time. It is also the basis of models at the stack and at the system levels in order to determine the most relevant mechanisms at each scale. It is required to combine kinetics and thermodynamics at molecular level with dynamical system effects, with the aim of integrating these with the models developed at adjacent scales (cell component and stack level).

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
To study the structure and the effective physical properties of the catalyst layer in order to improve its performances and durability	Develop multi-scale mathematical approaches able to combine kinetics and thermodynamics at molecular level with dynamical system effects and mathematical descriptions able to treat correctly biphasic phenomena and the influence of electric fields. Link with continuum kinectic model	Predictability of the cell component model based on *ab-initio* properties calculation and material properties characterization Validation of the model in the nominal conditions better that a target (mean difference (in the sense of L2 norm) between the model and the experiments, including the experimental uncertainty, on specific parameters (voltage, current,	ALL	From ab-initio calculation to continuum model: a database material properties for performance and ageing	1	2
To develop new numerical tools allowing to study the	Define their range of values relatively to the state of art, propose values to be reached in		ALL	Increase power density with optimal active layer structure by a model based approach	1	2

transport mechanisms from the smaller scale to the macro-scale in order to define the optimal materials structure, in the different components	order to obtain better performances Study the influence of material properties variation especially as caused by or leading to degradations Mapping of operating conditions which promote materials degradations	temperature…))	ALL	Fast and reliable degradation models covering multicomponents	1	4
To study the influence of the gas channels' geometry (two phase flow)	Propose relevant models simplifications in order to include them in stack and system models		PEM	Optimal design by simulation of bipolar plate including two phases flow with phase change	2	2

Topic 5.2: Unit cell modelling: single cell, bipolar plate, experimental validation

Rationale: Develop new and more robust models for cells scale with a multi-scale approach. Introduce degradation mechanisms in the cell scale.

Specific Challenges	Expected outcome	KPIs	Technologies Suited	Possible Project Title	Priority	Budget M€
To map all the main chemical-physical parameters (temperature, pressure, composition, flow rates, polarisation, current density)	Multi-scale mathematical approaches into full 3D geometry model with real design. Development on opensource codes. HPC simulations	3D CFD fuel cell stack model available on OpenSource format with documentation and database Database of reduce fuel	ALL	Fuel cell stack 3D CFD models with Open Source softwares	1	2

To study and model all the interfacial mechanisms and processes between the non-active cell components and the core cell (anode-electrolyte-cathode), looking at chemical, thermal and mechanical interactions, electrical conductivity and gas tightness	Reduction model for pseudo-3D model and 0D mapping Mathematical descriptions able to treat correctly all the phenomena involved in FC/EC operation, taking into account the specific cell structure by means of time integration of the specific kinetics model and considering the gas feeding system, geometry characteristics.	cell stack 0D model based on model reduction approaches	ALL	Co-optimization of bipolar plate design and MEA: toward the next generation of stack	1	3
To study the preparation of a modular-based approach that will allow to connect the unit cell models into stack models			ALL	From 3D model to p3D model for the fuel cell stack : cell reduction model stack level	2	2
Develop validation campaigns for the assessment of model validity and robustness		Definition of test cases for model validation and non regression		Models verification and validation: test cases	2	2

<u>Topic 5.3: Stack level modelling: thermal and fluid management, clamping and electrical architecture, stack models for simulation at the system level</u>

<u>Rationale</u>: Merging with results obtained in the frame of topic 5.2, there is a need to transfer cell level modelling towards developing new models for stacks.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**

Test new stack designs and find optimal parameters, geometry and configurations of bipolar plates (gas channels and the embedded cooling circuit), clamping plates, end plates, current collectors	Methods and rules to improve thermal and water management and the overall stack performance. Mechanical behavior are taken into account. Simplified thermal components in terms of design, manufacturing and maintenance	Mechanical fuel cell stack model to optimize conception and validation Lifetime add-ons in dynamic fuel cell stack model: Validation of the degradation models better that a target (mean difference (in the sense of L2 norm) between the model and the experiments, including the experimental uncertainty, on specific parameters (voltage, current, temperature…))	ALL	Optimization of stack design, with cell constraints and system dynamics	1	5
Develop models allowing to test the influence of auxiliaries on the stack performances (especially in transient regime) and to study the interactions of the stack with other electrical devices (hybrid systems).			ALL			
Reduce the time needed for stack design which can be used in the frame of SP 3	Robust and accurate simulation tools that can reduce the time needed for stack design		ALL	from 3D fuel cell stack simulation to specific rules of design and best practices	2	3

Topic 5.4: System modelling and control: dynamic system model, State-of-Health (SoH) indicators, predictive commands

Rationale: The operating conditions controlled by the system have direct influences on the local operation conditions into the cell and therefore a strong influence on the FC/EC durability.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
To develop a validated physical system model	Validated physical FC/EC system models at different operating range conditions and applications, with degradation mechanisms and validation	Fuel cell stack 0D model and auxiliaries librairies ready to be use in an opensource platform for system, with lifetime add-ons	ALL	Dynamic multi-physics fuel cell system model developement with lifetime prediction	2	2
Develop validation campaigns for the assessment of model validity and robustness **(see Topic 5.5)**			ALL	Build of a fuel cell system database (from the stack to the auxiliaries) and librairies	2	2

To develop energy management strategies with SoH constraints	SOH indicators as a function of the application and Algorithms for online identification		ALL	Degradations correlations between global operating conditions and lifetime, based on model approach	2	2
	Predictive commands for the improvement of the FC/EC durability and adaptive commands for the improvement of efficiency		ALL	Optimal FCMS (Fuel cell management system) including performance and durability constraints at the stack and system level	1	4
To develop and validate dynamic models for the various sub-system components (compressors, valves, exchangers, pumps, humidifiers etc.) in order to test by HIL simulation the commanding protocols	Simulation tools to optimize cost, performance and durability as a function of the application and constraints. Development of a MiL (Model in the Loop) simulation platform		ALL	Open fast prototyping simulation platform to optimise FC systems for transport applications taking into account battery hybridisation	1	4

<u>Topic 5.5: Development of characterization tools</u>

<u>Rationale</u>: The challenges concern the development of new experimental methods allowing the measurements of internal parameters without modifying the cell behaviour. They also concern the repeatability of experimental results that can be reached during round robin tests..

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
To develop validation campaigns for the assessment of model validity and robustness.	Further optimization of advanced 3D reconstruction techniques to fruitfully characterize the microstructure of cell components in terms of catalyst distribution, porous network, etc.	Definition of test cases for model validation and non regression Development of a experimental database for model validation	ALL	Multi-scale characterization, from the nano-scale to the micro-scale structure: high tomography resolution	1	3

To develop in-situ characterization techniques	Develop new and improved techniques and methods to monitor degradation mechanisms in real time with high time and spatial resolution during fuel cell operation.	and verification	ALL	Segmented bipolar plate for local investigation and real time diagnostic	1	3
To develop ex-situ cell tests for the characterization of individual phenomena and microstructure	Advanced ex-situ measurement procedures, analysis techniques and devices for the quantification of individual degradation phenomena.		ALL	Advanced local measurement in the fuel cell, for model parameters identification and model validation	1	3
To develop accelerated aging experiments and post-mortem analysis of the aged components and determine the chemical and morphological structure	To be able to assess the degradation of the unit cell or a cell component and quantify its influence on the performance of the electrode making use of accelerated tests.		ALL	Accelerating stress tests to validate degradations models (iterative approach between modeling and experiments)	2	2

Topic	Main Outcome	Nr. projects	Budget (M€)
5.1	Cell component modelling	4	10
5.2	Unit cell modelling	4	9
5.3	Stack level modelling	2	8
5.4	System modelling and control	5	14
5.5	Development of characterization tools	4	11
Total		**19**	**52**

5. Contact Point for the sub-programme on 'Modelling, validation and diagnosis'

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EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on
Fuel Cells and Hydrogen technologies (JP FCH)

SUB-PROGRAMME 6: *Hydrogen Production and Handling*

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

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Introduction

The sub Programme will focus on the development of novel low cost and efficient non-electrochemical hydrogen production systems which are not based on electrolysis (since this is covered by the other SP's). Current production methods of hydrogen are inefficient and further development of these technologies is required. The main issues are caused by poor materials and designs. This SP will thus aim to address these important issues by researching and developing new materials, processes, and component design.

The topics addressed are:

- Hydrogen production from Biomass/Biowaste
- Hydrogen production from Algae
- Hydrogen production from Thermolysis
- Hydrogen production from Photocatalysis
- Hydrogen Handling (improved compression and liquefaction)
- Hydrogen Purity, Safety, Codes and Standards

Over the initial seven year period of the programme substantial improvements are expected in the topics listed in order to enable industry to then employ these results in prototype developments. Progress will be mapped out during annual workshops and reviews in order to fine-tune and readjust the programme, if required.

The activities are not only centred around research but also encompass student and staff exchange in order to strengthen the networking between the groups involved, since the activities described here still appear fragmented across Europe.

The sub-programme encompasses around 26.25 person-years from 14 institutions across Europe.

Production of hydrogen by electrolysis is not covered by this Sub-Programme since it is an integral part of SPs 1 to 5.

1. Background

Hydrogen is already widely produced for a variety of industries, but it is only now being considered for use as an energy carrier for stationary and transportation applications. Around 20 million tonnes of hydrogen are produced in the world each year, enough to power around 60 million vehicles or 16 million homes. Hydrogen is currently utilised in industry such as: (i) oil refining, (ii) food production, (iii) metal treatment, and (iv) production of ammonia for fertilizer and other industrial uses.
Currently hydrogen production processes, from biogas and/or waste fuel, include steam reforming (SR), partial oxidation (POX) and autothermal reforming (ATR) of hydrocarbons. Recently the "tri-reforming process" is receiving growing attention: the process involves a combination of dry reforming, steam reforming and partial oxidation of methane in a single step, producing syn-gas with the desired H_2/CO ratio by modulation of feed composition.
In addition to the conventional hydrogen production methods of steam methane reforming (SMR) and grid-powered electrolysis, novel renewable production alternatives are emerging. These include various biogas production methods (using gasification), pyrolysis processes, biomass fermentation (using microorganisms), and newly developed photocatalytic and thermo-chemical processes that can facilitate water splitting into hydrogen and oxygen with lower energy requirements than 'conventional' electrolysis.
Codes and standards for hydrogen storage and transport have evolved dramatically over the past 20 years and now cover most hydrogen applications. Hydrogen is now being transported by trucks, pipelines etc, and is stored in vessels that are certified by ASME for stationary use only.
Challenges to expand the utilisation of hydrogen for stationary and automotive applications include better outreach, public engagement, education and training of local codes and standards on the processes for hydrogen systems. This would allow continued efforts to reduce the costs of renewable hydrogen production, improved efficiencies and performances with low to zero emissions of greenhouse gases.

2. Objectives

The sub-programme (SP) will concentrate on researching and developing cost effective and efficient non-electrochemical hydrogen production methods by improving materials and identifying superior novel materials, optimising materials processing, and developing new, break-through designs for hydrogen production systems. The SP will also be involved in the development and implementation of new Codes and Standards related to the aforementioned technologies, and strengthen the cooperation between the groups involved by promoting staff and student exchanges.

3. Description of foreseen activities

<u>*Main goals:*</u>
Development of novel low cost and efficient non-electrochemical hydrogen production systems by improving materials and identifying superior novel materials, optimising materials processing, and developing new, break-through designs for hydrogen production systems. Pre-normative research into Codes and Standards relevant to the technologies developed here.

<u>*Targets:*</u>
Reduce the production cost of hydrogen from the technologies covered here to well below 5 €/kg, including avoided costs of CO_2 emissions.

<u>*Justification of Programme:*</u>
The programme described here concentrates on the research and development of low cost and efficient non-electrochemical hydrogen production methods. The proposed programme is fully complementary to the FCH JU programme and most national programmes, since these concentrate on technology demonstration and market entry.

The work tasks will be performed using existing funding and programmes whose results are publicly available. Using additional funding, the scope and intensity of the task work could be considerably intensified.

<u>Topic 6.1: Hydrogen from Biomass/Biowaste</u>

There are two main routes for biomass/biowaste-based hydrogen production, namely thermo-chemical and bio-chemical. Thermo-chemical routes have three subheadings as pyrolysis, gasification, and supercritical water gasification (SCWG). Pyrolysis means that biomass is heated in absence of air. It can be taken bio-oil, char and tar after pyrolysis processes. Gasification is used as a well-stablished technology, in which biomass/ biowaste is heated at high temperatures and disengage to combustible gas (syngas). By using steam or oxygen as a gasification agent an increased energy value is obtained. Waste valorization to H2 and high-added value products can be also done through waste-to-energy and waste-to-hydrogen processes using gasification technologies. The third method of thermo-chemical routes is SCWG where water is miscible with organic substance above the critical point. This method is preferred especially for high moisture biomass.

Sub-Topic 6.1.1: Development of Novel Catalysts and Processes for Thermochemical Hydrogen Production

Generally, catalysts used in thermo-chemical methods of hydrogen production should effectively remove tars, be capable of reforming methane, be resistant to deactivation, be easy to regenerate, be inexpensive, and have significant strength (as fluidized beds are often used for gasification). Dolomites, zeolites, olivines, alumina, alkali metals salts and supported metal catalysts have all been used as catalysts for pyrolysis and gasification of biomass and clean-up. However, all these catalysts suffer from deactivation either by sintering and/or coke deposition. Thus, further work is needed to optimise the formulation of the catalysts: the metal content, the average particle size of metal, the catalyst support and the concentrations and type of doping additives.

Production of hydrogen from biomass gasification is faced with a multitude of problems ranging from tar cracking to sulphur and halogen removal. ew processes can take care of aspects of gas purification prior to later clean-up steps, thus reducing the cost and complexity in production of clean hydrogen and hydrogen-rich gases.

Objectives:
Improvement of catalyst robustness and lifetime, reduction of catalyst cost, reduction of overall cost of producing fuel cell fuels from biomass from thermochemical processes

Expected Outcomes:
Catalysts for fluidised bed and entrained flow biomass gasification with a lifetime of 40 000 hours, tar-cracking catalysts for gasifiers, novel processes for reducing tar content of biomass syn-gases

Sub-Topic 6.1.2: Optimisation of Super-Critical Water Gasification for Continuous Hydrogen Production

- Adaptation of SCWG to H_2 generation requirements
- Effect of biowaste material compositions on process parameters and hydrogen purity

Due to many wastes having a high fraction of water, thermal processes generally require a high amount of energy for drying. In SCWG any type of hydrocarbon can be reduced into its smallest components, thus even treating hazardous wastes in a safe manner.

Objectives:
Improve the process control with view on optimising the quality of the hydrogen produced and achievement of a continuous process; analyse the impact of various waste components on hydrogen and syn-gas quality and identify strategies to process specifically harmful components.

Expected Outcomes:
Increase the stability of conversion processes and identify prospects of reaching high hydrogen fractions.

Sub-topic 6.1.3: Hidrogen production from Waste/biowaste: Improvement of process efficiency and research on the influence of Biowaste Materials and compositions on Hydrogen production & purity

- Range of biowaste of several compositions for Hydrogen production
- Effect of biowaste materials on Hydrogen purity
- New approaches for improvement of process efficiency

In many countries biomass is not overly abundant. Wastes, though, may constitute a major problem for the infrastructure, including logistics and provision of landfill or incineration sites. Due to many wastes having a high fraction of hydrocarbons (plastics), biomass, MSW or other energetically useful components, conversion of waste to hydrogen rich gases (syn-gases) can be considered. The valorization of wastes following the waste-to-energy (W2E) and waste-to-hydrogen (W2H) processes can provide an optimum solution for reducing waste disposal in landfills with an effective reduction in final H2 production costs (by reducing biomass-feedstock costs). Additionally, new hybrid technological approaches based on combined solar heat and gasification process can provide an additional increase > 30% on process net efficiency.

The varying composition of the waste, though, will cause problems with the conversion process (fermentation or gasification) and subsequently (negatively) impact on the quality of hydrogen produced, so cleaning gas requirements should be carefully considered depending on the final application of the syngas. New approaches based on new gasification processes such as plasma gasification or thermal/catalytic gasification can take care of aspects of gas purification prior to later clean-up steps, thus reducing the cost and complexity in production of clean hydrogen and hydrogen-rich gases. Besides that further work is still needed to develop novel gas cleaning processes at high temperature

Objectives:
Improve the process control with view on optimising the quality of the hydrogen produced; analyse the impact of various waste components on hydrogen and syn-gas quality and identify strategies to avoid specifically harmful components
Improvement of process efficiency
Improve technology for valorisation of wastes

Expected Outcomes:
Increase the stability of conversion processes and identify prospects of reaching high hydrogen fractions above 50% at a variation of +/-5%
Novel high temperature syngas cleaning technologies
Novel gasification processes
Hybrid solar-heated gasification

Topic 6.2: Hydrogen from Algae

Since the pioneering discovery by Gaffron *et al.* over 60 years ago, the ability of green algae to produce Hydrogen upon illumination has been mostly a biological effect. Hydrogen evolution from green algae is usually induced upon a prior anaerobic incubation of the cells in the dark. A hydrogenase enzyme is expressed under such incubation and catalysed, with high specific activity, a light-mediated Hydrogen evolution. The monomeric form of the enzyme, a class of iron hydrogenases is encoded in the nucleus of the unicellular green algae. Light absorption by photosynthesis is essential for the generation of hydrogen as light energy facilitates the oxidation of water molecules, the release of electrons and protons, and the endergonic transport of these electrons to ferredoxin.

As far as fermentation processes are concerned the activities will concern the improvement of the processes in order to increase the volumetric H_2 productivity optimising culture conditions, biomass retention, or selecting highly productive species

The following activities are foreseen:

Sub-Topic 6.2.1: Influence of Algae materials and compositions on Hydrogen production

Objectives:
Analyse the dependency of hydrogen production of various species on insolation / illumination conditions and nutrition materials and supply; design optimised reactor configurations; test and evaluate hydrogen production rates; choice of algae suitable for high-efficiency lighting (e.g. LED)

Expected Outcomes:
Identification of algae species with photoconversion efficiencies above 5%

Sub-Topic 6.2.2: Influence of Algae materials and compositions on Hydrogen purity

Objectives:
Analyse the effect of algae types and nutrition on hydrogen purity; design and evaluation of hydrogen separation processes (membranes etc.) to receive high purity gases from algae conversion

Expected Outcomes:
Production of hydrogen with purities of minimum 99%

Sub-Topic 6.2.3: Novel Bioprocess Methods

For the designed 2-stage bioprocess, the volumetric H_2 productivity in the thermophilic fermentation step must be increased at least 10-fold in order to meet the production capacity of 425 m^3 H_2/h. This can be done by conventional methods such as optimisation of culture conditions, biomass retention, or selection of highly productive species or strains from the broad range of available hydrogen producing micro-organisms. The productivity of the photobiological fermentation step should be increased by at least a factor 15 through optimization of sunlight conversion efficiency. In this case the main improvement has to come from technological improvements of sunlight collection and light transfer systems, and photobioreactor development. To support the profitable utilisation of the effluent of the thermo-bioreactor, the conversion to methane should be considered as well. It is obvious that during the night, sunlight is lacking. Instead of storing the effluent, methane production might act as a substitute. When this option turns out favorable, the advantages of a partial photofermentation supplemented with a methane fermentation have to be weighed against a complete replacement of the photofermentation step. This issue needs to be evaluated together with the progress in the field of the application of methane in fuel cells and the utilisation of H_2/CH_4 mixtures as new energy carriers.

Objectives:
Improvement of process properties and efficiency; combination and balancing of hydrogen and methane production

Expected Outcomes:
Increase of current rate of production by a factor of ten

Topic 6.3: Hydrogen from Water Thermolysis

Water thermolysis is a reversible process and involves one-step direct thermal decomposition. Presently, the technically tolerable reaction temperature limit is around 2,500°C, which theoretically allows a dissociation level of slightly over 4% at atmospheric pressure. A water thermolysis reactor involves components manufactured of very special refractory materials able of enduring chemically active environment and very high temperatures generally in the range of 1,500 K and higher is expected to withstand temperature gradients of considerable magnitude and swift temperature swings without degradation.

In view of the prevailing material limitations, the possibility of lowering the operating temperature to some extent by catalysing the reaction appears as an attractive option.

Sub-Topic 6.3.1: Development of new catalyst materials on Hydrogen production

Objectives:
Develop novel catalyst materials at moderated temperatures on hydrogen production

Expected Outcomes:
Reduction of reactor temperature

Topic 6.4: Hydrogen from Photocatalyis

Semiconductor photoelectrolysis is currently being widely explored as a carbon-emission free route to convert the solar energy to chemical energy and generate low-cost hydrogen. If succeeded this technology has the potential to produce hydrogen to meet the fast growing world energy demand while producing almost no pollution. One approach to water-splitting uses light-absorption to excite an electron in a semiconductor from a filled valence band to a vacant conduction band. In a typical water splitting photoelectrochemical (PEC) cell, once the light is being absorbed by the semiconductor electrode and generated charges upon excitation, the majority carriers (electrons in a *n*-type semiconductor) travel to the substrate. The electrons collected at the substrate are transferred to the counter electrode where the H_2 evolution takes place. The remaining holes need to travel to the semiconductor/electrolyte interface to undergo water oxidation.
The activities will concern the development of nanostructured transition metal oxide semiconductor to maximise the light harvesting efficiency and to overcome the electron-hole

recombination losses occurring are key challenges in a PEC water splitting cell. A range of nanostructured transition metal oxide semiconductor electrodes with the emphasis of water oxidation on photoanodic semiconductor/electrolyte interface will be investigated with the aim of meeting those challenges. Effort will be dedicated to find a substitute for Pt developing Transition Metal Carbides as possible co-catalyst in photocatalytic water splitting

$$2H^{+} + 2e^{-} \rightarrow H_2$$
$$2H_2O + 4h^{+} \rightarrow O_2 + 4H^{+}$$

$$2H_2O \xrightarrow{hv} 2H_2 + O_2$$

Sub-Topic 6.4.1: Development of nanostructured transition metal oxide semiconductor

Maximising the light harvesting efficiency and overcoming the electron-hole recombination losses occurring are key challenges in a PEC water splitting cell.

A range of (nanostructured) transition metal oxide semiconductor electrodes with the emphasis of water oxidation on photoanodic semiconductor/electrolyte interface will be investigated with the aim of meeting those challenges.

Objectives:

- improved electrode performance by identifying materials and materials combination having optimal bandgaps and optimal bandedge positions with respect to the oxidation and reduction reaction.
- improve on today's best oxygen evolution catalyst (Co-phosphate) to further reduce the overpotential and enhance the oxygen evolution rate close to this minimal potential

Expected Outcomes:
Higher yield of the photocatalytic process

Sub-Topic 6.4.2: Development and characterisation of Transition Metal Carbides

Transition metal carbides (e.g. WC, Fe3C) offer a potential substitute for Pt. Their electronic structure is often called 'noble metal-like' but they also display distinct activity in their own right. Preliminary investigations showed WC to be a promising co-catalyst in photocatalytic water splitting.

Objectives:
Development of Pt-free catalysts for photocatalytic hydrogen generation; find methods to identify stable electrode materials (e.g. oxides) with an electronic diffusion length comparable to the light absorption depth

Expected Outcomes:
Cost reduction by replacing platinum as the catalyst

Sub-Topic 6.4.3: Effect of alcohol materials on photocatalysis

Nanostructured photocatalysts have to be investigated for the hydrogen production from visible-light driven photocatalysis of various fluids (ethanol, glycerol, etc.) since recent work showed promising results.

Objectives:
Using other fluids than water for photocatalytic hydrogen generation

Expected Outcomes:

Higher flexibility of hydrogen production from fluids

Sub-Topic 6.4.4: Preparing a water splitting device

The various components of a water splitting device need to be tuned to obtain the maximum total efficiency. The maximum efficiency obtained sofar in cheap oxide based technology is ~5% (solar-to-hydrogen).

Objectives:
Develop a water splitting device by developing materials combinations which are physically and chemically well-tuned to obtain the highest possible efficiency.

Expected Outcomes:
Demonstrator device with a 10%, based on cheap and abundant materials

Topic 6.5: Hydrogen compression, liquefaction and purification

Pure hydrogen has the best energy-to-weight ratio of any fuel, but also has the lowest storage density of all fuels at atmospheric pressure. There are a number of methods to store hydrogen for fuel cell applications, such as gas, liquid, metal, and/or chemical form; depending upon the application, hydrogen can be either compressed or liquefied.

(i) Compression of hydrogen is performed in the same way as for natural gas. It is often even possible to use the same compressors, as long as the appropriate gaskets are used and provided the compressed gas can be guaranteed to be oil free.

(ii) The energy density of hydrogen can be improved by storing hydrogen in a liquid form. Liquefaction plants operate nowadays with liquid nitrogen pre-cooling of the feed hydrogen with a pressure of at least 2 MPa. Before being liquefied, the hydrogen is cleaned and then free of CO_2, CO, CH_4 and H_2O. This is usually performed using a pressure swing adsorption process. The energy required to liquefy hydrogen reduces overall efficiency of the system; around 30% of the energy content of the gas. In all cases the liquefaction is achieved by compression followed by some form of expansion, either irreversible *via* use of a throttle valve or partly reversible *via* the use of an expansion machine. However, hydrogen losses become a concern and improved tank insulation is required to minimize losses from hydrogen boil-off.

Activities will dedicated to improve the storage of compressed and liquid H2 investigating various compressors using different gasket materials and physical processes with less energy input; developing new magneto-caloric processes & insulating materials in order to efficiently and rapidly transform ortho-hydrogen to para-hydrogen etc; improving tank insulation materials to (i) minimise loss and (ii) improve liquefaction efficiencies in views of reducing the energy required to cool and liquefy hydrogen gas

Sub-Topic 6.5.1: Development of novel compressors

- Investigate various compressors using different gasket materials and physical processes with less energy input
- Metal hydride compressors

Objectives:
Drastically reducing energy demand for hydrogen compression

Expected Outcomes:
Reduction of hydrogen compression work by a factor of two

Sub-Topic 6.5.2: Development of new magneto-caloric processes & insulating materials

- Investigate and develop novel magneto-caloric processes and other processes in order to efficiently and rapidly transform ortho-hydrogen to para-hydrogen etc
- Improving tank insulation materials to (i) minimise loss and (ii) improve liquefaction efficiencies in views of reducing the energy required to cool and liquefy hydrogen gas

Objectives:
Improve the efficiency of hydrogen liquefaction processes, incl. storage

Expected Outcomes:
Reduced liquefaction energy demand and heat gain during storage

Sub-Topic 6.5.3: Novel gas separation membrane materials

Various techniques have been used so far for hydrogen separation; such as pressure swing adsorption, cryogenic processes or hydrogen separation membranes. Among them, hydrogen separation membranes represent a potential pathway for economical hydrogen separation. Various materials have been tested for the production of membranes for separation, depending on the temperature range and the impurities tolerance (polymers, ceramics, carbon, precious metals). Among them, dense ceramic membranes based on perovskites (doped $SrCeO_3$ or $BaCeO_3$) or other proton conducting ceramics such as niobate ($LnNbO_4$) showed high hydrogen selectivity in the gas separation at 500-800°C. Furthermore, recently new mixed proton-electron conductors (such as cermets based on Nickel and perovskite ceramics) showed higher performances in hydrogen permeability. The membrane structure is also under study by comparing dense ceramic membrane to asymmetric membrane having a dense film on a porous membrane. Challenges in the development of these technologies are to derive materials that combine good hydrogen permeability with sufficient chemical and mechanical stability.

Objectives:
Improvement of hydrogen purification and permeability and/or of membrane chemical and mechanical stability by development of materials for gas separation membranes; development of gas separation techniques

Expected Outcomes:
High-diffusion membranes with low cost

Topic 6.6: Safety, Codes and Standards for Other Hydrogen Production Methods

A critical review of Safety, Codes and Standards requirements will be performed relevant to Work Tasks 1-5 in collaboration with international partners, including US Department of Energy. This Work Task will target a range of areas, including but not limited to general issues of hydrogen safety, like formation and mitigation of flammable mixtures, and specific issues such as toxicity of products and deterioration of materials for particular production processes. Pre-normative research findings will be suggested for inclusion into existing and development of new Codes and Standards to facilitate commercialisation of cost-efficient and safe hydrogen production technologies.

Currently it is anticipated that the work will focus on:
(i) purity of hydrogen produced using various technologies,
(ii) safety strategies and engineering solutions for inherently safer hydrogen production (using methods outlined in Work Tasks 1-5) and handling;
(iii) codes and standards

Sub-Topic 6.6.1: Purity of Hydrogen produced using various Technologies

International Standards specify two grades of hydrogen fuel, namely: ‘Type I, Grade E’ and ‘Type II, Grade E’. Three categories are specified under Type I Grade E for both fuel cell manufacturers and hydrogen suppliers.

The purpose of International Standards are to establish hydrogen quality supplied for stationary and automotive applications as well as the infrastructure of hydrogen can be implemented quickly and efficiently towards fuel cell commercialization. Quality verification requirements should be determined at the inlet point of fuel cell systems between the supplier and the user. Since fuel cell applications for stationary and automotive and related technologies are developing rapidly, International Standards need to be revised according to technological progress as required. Bearing in mind that the technical Committee ISO/TC 197, Hydrogen Technologies, will monitor this technology trend.

It is also important to emphasize that International Standards are currently being developed to assist in the deployment of fuel cell applications for stationary and automotive and related technologies.

Further research and development are required to generate specific information so that a final consensus can be reached. These efforts should focus on, but not be limited to:

- Impurity detection and measurement techniques and methods for laboratory, manufacturing and in-field operations
- Effects/mechanisms of impurities on fuel cell systems and related components

Objectives:
Define methodologies for monitoring hydrogen quality under every-day circumstances; develop sensors; assess impact of reduced quality on hydrogen appliances

Expected Outcomes:
Identification of effect and cost of reducing vehicle hydrogen delivery by two points (99.9 in place of 99.999 purity); cost effective methods of monitoring hydrogen quality

Sub-Topic 6.6.2: Safety Strategies and Engineering Solutions

All aforementioned technologies (WT1-WT5) require safety studies starting from design stage through pilot installation use to industrial scale exploitation and decommissioning. Safety strategies relevant to hydrogen production (WT1-WT5) will be developed in WT6 based on the recent developments in the HySAFER centre at the University of Ulster and this research project. This will be underpinned by access of partners to the best European Infrastructure for Hydrogen and Fuel Cell Research (FP7 project H2FC European Infrastructure, 2011-2015, €8M).

Safety of each of the methods outlined in Work Tasks 1-5 will be assessed from the perspective of large-scale industrial production based on the analysis of published accident case studies. For example, industrial experience shows that bio-generated hydrogen can cause devastating accidents with life and property losses. Different routes of hydrogen production will be assessed by their toxicity level, pyrophoric properties, effect of reacting components on materials, propensity to self-heating and self-ignition when stored at large quantities, potential to create flammable mixtures with hydrogen and combust them in deflagrative and/or detonative regime, etc. Safety strategies will be developed following principles of avoiding formation of flammable mixture at operation temperature, pressure and composition, avoiding ignition sources or spontaneous ignition, and finally mitigation of accidental combustion if previous is impossible by technological reasons. ”Standard” safety issues like hydrogen leaks and dispersion in confined spaces, ignition and jet fires, deflagrations and potential for detonations (minimisation of deflagration-to- detonation transition potential in case of accidents) will be considered based on particularities of hydrogen production and handling methods.

Objectives:
assessment of hydrogen handling, especially within spaces (buildings)

Expected Outcomes:
guidelines for hydrogen use in confined spaces

Sub-Topic 6.6.3: Codes and Standards for Safe Production and Handling of Hydrogen

International Standards are intended to consolidate the hydrogen product specification needs anticipated by fuel cell manufacturers and hydrogen suppliers as industry proceeds towards achieving commercial opportunity and viability. Methods to monitor the hydrogen fuel quality that is produced and delivered require to be addressed and are necessary due to specific impurities which will adversely affect the fuel cell system. In addition, there may be drastic performance loss implications in the fuel cell system if non-hydrogen constituent levels are not properly controlled.

Objectives:
assessment of safety and risk in hydrogen production

Expected Outcomes:
guidelines for hydrogen safety in production and handling plants

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

Topic 6.1: Hydrogen from Biomass/Biowaste

Rationale: The activities will concern the improvement of the processes in order to increase the H2 purity and production, and develop a steady output of hydrogen from currently partly batch processes (SCWG and sub critical WG or APR). Catalyst development is targeted at avoiding impurities and pollutants at an early stage in the thermal processes and at lowering reactor temperature.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Improvement of catalyst robustness and lifetime, reduction of catalyst cost, reduction of overall cost of producing fuel cell fuels from biomass from thermochemical processes	Catalysts for fluidised bed and entrained flow biomass gasification with a lifetime of 40 000 hours, tar-cracking and tar and light hydrocarbon reforming catalysts for gasifiers, novel processes for reducing tar content of biomass syn-gases	Lifetime 40000hrs Cost target 3 $/kW Electrical conductivity >100 S / cm	High-performance gasifiers	Hydrogen production from biomass using non-noble metal catalysts	2	4

Improve the process control with view on optimising the quality of the hydrogen produced and achievement of a continuous process	Increase the stability of conversion processes and identify prospects of reaching high hydrogen fractions above 50% at a variation of +/- 5%		High-performance gasifiers	Continuous operation of waste gasification >10.000 hours	1	6
Increase the catalyst activity and selectivity in the continuous process. Increase the type of biowaste used in the process and its complexity	Increase the hydrogen productivity and widen the range of wet residues used in the process.	water content of feedstock up to 50% p(H2) > 50%"	High-performance gasifiers	Continuous operation of waste gasification with improved catalysts using optimised control (follows 6.2 & 6.4	2	4
Analyse the impact of various waste components on hydrogen and syn-gas quality and identify strategies to process specifically harmful components; standardise fuel quality prepared from waste	Develop control mechanisms that take varying fuel quality into account; develop in-process fuel quality assessment	demonstrati on run on standardised feedstock >1000 hours	High-performance gasifiers	Standardising waste-drived fuels and developing in-process fuel analysis methods	1	6

Topic 6.2: Hydrogen from Algae

Rationale: Hydrogen production by bacteria, algae or direct sunlight offer highly energy efficient and facile opportunities for energy supply and storage. The activities will concern the improvement of biological (algae or fermentation) and photocatalytic processes in order to increase the volumetric H2 productivity and simplify the reactors.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**

Analyse the dependency of hydrogen production of various species on insolation / illumination conditions and nutrition materials and supply; design optimised reactor configurations; test and evaluate hydrogen production rates; choice of algae suitable for high-efficiency lighting (e.g. LED)	Identification of algae species with photoconversion efficiencies above 5%	photoconversion efficiencies above 5%	Biological selection	Systematic selection of high-performing algae and bacteria	1	16
Analyse the effect of algae types and nutrition on hydrogen purity; design and evaluation of hydrogen separation processes (membranes etc.) to receive high purity gases from algae conversion	Production of hydrogen with purities of minimum 99%	hydrogen purities >99%	Polymer and metal membranes	Membrane development for algal and bacterial H2 production	3	8
Improvement of process properties and efficiency; combination and balancing of hydrogen and methane production	Increase of current rate of production by a factor of ten	n/a	Supporting bio-processes in algae and bacteria	In vitro biological water gas-shift reaction : Biofunctionalisation of carbon nanotubes with carbon monoxide dehydrogenase (CODH) and [NiFe]-hydrogenase	3	12

Topic 6.3: Hydrogen from Water Thermolysis

Rationale: In view of the prevailing material limitations, the possibility of lowering the operating temperature to some extent by catalysing the reaction appears as an attractive option.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€

Develop novel catalyst materials at moderated temperatures on hydrogen production from water, and CO production from CO_2	Reduction of reactor temperature	T<2500degC	Solar tower, solar concentration, coupling with SOE, combination with photocatalysis?	Novel catalysts for low-temperature thermolysis of water and CO_2	3	6

Topic 6.4: Hydrogen from Photocatalysis

Rationale: The activities will concern the development of nanostructured transition metal oxide semiconductor to maximise the light harvesting efficiency and to overcome the electron-hole recombination losses occurring are key challenges in a PEC water splitting cell. A range of nanostructured transition metal oxide semiconductor electrodes with the emphasis of water oxidation on photoanodic semiconductor/electrolyte interface will be investigated with the aim of meeting those challenges. Effort will be dedicated to find a substitute for Pt developing Transition Metal Carbides as possible co-catalyst in photocatalytic water splitting

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Improved electrode performance by identifying materials and material combinations having optimal bandgaps and optimal bandedge positions with respect to the oxidation and reduction reaction.	Higher yield of the photocatalytic process	Efficiency >5% and up to 10%	Photocatalysis	Co-doped $TiO_2 \vert Co_3O_4$ nanostructured heterojunction as photoanode for H_2 production by solar water splitting	2	3
Improve on today's best oxygen evolution catalyst (Co-phosphate) to further reduce the overpotential and enhance the oxygen evolution rate close to this minimal potential	Higher yield of the photocatalytic process	Efficiency >5% and up to 10%	Photocatalysis	Improved catalysts	2	3

Development of Pt-free catalysts for photocatalytic hydrogen generation; find methods to identify stable electrode materials (e.g. oxides) with an electronic diffusion length comparable to the light absorption depth	Cost reduction by replacing platinum as the catalyst	n/a (no costs associated to devices of technically relevant scale)	Photocatalysis	Nano-structured non-precious catalysts for water photo-dissociation and production of solar fuels	3	2
Using other fluids than water for photocatalytic hydrogen generation; due to limitations in the O2 generation process during photocatalytic water splitting, the use of alcohols as sacrificial reagents leads ro the concept of photocatalytic reforming of alcohols.	Higher flexibility of hydrogen production from fluids. Valorisation of a wide range of biomass-derived substances by photocatalytic reforming in aqueous solutions.	Efficiency >5% and up to 10%	Photocatalysis	Catalysts for H2 production by alcohols photoreforming	2	3
Development of efficient and robust photoreforming catalyst using residual biomass as sacrificial agent	Higher flexibility of hydrogen production from fluids	Efficiency >5% and up to 10%	Photocatalysis	Catalysts for H2 production by biomass photoreforming	2	3
Develop a water splitting device by developing materials combinations which are physically and chemically well-tuned to obtain the highest possible efficiency	Demonstrator device with a 10% efficiency, based on cheap and abundant materials	efficiency 10%	Photocatalysis	Development of multi-scale models for the engineering of artificial photosynthesis	3	2

Topic 6.5: Hydrogen compression, liquefaction and purification

Rationale: Pure hydrogen has the best energy-to-weight ratio of any fuel, but also has the lowest storage density of all fuels at atmospheric pressure. Preparing hydrogen for storage (purification, compression, liquefaction) requires considerable energy – this requires efforts in reducing energy demand. Biological purification processes often result not in pure hydrogen but syn-gas mixtures.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Drastically reducing energy demand for hydrogen compression	Reduction of hydrogen compression work by a factor of two	Reduction of hydrogen compression work by a factor of two	electrochemical compression by metal hydrides	Implementation of metal hydride pressure compressors for 70 MPa delivery applications	3	2
Improve the efficiency of hydrogen liquefaction processes, incl. storage	Reduced liquefaction energy demand and heat gain during storage	Reduced liquefaction energy demand and heat gain during storage	coupled technologies	Reducing H2 liquification energy demand by a factor of three	3	2
Improvement of hydrogen purification and permeability and/or of membrane chemical and mechanical stability by development of materials for gas separation membranes; development of gas separation techniques	High-diffusion membranes with low cost	not yet definied sufficiently	metal and ceramic membranes	Chemical stability and selectivity of hydrogen purification membranes in harsh atmospheres: H2O,CO,H2S, SOx,NH3,organics…Mechanical and chemical stability of hydrogen purification membranes at high working pressures and temperatures	2	3

Increase integration of H2 production and membrane separation processes; improve the efficiency of the production and separation on site, improve the stability of the membrane under reaction conditions, develop an integrated technology.	Increase the efficiency of small scale plant producing pure hydrogen.	not yet definied sufficiently	integrated membrane reactors	Implementation of metal hydride pressure compressors for 70 MPa delivery applications	2	3

Topic 6.6: Safety, Codes and Standards for Other Hydrogen Production Methods

Rationale: Pure hydrogen has the best energy-to-weight ratio of any fuel, but also has the lowest storage density of all fuels at atmospheric pressure. Hydrogen handling in the public domain will drastically increase in the close future and require a new look at safety standards.
Preparing hydrogen for storage (purification, compression, liquefaction) requires considerable energy – this requires efforts in reducing energy demand. In this respect, the importance of evaluation and proper benchmarking in hydrogen production technologies (catalysts for photocatalysis, e.g.) cannot be underestimated.

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Define methodologies for monitoring hydrogen quality under every-day circumstances; develop sensors; assess impact of reduced quality on hydrogen appliances	Identification of effect and cost of reducing vehicle hydrogen delivery by two points (99.9 in place of 99.999 purity); cost effective methods of monitoring hydrogen quality	Reduction from 99.999 to 9.99 quality	Monitoring, sensors, de-sensitivation of fuel cells	Hydrogen quality sensors PEFC for lower quality hydrogen	1	4
Assessment of hydrogen handling, especially within spaces (buildings)	Guidelines for hydrogen use in confined spaces	Guidelines draft delivered to stakeholders	Monitoring, sensors, compressors		1	1

Assessment of safety and risk in hydrogen production	Guidelines for hydrogen safety in production and handling plants	Guidelines draft delivered to stakeholders	Risk assessment		1	1
Assessment on measuring and reporting heterogeneous photocatalysis efficiencies	Guidelines for comparison of catalysts and water splitting devices efficiencies	Guidelines draft delivered to stakeholders	Photocatalysis	Risk assessment and guidelines for hydrogen use in buildings	2	2

Topic	**Main Outcome**	**Nr. projects**	**Budget (M€)**
6.1	Hydrogen from Biomass/Biowaste	4	20
6.2	Hydrogen from Algae	3	36
6.3	Hydrogen from Water Thermolysis	1	6
6.4	More efficient photocatalytic H2 production	6	16
6.5	Hydrogen compression, liquefaction and purification	4	10
6.6	Safety, Codes and Standards for Other Hydrogen Production Methods	4	8
Total		**22**	**96**

5. Contact Point for the sub-programme on 'Hydrogen Production and Handling'

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EERA

EUROPEAN ENERGY RESEARCH ALLIANCE

Joint Research Programme on Fuel Cells and Hydrogen technologies (JP FCH)

<u>SUB-PROGRAMME 7: *Hydrogen Storage*</u>

A sub-programme within the
Joint Programme FCH

IMPLEMENTATION PLAN 2018 - 2030

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Introduction

The Sub-Programme (SP) Hydrogen Storage will focus on the development of novel low cost and efficient hydrogen carriers and storage systems. All currently available hydrogen storage technologies fail to meet all requirements for application with respect to storage density, performance and cost of the storage systems at the same time. The main issues are caused by materials, designs and non-optimized integration with applications. Many different hydrogen carrier technologies are currently investigated, both in the solid and liquid state. These include hydrogen chemisorption (i.e. metal hydrides, complex hydrides, etc,) or physisorption in highly porous materials, as well as liquid organic carriers. Several basic aspects of these technologies are well established, but they are in an early stage of industrial development and need further fundamental research. SP7 on hydrogen storage will thus aim to address these important issues by researching and developing new materials, processes, and design of components, integration and BoP.

The Topics addressed in the Sub Programme are:

1. Compressed and Liquid Hydrogen Storage
2. Hydrogen carriers
3. Hydrogen Storage Systems

The activities cover different timeframes (short, medium and long term) and the programme scope will be evaluated and discussed thoroughly after a state of the art review. SP7 focuses on existing technologies, R&D status and needs, as well as safety related issues. Based on this, research orientations will be given and main challenges towards industrialization will be identified. SP7 addresses the evaluation of the different hydrogen storage technologies through multiple criteria: technical performances, safety, social acceptance, economics and environmental impact. After the identification of the evaluation criteria, a database will be initiated to collect and share all the information gathered from the state of the art. Finally, the developed evaluation methodology will be implemented on selected cases, both for transport and stationary applications, as these applications have to face different challenges.

Over the initial period of the programme, substantial improvements are expected in the topics listed in order to enable industry to then employ these results in prototype developments. Progress will be mapped out during periodic workshops and reviews in order to fine-tune and readjust the programme, if required.

The activities are not only centred around research but also encompass student and staff exchange in order to strengthen the networking between the groups involved, since the activities described here still appear fragmented across Europe.

1. Background

The main motivation for this EERA initiative on hydrogen storage is to complement existing European programs, especially in the Energy part of the H2020 Program and in the Fuel Cell and Hydrogen Joint Undertaking (FCH JU) by sharing and harmonising regional, national and European initiatives. Whereas running EU projects gather limited number of partners on highly focused subjects, the main ambition of this EERA Sub-Programme, on the contrary, is to contribute in building a comprehensive and consistent picture of all the R&D activities related to hydrogen storage that are on-going in the member states, being either funded by the regions, by national grants or by European ones. This picture will be based on non-confidential information shared by the EERA partners and also on information coming from other European and international institutions.

Based on this consensual picture, together with well-established and mature technologies on compressed gas and liquid hydrogen storage, it will be possible to identify the hydrogen carriers that have already reached a high technology readiness level and those that are less mature but are found to be promising and to deserve more research work.

2. Objectives

The overall objective of this sub-programme is to build a comprehensive and consistent picture of all the R&D activities related to hydrogen storage that will serve as a technical-scientific basis to orientate further development on hydrogen for the storage of energy. The maturities of the technologies considered in this

SP are extremely diverse and the challenges to address are multiple. A common state of the art review will be achieved that will allow establishing a research and development agenda for each technology.

Depending on the knowledge bases and the technology readiness levels of each technology, an aggregation of the R&D work done by the partners will pave the way towards system engineering. As hydrogen storage in carriers is a less mature technology than gaseous or liquid storage, the activities will specifically focus on R&D status and identification of technical challenges. Specific attention will be given to the identification of common testing methodologies and of common evaluation criteria, in order to build and introduce a consistent and harmonised research approach.

After identification of the main technological gaps, the SP will present a set of concrete recommendations and priorities for future research and development liable to accelerate the deployment and market entry of most advanced hydrogen storage in complete system. The main conclusions will be proposed as R&D orientations for removing technology barriers and accelerating future implementation of hydrogen storage for both transport and stationary applications.

3. Description of foreseen activities

This SP aims to provide contributions for the developments of systems for the storage of hydrogen. Various approaches for hydrogen storage will be investigated: gaseous and liquid (Topic 1) or using hydrogen carriers (Topic 2), such as absorption in hydrides, adsorption on surfaces or via chemical hydrides. Combined technologies of hydrogen storage, as well as the integration of hydrogen storage system with fuel cells for mobile and stationary applications, will be investigated (Topic 3). Activities will be performed in collaboration with other SPs of the Joint Program on Fuel Cells and Hydrogen, considering also safety issues and Standard and Codes for hydrogen storage.

The activities considered in this sub-programme description cover a 5 year time frame. A preliminary analysis of the state-of-the-art will allow the partners to build the full picture representation of the different hydrogen storage technologies. It will reflect the current understanding of the general research needs with respect to the storage of hydrogen.

SP7 addresses the use of hydrogen as an energy storage media and will focus on storage of hydrogen in gaseous form, at pressures high enough to provide 700 bars service pressure of tank, liquid form and via hydrogen carriers, i.e. absorbed (metal hydrides and chemical hydrides, etc.) or adsorbed on surfaces (carbon nanotubes, Metal Organic Frameworks. etc.), as well as bonded in organic compounds. Developed hydrogen tanks will be analyzed in light of systems integrated with fuel cells, in small to medium size power-to-power systems as well as photoelectrochemical and biomass based hydrogen production systems. Hydrogen storage will be considered for various applications, including stationary storage of renewable energy, and mobile storage for FC-based vehicles. Different uses of stored hydrogen will be also considered, such us industrial needs, conversion in turbines, as well as a reactant for CO_2 conversion into synthetic fuels.

Topic 7.1: Compressed Gas and Liquid Hydrogen Storage

Sub-Topic 7.1.1: Compressed Gas Hydrogen Storage

Objectives:
Studies for gaseous storage are related to innovative tank manufacturing processes, hydrogen enhanced fatigue understanding, or instrumentation for crack initiation detection, etc. Safety, reliability, test methodologies are the key challenges for introduction of gaseous hydrogen for hydrogen storage, both for transport applications and for hydrogen storage vessels in Hydrogen Refuelling Stations.
Focus of the research on compressed hydrogen storage is expected to be on

- Enhancing the safety of the stores
- Identifying potentials for decreasing cost
- Materials selection for tank production
- Control of charging and discharging process

Key Actions:

- Investigation of materials alternative to carbon fibres at pressures lower than currently used, e.g. glass or aramid fibres
- Investigation of materials alternative to polyamide 6 or ultra-high polyethylene density for manufacture the liners

- Use of graphene in small percentages in carbon fibres, glass or aramid fibres in order to improve the mechanical resistance and decrease the weight
- Effect of materials selection on hydrogen lines, valves, P regulators, etc.
- Use of active temperature control system of the tank during fast discharging, artificial neural networks, artificial immune control systems, model based predictive control, etc

Expected outcome:
- Innovative tank manufacturing processes
- Innovative control system of the fast recharging high pressure hydrogen tank

Sub-Topic 7.1.2: Liquid Hydrogen Storage

Objectives:
As for liquid hydrogen storage, due to the maturity of cryogenic liquid hydrogen storage technologies, little fundamental research is expected. Investigations on materials for tank production will be carried out. Efficiency of liquefaction processes will be investigated, in order to reduce hydrogen storage costs. Boiling-off problems will be considered.
Focus of the research on liquid hydrogen storage is expected to be on
- Enhancing the safety of the stores
- Identifying potentials for decreasing cost
- Liquefaction processes
- Cryomanagement for tanks
- Materials selection for tank production

Key Actions:
- Effect of liquid hydrogen on materials selection for connection lines, valves, P regulators, etc.

Expected outcome:
- Enhanced understanding on effects of cryogenic liquid hydrogen to materials.

Topic 7.2: Hydrogen Carriers

Sub-Topic 7.2.1: Solid State Hydrogen Storage in Complex and Metal Hydrides

Objectives:
This work package will focus on storage of hydrogen in solids, i.e. absorbed in metal and complex hydrides. A state-of-the-art review will allow identifying the most relevant on-going research work and future research directions. In this Sub-Topic, partners will share experimental results, methodologies, analysis methods and will contribute to define research work orientations.

Work on complex and metal hydrides will include synthesis of materials for reversible hydrogen storage from the gas phase, structural and spectroscopic investigation, and hydrogen absorption-desorption characterization. Thermodynamic and kinetic aspects of hydrogen sorption reactions will be investigated in detail. Modelling on atomic-molecular level, as well as assessment of thermodynamic and kinetic properties of investigated materials, will support experimental investigations.

New materials for (reversible) hydrogen storage will be investigated. Characterization of phase-structural composition, kinetics and thermodynamics of the metal-hydrogen interaction. The analysis of possible reversible reactions will be considered. The goal is to develop materials with hydrogen storage capacities in the 5 – 10 wt.% range and > 50 g H_2/l at working temperatures lower than 200 °C. Scale-up and cost decrease will be also investigated.

Collaboration with SP6 Hydrogen Production and Handling is expected in the field of hydrogen compression based on use of metal hydrides for the compressors, e.g. with respect to characterisation of hydrogen sorption properties, thermodynamics and kinetics, and selection of optimal materials for both, storage and compression.

Focus of the research on complex and metal hydrides is expected to include:
- Development of new materials (metal hydrides, intermetallics, alanates, borohydrides, amides/imides, ammoniaborane, etc.)
- Characterization of phase-structural composition, kinetics and thermodynamics of the metal-

hydrogen interaction.
- Basic understanding of hydrogen sorption mechanisms and properties in complex and metal hydrides
- Efficient synthesis and nanostructuring of hydrides (wet chemistry, ball milling, etc.) for scale-up and cost decrease
- Avoidance of Critical Raw Materials as far as possible
- Consideration of recyclability of hydrogen storage materials
- Hydrogen storage materials for stationary and mobile applications.

Key Actions:

- Complex hydrides based on light elements.
- Amide/imide based materials
- Hydrogen storage in novel intermetallic alloys, e.g. bcc alloys, FeTi, high entropy alloys
- New RE-Mg-TM ternary hydrides for hydrogen storage at ambient conditions
- Mixed systems based on ammonia borane and/or borohydrides
- Highly substituted complex hydrides
- High entropy hydrides
- Materials being unstable at ambient conditions, but stabilised under higher hydrogen pressures

Expected outcome:

- Materials with capacities in the 5 - 10wt.% range and >50 g H_2/l
- Working temperatures <<200 °C
- Scale-up and cost decrease

Sub-Topic 7.2.2: Solid State Hydrogen Storage in porous materials

Objectives:
Hydrogen storage via absorption on surfaces of porous materials (e.g. carbon based structures, Metal Organic Frameworks, etc.) will be investigated in this Sub-Topic. The characterization of phase-structural composition, kinetics and thermodynamics of the metal-hydrogen interaction will be performed. An analysis of possible reversible reactions for different materials will be carried out. The goal is to develop materials with high hydrogen storage capacities at suitable working temperatures. Scale-up and cost decrease will be also investigated.

Focus of the research on porous materials is expected to include:
- Synthesis of porous materials for H_2 storage.
- H_2 storage capability characterization.
- Nanoconfinement of metallic/complex hydrides in porous materials
- Novel nanomaterials design pathways for hydrogen storage

Key Actions:

- Hybrid materials using TM-alloys@MOFS for combining hydrogen ad- and absorption at low temperature
- Increase of adsorption heat and hydrogen storage by the a combined effect of chemisorption on well dispersed metallic particles and appropriate textural properties
- Hydrogen storage in clathrates and porous ice

Expected outcome:

- Materials with capacities in the 5 – 10 wt.% range and >50 g H_2/l
- Working temperatures <<200 °C
- Scale-up and cost decrease

Sub-Topic 7.2.3: Hydrogen Storage in Liquid Compounds

Objectives:
In this Sub-Topic, hydrogen storage will be considered through chemical hydrides. When applicable, some of these chemicals will be also considered as energy carriers themselves. Liquid energy carriers will be specifically investigated. e.g. liquid organic compounds for hydrogen storage (LOHC). In this Sub-Topic, also investigations will be carried out on solid materials (e.g. LiH and $NaBH_4$) for hydrogen storage, via hydrogen release due to reactions with suitable liquid solvents (e.g. hydrolysis with water).

Focus of the research on liquid compounds is expected to include:
- Liquid organic compounds for hydrogen storage.
- Catalysts development.
- "Green" Ammonia, Methanol and Ethanol as liquid hydrogen carrier
- H_2 storage capability characterization.
- Mechanism of hydrogen sorption reactions.
- Development of heterogeneous catalysis processes without Pt and/or Critical Raw Materials (CRM)
- Selection of chemical hydrides for irreversible hydrogen storage.
- Hydrogen release from suitable compounds via solvent reactions (e.g. hydrolysis with water). Analysis of recovery of the compounds and reloading.

Key Actions:
- Novel LOHC's (aromatics, alcohols, etc.)
- Formic acid as organic liquid hydrogen carrier
- Green ammonia, methanol and ethanol process production, storage and hydrogen remove (catalytic, electrochemical, etc.).
- Materials for hydrogen generation via solvent reactions
- Controlled hydrolysis and recovery of by-products of low-cost metal and hydride compounds

Expected outcome:
- Materials with capacities in the 5 – 10 wt.% range and >50 g H_2/l
- Working temperatures <<200 °C
- Catalysts development for operation at low temperatures as well as replacing noble metals
- Improving catalytic activity and durability
- Scale-up and cost decrease

Topic 7.3: Hydrogen Storage Systems

Sub-Topic 7.3.1: Hydrogen Storage in Combined Technologies

Objectives:
The development of combined technologies will be considered in this Sub-Topic. In particular, the benefit obtained by hydrogen gas-compression will be coupled with solid-state hydrogen storage materials. Mix between high pressure storage and LOHC, ammonia, methanol and ethanol for Hydrogen Refuelling Stations will be also investigated. The goal is to provide a proof-of-concepts of combined hydrogen storage technologies in real systems.

Focus of the research on combined technologies is expected to include:
- Cryo-compressed hydrogen storage
- Compressed – solid state hydrogen storage
- Compressed – liquid hydrogen carrier storage
- H_2 storage capability characterization.
- Identification of potentials for lowering cost compared to SoA hydrogen stores

Key Actions:
- Cryo-compressed systems
- Compressed - solid-state hydrogen storage systems
- Compressed – liquid hydrogen carrier storage systems

Expected outcome:
- Proof-of-concepts of combined hydrogen storage technologies

Sub-Topic 7.3.2: Integration of Hydrogen Storage Systems

Objectives:
Within this Sub-Topic, challenges related to system engineering will be identified and a set of recommendations and priorities will be defined. Reliability, cost optimization and energy efficiency will be the main topics to be addressed. Partners will define methodologies and roadmaps to favour the

industrialization of hydrogen storage technologies for transport and stationary applications. System integration of H_2 storage tanks with fuel cell systems for mobile applications will also be addressed in regard to thermal and energy management, as well as operating strategies. Storage systems from H_2 sources at low pressures (bio-production, electrolyzers, etc.) will be developed. Connections of hydrogen storage with chemical reactors and turbines will be also considered. Reliability, cost optimization and energy efficiency will be specifically considered. Demo systems at a lab scale will be provided when applicable.

Like in Sub-Topic 7.2.1., collaboration with SP6 on Hydrogen Production and Handling is expected with respect of integration of hydrogen compression and hydrogen storage technologies, which e.g. might lead to integrated hydrogen compression and storage systems, both based on hydrogen carriers.

Focus of the research on system integration is expected to include:

- Hydrogen carrier based hydrogen storage systems for stationary and mobile applications
- Development and experimental proof of new storage reactor concepts (kinetics, simulation, thermal management and innovative material concepts).
- Integration with fuel cell systems.
- Thermal management.
- Techno-economical assessment.
- Life Cycle Analysis

Key Actions:

- Integration of hydrogen carrier based stores with FC systems
- Integration of hydrogen carrier based stores with low pressure hydrogen generation systems (e.g. electrolysers, photoelectrochemical hydrogen generation, hydrogen from biomass)

Expected outcome:

- Demo systems at a lab scale

Sub-Topic 7.3.3: Safety Strategies

Objectives:
A critical review of Safety requirements will be performed, based on results of other topics, also in collaboration with international partners, including US Department of Energy.
This Sub-Topic targets a range of areas, including but not limited to general issues of hydrogen safety, like formation and mitigation of flammable mixtures, and specific issues such as toxicity of products and deterioration of materials for particular production processes. Assessment of safety strategies for hydrogen storage, both in mobile (e.g. FC vehicles) and stationary applications (e.g. buildings).

Focus of the research on safety is expected to include:

- Safety strategies for hydrogen storage
- Engineering solutions for hydrogen storage

Key Actions:

- Guidelines for safe hydrogen storage in confined spaces
- Demo systems development

Expected outcome:

- Safety strategies, guidelines and engineering solutions

Sub-Topic 7.3.4: Codes and Standards for Hydrogen Storage

Objectives:
Pre-normative research findings will be suggested for inclusion into existing and development of new Codes and Standards to facilitate commercialisation of cost-efficient and safe hydrogen storage technologies.

Focus of the research on Codes and Standard is expected to include:

- Testing procedures for hydrogen tanks
- Codes and Standards related to hydrogen storage worldwide
- Deficits with relation to novel storage technologies like hydrogen carriers and hybrid storage systems
- Codes and Standards for integrated fuel cell and/or hydrogen generation – hydrogen storage

systems
- PNR on hydrogen carrier based hydrogen storage systems

Key Actions:
- Assessment of codes and standards for hydrogen storage.
- Definition of normatives for hydrogen storage in European Countries.

Expected outcome:
- Definition of normatives for hydrogen storage in European Countries

4. Approximate project implementation and required budget

The topics described above are here schematized, prioritized and given a preliminary indication of required budget for their adequate addressment.
In terms of the prioritization, the following legend applies:

1. **Urgent Priority: implement as soon as possible**
2. **High Priority: implement after 2020**
3. **Medium Priority: implement after 2025**

Topic 7.1: Compressed gas and Liquid Hydrogen Storage

Rationale: Safety, reliability, test methodologies are the key challenges for introduction of gaseous hydrogen for hydrogen storage, especially for transport applications. Due to the maturity of cryogenic liquid hydrogen storage technologies, little fundamental research is expected. Materials for tank production and efficiency of liquefaction processes need to be investigated

Specific Challenges	**Expected outcome**	**KPIs**	**Technologies suited**	**Possible Project Title**	**Priority**	**Budget M€**
Enhancing the safety and decreasing cost of the gaseous hydrogen stores	Innovative tank manufacturing processes	Tank capacity 2-3 kg/tank module Tank Capex 500 €/kg H2 for large scale production Tank charging time 3 min	Hydrogen stored as compressed gas	Investigation of materials alternative to carbon fibres at pressures lower than currently used, e.g. glass or aramid fibres	1	3
				Effects on hydrogen lines, valves, P regulators	1	1
				Control systems for fast recharging of high pressure hydrogen tanks	1	1
Identify potentials for decreasing cost of liquefied hydrogen stores	Enhanced understanding on effects of cryogenic liquid hydrogen to materials.	Liquefaction efficiency ≤6.5 kWh/kg H2 Tank Capex H2 Tank Boiloff time H2 Tank offloading time	Hydrogen stored as cryogenic liquid	Effects of liquid hydrogen on connection lines, valves, P regulators, etc.	3	1

Topic 7.2: Hydrogen Carriers

Rationale: Hydrogen Storage in complex and metal hydrides, in porous materials, or in liquid compounds as well as materials based hydrogen compression is expected to improve hydrogen storage density and/or overall energy efficiency and thus decrease its cost, when compared to SoA compressed or liquefied hydrogen storage.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
New materials for (reversible) hydrogen storage. Characterization of phase-structural composition, kinetics and thermodynamics of the metal-hydrogen interaction. Analysis of possible reversible reactions.	Materials with capacities in the 5 - 10wt.% range >50 g H2/l at working temperatures <<200°C.	Working temperature < 200 °C Charge / discharge efficiency >95 % Discharge energy use up to 10 kWh / kg H2 Loss of storage capacity less than 0.2 % per cycle Carrier gravimentric density up to 10 wt% H2, depending on application Carrier volumetric density ≥ 50 kg H2/m3	Hydrogen Storage in Solid Materials	Amide/imide based materials	1	2
			Hydrogen storage for stationary applications.	Hydrogen storage in bcc alloys	2	1
			Hydrogen storage for niche mobile applications	Complex hydrides based on light elements.	2	1
			Stationary hydrogen storage tank. Long-term energy storage of renewable energy sources	New RE-Mg-TM ternary hydrides for solid hydrogen storage at ambient conditions	2	1
			Hydrogen Storage in Solid Materials	mixed systems based on ammonia borane and/or borohydrides	2	1
			Basic understanding of properties of complex hydrides	Highy substituted complex hydrides	2	1
			Basic understanding of properties of metal hydrides	High entropy hydrides	2	1
			Hydrogen Storage in Solid Materials	Materials being unstable at ambient conditions, but stabilised under higher hydrogen pressures	2	1
Characterization of phase-structural composition, kinetics and thermodynamics of the metal-hydrogen interaction. Analysis of possible reversible reactions. Examples: graphene-based porous materials, organometallics for H2 storage.			Nanoconfinement of metallic/complex hydrodes in porous materials	Hybrid materials using TM-alloys@MOFS for combining hydrogen ad- and absorption at low temperature	3	1
			Hydrogen Storage in Porous Materials	Clathrates, porous ice	3	2
Liquid organic compounds for hydrogen storage (i.e. LOHC). Chemical hydrides and	Materials with capacities in the 5 - 10wt.% range and >50 g H2/l		Development of heterogeneous catalysis processes	1.-Sodium borohydride solutions for liquid-state chemical hydrogen storage. Other compounds like ammonia borane are also included.	1	3

reactions in the liquid phase (i.e. hydrolysis of complex hydrides).	at working temperatures <<200°C. Catalysts development for operation at low temperatures as well as replacing noble metals. Improving catalytic activity and durability. Scale-up and cost decrease.		Development of heterogeneous catalysis processes (no Pt, CRM)	2.-Formic acid as organic liquid hydrogen carrier.	1	3
			Synthesis, catalysis	novel LOHC's (aromatics, alcools, etc.)	1	2
			Synthesis, catalysis	Controlled hydrolysis and recovery of by-products of low-cost metal and hydride compounds	2	2
Materials for hydrogen compression up to 900 bar and more (in collaboration with SP6)	Decrease of cost of hydrogen compression, especially energy cost and OPEX	Input pressure ≤ 20 bar Output pressure up to 900 bar	Hydrogen carriers, being able to release hydrogen at high pressures up to 900 bar and more for materials based hydrogen compressors	Metal hydrides	2	2

Topic 7.3: Hydrogen Storage Systems

Rationale: Hydrogen Storage in combined technologies, integration of hydrogen storage systems in the suitable applications (e.g. electrolysis, fuel cells, direct supply of hydrogen to refuelling stations, glas or metal industries, etc.) and research on corresponding Codes and Standards are necessary development steps, to bring optimised storage technologies into application and the market.

Specific Challenges	Expected outcome	KPIs	Technologies suited	Possible Project Title	Priority	Budget M€
Coupling the benefits obtained by hydrogen gas-compression with solid-state hydrogen storage	Proof-of-concepts of combined hydrogen storage technologies	Working temperature << 200 °C Charge / discharge efficiency >95 % Discharge energy use max 10 kWh/kgH2 Tank gravimentric density up to 5 wt% H2, depending on application Tank volumetric density ≥40 kgH2/m3	Hydrogen Storage in Solid Materials and gas phase	Cryo-compressed, compressed-solid-state	1	3
				Cryo-compressed, compressed-solid-state, based on porous ice	2	2
Reliability, cost optimization and energy efficiency	Demo systems at a lab scale		Hydrogen carrier based hydrogen storage systems for stationary applications	Integration of hydrogen carrier tank with FC system	1	2

Formation and mitigation of flammable mixtures, toxicity of products and deterioration of materials for particular production processes	Safety strategies, guidelines and engineering solutions	Not applicable	PNR on safety for hydrogen storage systems	Normative definition	2	1
Deficits of normative with relation to novel storage technologies like hydrogen carriers and hybrid storage systems	Definition of normatives for hydrogen storage in European Countries	Not applicable	PNR on hydrogen carrier based hydrogen storage systems	Normative definition	2	1

Topic	Main Outcome	Nr. projects	Budget (M€)
7.1	Compressed gas and Liquid Hydrogen Storage	4	6
7.2	Hydrogen Carriers	15	24
7.3	Hydrogen Storage Systems	5	9
Total		**24**	**39**

5. Participants

Name	Country
CEA	France
CNH2	Spain
CNR	Italy
CNRS	France
CSIC	Spain
DLR	Germany
DTU	Denmark
ENEA	Italy
FBK	Italy
HZG	Germany
IFE	Norway
IPE, WUT	Poland
JRC	The Netherlands
TECNALIA	Spain
TU DELFT	The Netherlands
UNIBHAM	UK
UNIBO	Italy
UNIPD	Italy
UNITO	Italy
UNIUTRECHT	The Netherlands
WUT	Poland

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