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Deliverable

D4.1 Scientific Bottlenecks for Commercialization of H₂ & FC Technologies

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1 Introduction

For successful entry into relevant markets, hydrogen and fuel cell technologies face a series of technical challenges as previously documented e.g. by the European Commission and the U.S. Department of Energy. They are also facing institutional and economic challenges as they have to enter a marketplace where neither regulations nor economical business models are ready for them.

The present deliverable report is framed within the H₂FC European Infrastructure projects WP4 - Foresight, Knowledge, Innovation, which is one of the 5 networking activities within the project. In this WP, Task N3.1 – Specification of key scientific bottlenecks aims to "translate" the technology requirements for hydrogen and fuel cell technologies into a specification of the fundamental scientific bottlenecks these correspond to. This report also considers which approaches should be pursued to solve them, including the use of advanced research methods and the related infrastructures. The scientific bottlenecks may include aspects such as need of enhanced understanding of material properties at micro and nanoscale, detailed study on the stability issues (caused by materials degradation), the need for new and low cost materials (e.g., catalysts) with better performance, or need for better modelling tools etc.

It is worth noting that the maturity of the different technologies considered here are very different. Many technologies are already technologically mature for deployment and are facing essentially institutional and economic challenges. It is however possible for them to identify from return of experience, some weaknesses to be addressed for preparing a second generation. On the contrary for some less mature technologies, technical bottlenecks remain numerous.

In this deliverable report, scientific bottlenecks are extracted and compiled from a selection of reports and from the partners of the consortium who, as experts in the field, have provided specific information on different technologies. From comparison of these data, the final aim of this WP task is to validate the relevance of existing infrastructures for solving current scientific bottlenecks in the field of hydrogen and fuel cells related technologies, to develop suggestions for revision of the on-going research in the Joint Research Activities (JRA) in order to adapt current infrastructures to the needs highlighted and finally to identify, if any, totally missing infrastructure.

2 Relevant reports

In this section the reports used as background material/references in this deliverable are presented. The detailed content of each report is not repeated in full here, however, is meant to be used for further discussion of the input provided by the H_2FC consortium. As indicated in the following, the reports considered here have different approaches with respect to how to categorize the hydrogen and fuel cell technologies. There is a significant overlap between the defined challenges and focus areas for different topics and the essence of each report is summarized in the following paragraphs. However, for a complete overview and exact details, we refer to the original documents which are accessible to the public through the sources indicated in footnotes.

2.1 European Commission - Materials Roadmap Enabling Low Carbon Energy Technologies¹

This materials roadmap is prepared to complement and expand the technology roadmaps previously developed in the context of the SET-Plan as the basis for its implementation. It intends to facilitate development of key materials research and innovation activities for advanced energy technologies. The roadmap aims at serving as a guide for basic R&D activities in the field of materials for energy applications, including hydrogen and fuel cell technologies, to assess and/or to improve the properties of current materials and orientate ground breaking researches towards preparing second generation of materials. As such, it defines challenges that are much more basic and long-term oriented than the DOE research program. The document defines 5 specific focus areas for *materials R&D and related product development* for hydrogen and fuel cells:

1. *Ionic and electronic conductors (for electrolytes, catalyst carriers, bipolar plates, gas diffusion layers)*

For electrolytes, technical challenges concern the development of proton conducting polymers and high temperature proton and oxygen ion conducting materials with improved properties and reduced cost, along with the need for Health, Safety and Environment (HSE) considerations (i.e. for recycling of materials). For the electronic conductors, development of more efficient and cheaper bipolar plates, cell spacers and current collectors, improved corrosion and mechanical stability of gas distribution layers along with development of stable and conductive catalyst-carriers with large surface areas are highlighted.

2. Catalysts (for low and high temperature applications and steam methane reforming) The need for development of supported catalysts with reduced loading of novel metals for low temperature application is pointed out along with challenges with carbon corrosion and Pt dissolution in PEM fuel cells and need for improved catalysts for alkaline media. For high temperature applications, need for improved efficiency, durability and tolerance to fuel and steam impurities is a key material challenge.

¹ <u>http://ec.europa.eu/research/industrial_technologies/pdf/materials-roadmap-elcet-13122011_en.pdf</u>

3. **Other functional materials** (for hydrogen purification, storage and thermomechanical cycles)

For hydrogen purification materials, development of gas-adsorption materials with improved sorption kinetics and selectivity along with new improved hydrogen separation membrane materials (ceramic, Pd-alloy, organic) and optimization of membrane thickness/microstructure- are highlighted as challenges.

For hydrogen storage materials, metal-hydrides & physisorption-based storage materials, chemical hydrides and complex hydrides need further research work and specific improvements. The development of materials for innovative concepts like solid-pressurized hydrogen storage is also mentioned as a need. Improved reactor chemical stability and reaction kinetics for metal/oxide systems for application in thermochemical cycles are also highlighted.

4. **Structural materials** (for storage of pressurized (small and large scale), cryogenic and cryo-compressed H₂, transport of H₂, coal gasification, thermochemical cycles and sealants)

The need for development of new and innovative materials for storage of pressurized, cryogenic and cryo-compressed hydrogen is highlighted along with investigation of corrosion mechanisms and effects of sulphur on materials for large scale storage, corrosion and embrittlement of materials for transport, coal gasification and thermochemical cycles. Furthermore the need for satisfactory seal materials is underlined.

5. **Novel materials** (advanced electrolytes, advanced catalysts, advanced photo-materials, advanced materials for H₂ storage)

More basic research on innovative concepts is needed for ionic conductors, for developing new non-Platinum Group Metals (PGM) catalysts for low T acidic applications such as PEMFC or PEM-electrolysis. It is suggested as well that development of advanced materials for photo-electrochemical applications and innovative hydrogenated materials with enhanced capacity/reversibility and high tensile strength materials for hydrogen storage is required.

Regarding *materials integration and component technologies*, guidelines for further development of manufacturing processes and technology testing is given. A paragraph related to hydrogen and fuel cells *research infrastructure* discusses and indicates needs for test facilities and virtual centres.

2.2 Fuel Cells and Hydrogen Joint Undertaking (FCH JU)²

The Multi-Annual Implementation Plan (MAIP) of the FCH JU outlines the scope and details of the initial planning of the research, technological development and demonstration (RTD) activities for the time frame 2008 - 2017. It also describes the objectives of the FCH JU, the policy and global context, technical targets, required actions for the implementation of the JTI and governance structure. The document covers the priority areas listed below; by construction it is focused on the short and medium term research contrarily to the Materials roadmap.

• Transport & Refuelling Infrastructure

² <u>http://www.fch-ju.eu/sites/default/files/documents/fch_ju_multi_annual_implement_plan.pdf</u>

Large scale fleet demonstration is in focus here in order to demonstrate durability, robustness, reliability, efficiency and sustainability of vehicles and infrastructures. Integration of fragmented PEMFC stack R&D is needed, mainly addressing PEMFC technology for transport applications. Other RTD activities of importance are hydrogen quality requirements and standards, design and test criteria for high pressure composite and solid state storage tanks, fast refueling protocols and standards, crash tests and safety for hydrogen powered vehicles.

• Hydrogen Production & Distribution

On a long term there is a goal to develop and implement a portfolio of costcompetitive, energy efficient and sustainable hydrogen production, storage and distribution processes, however, on short term the focus is suggested to be put on R&D related either to mature technologies or to long term and breakthrough oriented research. Among the mature technologies in focus are (i) reforming based on bio and fossil fuels, (ii) low T electrolysers, (ii) biomass to hydrogen (BtH). Cooperation with the Zero Emission Platform is recommended to demonstrate carbon lean/free hydrogen production.

Also highlighted is demonstration of high volume, high safety hydrogen storage in synergy with energy storage requirements from variability/intermittency of renewable energy sources connected to the grid.

• Stationary Power Generation & Combined Heat & Power

Stationary power generation and CHP markets require improved technology for fuel cell stack and BOP components. Product validation and up-scaling of manufacturing capabilities are proposed for deployment for the main fuel cell technologies (i.e. SOFC, PEMFC). Long term and breakthrough oriented R&D on materials degradation/lifetime fundamentals is however also required. Technology validation and market capacity in form of proof-of-concept fuel cell systems are needed as well as full scale demo plants. Coordination with R&D for on-board power generation (Transport & refuelling) is required to promote and take advantage for synergies.

• Early Markets

Short term demonstration and ready-to-market products; (i) portable and micro fuel cells, (ii) portable generators, back-up power and UPS-systems, (iii) specialty material handling vehicles incl. related hydrogen refuelling infrastructure. Main foreseen research areas include; reduce cost for FC systems/optimization of BOP, improve efficiency and lifetime, enhance fuel supply for FC application (reduced hydrogen delivery cost, expand fuel cell sources, extend system operation time – improved storage systems). Better integration of SMEs in industrial supply chains for utilization of innovative ideas and product development.

• Cross-Cutting Issues

Evaluation of socio-economic, environmental and energy impact of FCH technologies. Coordination of Regulations, Codes and Standards strategy. Frameworks and schemes to help SMEs develop a supply chain for FCH technologies.

2.3 U.S. Department of Energy – Hydrogen and Fuel Cells Program Plan³

In this document the complete plan for the Department of Energy's Hydrogen and Fuel Cells Program is presented. This includes the technology requirements for widespread application of hydrogen and fuel cell technologies which are summarised in Figure 2.1.

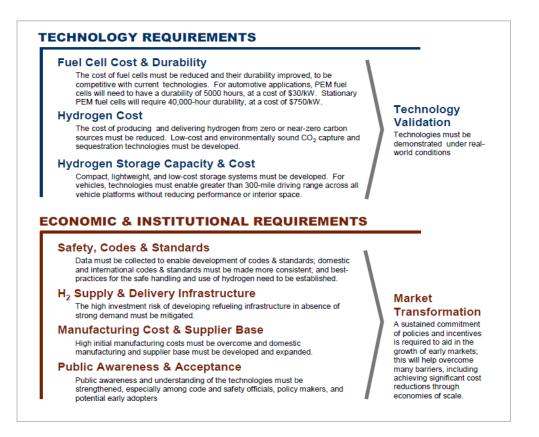


Figure 2.1 The Technology and Economic& Institutional Requirements for widespread Commercialization of Hydrogen and Fuel Cells (US Dept. of Energy³)

2.4 U.S. Department of Energy – Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan⁴

This document describes the planned research, development, and demonstration activities for hydrogen and fuel cell technologies in the U.S. Chapter 3 of this report, *Technical Plan*, provides a detailed outline of the various activities occurring within the technical sub-programs as defined as follows;

³ The Department of Energy Hydrogen and Fuel Cells Program Plan, US Department of Energy, Information Centre, <u>http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/program_plan2011.pdf</u>

⁴ <u>http://www1.eere.energy.gov/hydrogenandfuelcells/mypp/</u>

3.1 Hydrogen Production, 2011 Interim Update Updated September 2011

For *Hydrogen Production with a low carbon footprint* the main t challenge is the cost of delivered hydrogen which with current technologies is too high. More specific challenges are i.e. capital costs of water electrolysis systems along with high electricity prices (and need for cleaner power) and high cost of bio-derived liquids for reforming of e.g. ethanol and pyrolysis oil. For less mature technology such as biomass conversion, a technical challenge is the low efficiency of the process. Immature technologies like high-temperature, solar driven, thermochemical production using water splitting chemical cycles, photoelectrochemical production – direct water splitting (efficiency, material cost) and biological production are also mentioned as deserving basic research work prior to any demonstration and deployment.

<u>3.2 Hydrogen Delivery, 2007</u>

The main challenge for *Hydrogen Delivery* is not technical by nature but economical: it is the high investment costs of the technology/high risk for not obtaining profitable return for stakeholders. However, several technical challenges are listed. They include need for improved energy efficiency of delivery, high purity requirements and issues related to hydrogen leakage. Further analysis of options and trade-offs for hydrogen delivery from central, semi-central, and distributed production to the point of use is needed.

3.3 Hydrogen Storage, 2011 Interim Update Dpdated September 2011

For *Hydrogen Storage* in general the main challenge for transportation applications is predominantly technical, being related to driving range which is constrained by weight, volume, durability, efficiency and total cost of storage units. Furthermore durability/lifetime of performance still needs to be verified (as such it is not really a technical challenge but a mandatory step for going to the market). On the contrary the improvement of charging/discharging rates constitutes a real technical challenge and the establishment of dedicated codes and standards an institutional challenge. Other general issues are BoP components, dispensing technology, thermal management during dispensing, and system life-cycle assessments. Specific challenges for compressed gas systems are related to the requirement for high-pressure tank conformability and to the lack of available tank performance data. For cryogenic liquid systems the liquefaction energy penalty and hydrogen boil-off are additional issues. For reversible materialsbased storage systems, that are less mature than the two previous technologies, the lack of understanding of hydrogen physisorption and chemisorption is mentioned as well as the need of defining standard test protocols for evaluation of materials, including reproducibility of synthesis and materials properties. Finally the need for establishment of regeneration processes and removal of by-product/spent material are highlighted as critical challenges for chemical hydrogen storage systems.

3.4 Fuel Cells, 2011 🖉 Updated March 2012

Cost and durability are defined as the two most significant challenges for obtaining clean, reliable and cost-effective fuel cell systems. The need to define quantified performance criteria to position fuel cell versus competing alternative technologies is highlighted as well as the need for validation of durability and reliability upon operation for BoP components and subsystems.

Several other specific technical challenges are also listed.

- PEMFC stacks durability, including tolerance to impurities (air, fuel, and systemderived) and chemical and mechanical integrity needs to be established. Sufficient durability of fuel cell systems in conditions realistic for automotive applications (including operation in low humidity) is not demonstrated. Degradation and failure mechanisms are not yet fully understood.
- For stationary fuel cells, durability under start-up and transient operation needs to be improved.
- Accelerated testing protocols need to be developed to predict durability and allow timely iteration in the technology development.
- BoP components durability need to also be improved.
- Materials and manufacturing costs for stack components (membrane, catalysts, bipolar plates) need to be reduced while maintaining high performance. BoP components and subsystems need further development to reach cost targets. Development of a cost-effective process and subsystem for removing contaminants is underlined, allowing reduced overall cost and higher fuel flexibility.
- Regarding fuel cell and fuel cell system performance and efficiency, technical challenges at different levels are mentioned with variable priority; cell issues, stack water management, system thermal and water management, system air management, system start-up and shut-down time and energy/transient operation.

3.5 Manufacturing R&D, 2011 🖉 Updated February 2012

- *Manufacturing R&D* is needed for hydrogen production, delivery, storage and fuel cells. For *Hydrogen Production* specific need for manufacturing R&D is highlighted for joining of reformer components, reformer reactor vessels, stamping and extrusion of reformer components as well as deposition of catalyst coatings onto non-conformable surfaces in reformers and hydrolyzers.
- For *Hydrogen Delivery* the following challenges for manufacturing of components and systems are highlighted; high cost of fiber-reinforced polymer pipelines, Department of Transportation's (DOT) requirements for composite tube trailer vessels, reliability and cost of compressors.
- For *Hydrogen Storage* reduction in the amount of composite tank material needed and cost of carbon fibers are underlined along with need for higher manufacturing efficiency.
- For *Fuel Cells* production of MEA and gas diffusion media, fuel cell stack assembly, fabrication of bipolar plates, BoP subsystem assembly and quality control are highlighted.
- *Cross Cutting Issues* concern cost of carbon fiber for vehicular, tube trailer and stationary hydrogen tanks, modelling and simulation for development and optimization of manufacturing processes, materials knowledge (new materials), sensing and process control as well as metrology and standards.

3.6 Technology Validation, 2011 Updated February 2012

With respect to *Technology Validation* the primary technical challenge is that of integration of complex systems (i.e. integration of fuel cell systems into existing thermal/electrical systems in vehicles or buildings). Several specific technical barriers are defined, many dealing with the lack of data extracted from demonstration and first deployment, e.g. lack of fuel cell electric vehicle and fuel cell bus performance and durability data, lack of data on stationary fuel cells in real-world operation, lack of hydrogen refuelling infrastructure performance and availability data, limited data on coal-to-hydrogen plants with carbon sequestration – need for high T and P hydrogen separation systems, little information and lack of demonstration of hydrogen from renewable resources as well as co-production of hydrogen and electricity. Some technical challenges are more basic in nature, such as the lack of understanding of storage tank operating cycle life and failure mechanisms, The lack of adopted or validated codes and standards constitutes a technical and institutional challenge.

3.7 Hydrogen Safety, Codes and Standards, 2012 - Updated July 2012

For Hydrogen Safety, Codes and Standards barriers to be overcome are; limited access and availability of safety data and information, availability and affordability of insurance, safety is not always treated as a continuous process, lack of hydrogen knowledge among authorities having jurisdiction, lack of hydrogen training materials/facilities for emergency responders, lack of consistency for RCS limits international trade and markets, insufficient technical data to revise standards, insufficient synchronization of national codes and standards, lack of consistency in training officials, limited participation of business in the code development process, no consistent codification plan and process for synchronization of R&D and code development, need for developing codes and standards for usage and access restrictions.

3.8 Education, 2011 Pdated May 2012

With respect to education the following barriers are defined; lack of readily available, objective and technically accurate information, conflicting messages about hydrogen and fuel cells, poor connection between hydrogen information sources and dissemination networks, lack of educated trainers and training opportunities, regional differences and difficulty of measuring success of education activities. It is worth noting that these barriers are more institutional by nature than technical.

3 Input from partners of the H₂FC consortium

A spread sheet matrix was prepared and distributed to all partners of the H_2FC consortium for identification of scientific bottlenecks indicated by the experts on various hydrogen and fuel cell technologies. Four main topics were defined for grouping the different technologies and related challenges;

- Hydrogen production (including purification)
- Hydrogen storage and distribution
- Hydrogen end-use / systems
- Cross-cutting issues

Various technologies (sub-topics) were defined under each topic and challenges/bottlenecks identified related to key aspects;

- Main materials challenges
- Limiting cost factors
- Limitations in characterization/modelling tools
- Main system challenges
- Main safety issues
- Main market challenges
- Other challenges

All input obtained from project partners can be found summarized in Appendix A.1 of this report. Since the consortium of the H_2FC project does not possess competence and experience within the whole chain of hydrogen and fuel cell technologies, the input given should not be interpreted as a complete survey. In an attempt to condense the identified bottlenecks, the following sections list the main issues for the 4 defined topics.

3.1 Hydrogen production (including purification)

The key bottlenecks for *hydrogen production* defined by the H_2FC consortium are listed in Table 3.1.

Table 3.1 Key scientific bottlenecks for hydrogen production as defined by the H₂FC consortium

Main materials challenges	For all technologies, materials with increased stability in operating conditions are required. E.g. Catalysts for reforming or partial oxidation and for PEM water electrolysis, membrane, bipolar plates/current collectors for PEM water electrolysis
Limiting cost factors	High cost materials required to withstand system conditions/specs. Either develop better materials or change system
Limitations in characterization/modelling tools	Are related to the lack of understanding of degradation mechanisms, to the need to predict remaining system lifetime. Need for in situ characterisation is expressed. On-line data monitoring and processing from real-world operation
Main system challenges	Lack in suitable BoP components and coupling of hydrogen production technologies with grid and (other) energy sources
Main safety issues, incl. RCS	Gas leaks, high pressure hydrogen and oxygen
Main market challenges	Combined technology and market maturity Reduction of the production costs
Other challenges	

3.2 Hydrogen storage and distribution

The key bottlenecks for *hydrogen storage and distribution* defined by the H2FC consortium are listed in Table 3.2.

Table 3.2 Key scientific bottlenecks for *hydrogen storage and distribution* as defined by the H2FC consortium

Main materials challenges	Limited gravimetric hydrogen capacity from current materials, unpractical conditions for hydrogen sorption, reversibility, fundamental understanding of hydrogen sorption mechanisms in solids Effect of H ₂ purity on pressure vessel materials. Innovative structural materials cheaper than carbon fibre.
Limiting cost factors	High production cost for storage materials and storage components
Limitations in characterization/modelling tools	On solid storage, need for harmonised measurement protocols and for in situ characterisation On pressurized storage need for harmonization, for more experiments to validate CFD models and for inter-comparison.
Main system challenges	Correct integration (placement, alarm levels, communication with safety design features) of devices for detection of leaked hydrogen. Improve the energy efficiency of storing/extracting hydrogen. Component cost reduction. Thermal management
Main safety issues, incl. RCS	In-depth understanding of hydrogen behaviour under possible accident "situations". Availability and correct use of reliable hydrogen sensors .Safety issues linked to material based storage technologies.
Main market challenges	Market with various maturity level depending on the technology and the application (hydrogen for industry is a mature market but hydrogen-fuel is a very immature one).
Other challenges	Lack of field experience. Guidelines/best practices on technology (e.g. detection) application

3.3 Hydrogen end-use / systems

The key bottlenecks for *hydrogen end-use / systems* defined by the H_2FC consortium are listed in Table 3.3.

Table 3.3 Key scientific bottlenecks for hydrogen end-use / systems as defined by the $\rm H_2FC$ consortium

Main materials challenges	For all technologies, materials with high
	performance and increased stability in operating
	conditions are required. Catalyst,
	membranes/electrolytes, bipolar
	plates/interconnectors
Limiting cost factors	For all technologies, high cost materials with low
	volume production
Limitations in characterization/modelling tools	Verified, harmonized and standardized
	accelerated stress test protocols, advanced
	tools/methods
	In situ characterisation
	More "complete" models, describing all
	interlinked processes supported by experimental
	validation, to predict system remaining system
	lifetime
Main system challenges	Lack in suitable balance of plant components for
	all technologies, for water handling in PEMFC,
	temperature management, for clean-up systems
	in high temperature fuel cells
Main safety issues, incl. RCS	Hydrogen/fuel leakage and accumulation indoors
	with consequent ignition and combustion
	Detection of leaked hydrogen and activation of
	safety procedures
Main market challenges	High cost of these technologies
	Competing technologies are cheap, mature and
	accepted in the market. No market for CO_2
	emission reduction
	Cost, availability and quality of hydrogen fuel
Other challenges	

3.4 Cross-cutting issues

The key bottlenecks for *cross-cutting issues* defined by the H_2FC consortium are listed in Table 3.4.

Table 3.4 Key scientific bottlenecks for cross-cutting a	<i>issues</i> as defined by the H ₂ FC consortium
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Main materials challenges	Light materials for hydrogen storage (type 3 and 4 tanks) have low fire resistance.				
Limiting cost factors	Cost of safety system is not a part of FCH system or infrastructure cost.				
Limitations in characterization/modelling tools	Absence of protocols for testing of whole systems, e.g. vehicle behaviour in fire. Difficulties with use of full chemistry models for predictive simulation of real (large) scale accident scenarios.				
Main system challenges	Low hydrogen safety knowledge at designer/regulator/managerial levels.				
Main safety issues, incl. RCS	Low fire resistance of on-board hydrogen storage.				
	Lack of higher education on hydrogen safety at national level.				
	RCS have unacceptably little information on safety strategies and engineering solutions.				
	Lack in harmonization and standardization of safety issues, add legal requirements to harmonisation and standardisation				
Main market challenges	Lack in standards and approval of systems				
	Build public confidence in hydrogen through demonstration to public of safety performance of systems (e.g. vehicles) and infrastructure (e.g. refuelling stations).				
Other challenges	Public awareness: Unfamiliarity with the new technologies and resistance to adoption of the technologies				
	Lack of installers that are accredited to install and service systems				
	Some stakeholders claim that "there are no safety issues" for their systems. An accident with a poorly designed/constructed system might have bad reputational knock on effects on serious companies.				

4 Discussion and Summary

Considering all the input combined from three different sources in this report, it is evident that the barriers against a hydrogen-based economy are not limited to only a few central issues for further hydrogen and fuel cells research. Depending on the maturity of the different technologies from hydrogen production to end-use, there are different ways and requirements to focus on harmonizing test protocols, safety standards, develop modelling in addition to further improvements on scientific areas, before large scale commercialization is possible.

This can be illustrated with hydrogen storage for which the preferred technology is very much dependant on application. For automobile applications, high pressure composite tanks are typically used, while solid storage may be a preferred solution for smaller vehicles/systems and applications like materials handling. Regarding high pressure composite tanks, standards and certifications for the materials used and safety tests are required. Feedback data on materials performances and on-field test behaviours are also required to assess the condition and safety of the tank on-board. Regarding solid materials, more fundamental understanding is required as this technology is less mature.

Generally, for more mature technologies such as natural gas reforming to produce hydrogen, pressurized hydrogen storage and PEMFC as end-use, some challenges are more economical and institutional than technical. In addition to the lifetime/cost issue, the technical requirements that are commonly expressed are the need for harmonised tests and standards, the poor range of available BoP components and further need for improvement of process integration.

For less mature technologies such as electrolysis for hydrogen production, solid storage and SOFC as end-use, challenges are still more scientific, as these technologies require more research and development before potentially being ready for market entry. The need for better understanding of materials and systems, for advanced characterisation methods including in situ characterisations and for concerted modelling is commonly mentioned. It is also worth noting that harmonised approaches stand as facilitating vector for increasing the technology readiness level of all technologies.

According to the input obtained within the H₂FC project, several material challenges still remain for hydrogen production, storage and end-use linked with their stability and performance under operating conditions and their production cost. This indicates that significant attention is needed for improving catalysts, membranes, bipolar plates/interconnectors with respect to both durability and cost, which is in line with the long term vision of the EC materials Roadmap. Challenges related to high production cost of materials and components for various technologies may alleviated with time as a cost reduction is naturally expected upon break-through of a technology and start-up of mass production.

In the selection of available reports used for comparison there is only limited attention given to the need for characterization tools and modelling/simulation tools. However two documents are short or medium term oriented (Road map of DOE in chapter 2.1 and MAIP of the FCHJU in chapter 2.3) and list the properties to be improved and the missing data to be provided rather that the way to do it. The third document is medium to long term oriented with a focus given on material (EU material roadmap in chapter 2.2). Here again the properties to improve are listed but not the way to reach them. Despite not being mentioned

explicitly, there is however little doubt that such tools are necessary for efficient characterization, understanding of mechanisms (e.g. hydrogen absorption, catalyst deactivation, material destabilisation upon operation, etc.) and development of relevant solution for all technologies. Within the H₂FC project consortium, as a dedicated question was asked, the need for specific tools including in situ characterisation and for modelling is clearly mentioned; see Appendix A.1 for more details.

Safety is also specially highlighted within the H_2FC consortium, where modelling in general as well as safety related regulations, codes and standards for the various technologies and use of hydrogen in general is defined as bottlenecks. One of the most challenging safety issues is a low fire resistance of on-board hydrogen storage and consequences of accidental leaks from vehicles outdoors and indoors.

This analysis of the Scientific Bottlenecks for Commercialization of H_2 & FC Technologies confirms that the H_2FC European infrastructure project is positioned on these key issues:

- Test harmonisation and protocols
- Accelerated tests development
- Mechanisms understanding and modelling thanks to advanced characterisation means including in situ characterisation
- Safety
- Other cross cutting issues such as public demonstration and awareness

The report from TASK N3.2 "Mapping the existing European Research Infrastructure facilities", also in WP4, will give an overview of relevant infrastructure available. By processing the information in the two reports on bottlenecks and infrastructure, priorities for further hydrogen and fuel cell infrastructure will be ranked. Based on this current report on bottlenecks, some infrastructure development and/or adaptation should be considered for in situ analysis to further sustain basic understanding, and infrastructures for system integration may be foreseen. The latter is commonly mentioned as a technical bottleneck for mature technology close to commercialisation.

APPENDIX A.1

- Overview of identified bottlenecks for HYDROGEN PRODUCTION (incl. purification)
- Overview of identified bottlenecks for HYDROGEN STORAGE AND DISTRIBUTION
- Overview of identified bottlenecks for HYDROGEN END-USE / SYSTEMS
- Overview of identified bottlenecks for CROSS-CUTTING ISSUES

	Identified bottlenecks for HYDROGEN PRODUCTION (incl. Purification)						
Торіс	What are the main materials challenges (i.e. performance, stability, lifetime)? Please specify.	List the limiting cost factors related to the technology.	Is the research limited by lack of characterization and/or modelling tools and techniques? Please specify.	What are the main system challenges related to this technology (i.e. BoP)? Please specify.	What are the main safety issues (incl regulations, codes, standards)? Please specify.	What are the main market challenges inhibiting further/early development of the technology? Please specify.	Are there other challenges regarding this technology? Please specify.
Reforming / partial oxidation of fossil fuels	of coke-resistant catalysts for steam and dry reforming. Catalyst stability (hydrothermal,	Process endothermic so it would have a high heat input. Identification of reliable and cost effective selective membranes for H2 separation and purification to the required FC-grade. Effective methods for heat supply (internal via oxygen, or external), air separation. Compact units (reactors, etc.)	No, not especially limited. Purification by membranes, both ceramic and polymeric could require more characterization and modelling efforts	Cyclone which retains particles present in the syngas. Heat exchanger for water and tars condensation. Pressure Swing Adsorption system or hydrogen permeable membranes. URAS analyser of CO, CO2 and O2 to monitor the process. Development of efficient systems (> 80% thermal efficiency) for small-scale distributed H2 generation. System (many integrated units) operation at dynamic conditions. Routines and conditions preventing coke formation and performance losses, for example keeping the active catalysts in desired state.	Gas leaks. Reliable and cost effective detection tools/sensors. Safe control of oxygen handling in case of CPO, ATR, etc.	High energy consumption. Low hydrogen production (68% max.) and quite tras generation. Directives which drivers the consumers/end users to switch towards hydrogen economy: FC cars, decentralized energy production, emissions limits	
Reforming / partial oxidation of biomass	Poison resistant materials (S, Cl, F, siloxanes) that make biogas/bio syngas clean up quite difficult step. Syngas hot conditioning (catalysts and adsorbents for removal of S, inorganics, halides, tar and CH4 removal or conversion). Multifunctional materials/reactors.	biomass have a hydrogen deficit making optimization and efficiency	Understand poisoning and recovering mechanisms. Model to predict life time. Complex feed stocks gives complex processing and material challenges.	Optimized integration among at least 4 different units: anaerobic digester/gasifier, clean up/up grading, reforming, fuel cell		First be aware that there is quite big market taking into account both cultivated biomasses and waste derived biomasses Secondly that in this field the suitable power range could be from a few kWs to some MWs	
PEM Water electrolysis	Materials for bipolar plates and current collectors: Stability and performance (oxidation of titanium, high contact resistance). Membrane materials with lower gas crossover and higher temperature stability. Catalysts with higher activity for oxygen evolution and long term stability.	Bipolar plates are expensive. Materials cost and machining costs. Noble metal catalysts, high loadings, usually 2-5 mgcm2	No, not especially limited.	BoP components for high gas pressures. Dryers, separators and production of DI water	High pressure hydrogen and oxygen, danger of mixing, danger of spontaneous combustion of construction materials. Burn of electrolyser shell from inside by H2-02 flame and release of content outside (high pressure) with toxic products of membrane combustion, etc.	Challenge for PEM electrolysers is to reduce cost and improve lifetime. Competition with other electrolysis technologies and hydrogen from fossil sources.	Develop new ideas such as, for example, photo catalysis, thermo assisted water electrolysis, pyrolysis, etc.
Alkaline Water electrolysis	Membrane materials with low gas crossover and high temperature stability (120°C); durability against bases (30%KOH), high ion conductivity (low overvoltage)	no specific materials cost, but total system cost	in-situ characterization	BoP components for high gas pressures (> 30 bar). Dryers, separators and production of DI water		price of produced H2, electricity consumption	
High-temperature water electrolysis (SOEC)	High-temperature stability of materials,and interfaces, materials aging and interactions, long term stability, mechanical stability	Cost of materials, i.e. cathode, anode and solid electrolyte (ceramics), sealings and interconnectors, may be significantly reduced, if temperature is lowered (900°=> 700°C)	in-situ characterization, mutiscale modeling of coupled processes (electrochemical / thermal / mechanical)	High temperature sealing, material and cell and stack durability	High pressure hydrogen and oxygen, danger of mixing, danger of spontaneous combustion of construction materials. Burn of electrolyser shell from inside by H2-O2 flame and release of content outside (high pressure) with toxic products of membrane combustion, etc.		
By-product hydrogen		Hydrogen purification			Increase of mixture flammability due to presence of hydrogen.		
Pyrolysis (Biomass to Hydrogen, BtH)	Fouling, high temperature stability.			Suitable feedstock and properties. Waste limiting processing.			
H2O splitting	Catalyst stability over > 1,000 hours (e.g. for intermediate acid decomposition)	Construction materials to withstand the harsh acid environment in suphur-based thermochemical cycles. Thermal efficiency should be increased.	Some basic unit operations in some thermochemical water-splitting cycles still need to be experimentally explored (e.g. reactive distillation option in the Suffur-lodine process, side reactions/products hindering closed cycle operation,)	Absence of reliable flame and detonation arrestors for H2-O2 mixtures. Some thermittent primary source (like solar) by cost effective systems with borrful depointed like locing		Lack of large H2 distribution infrastructure to deliver the massive H2 produced from large thermochemical water-splitting plants.	Proof-of-concept and demonstration at the pilot scale for thermochemical water- splitting cycles is missing yet.
Photo-electrochemical production	New materials such as more performing Titanium oxide to be able to use even "visible light" not only infrared	Develop cost effective systems to make nano structured materials	Nano structured materials characterization. Modelling of photo catalysis mechanisms				
Purification - Fuel quality	Development of sulphur-resistant catalysts and processes for steam and dry reforming.	Identification of reliable and cost effective selective membranes for H2 separation and purification to the required FC-grade					
Links to Energy resource (e.g., wind, PV, hydroelectric)				Determination of strategies for the coupling between the production plant and the intermittent primary energy source like solar and wind by energy storage, buffering, shortening of start up periods, management of transients, etc.			

	Identified bottlenecks for HYDROGEN STORAGE AND DISTRIBUTION						
Торіс	What are the main materials challenges (i.e. performance, stability, lifetime)? Please specify.	List the limiting cost factors related to the technology.	Is the research limited by lack of characterization and/or modelling tools and techniques? Please specify. What are the main system challenges related to this technology (i.e. BoP)? Please specify. What are the main safety issues (incl regulations, codes, standards)? Please specify.			What are the main market challenges inhibiting further/early development of the technology? Please specify.	Are there other challenges regarding this technology? Please specify.
Liquefied H2	Thermally insulated containers Leakage Hydrogen quality	Cryogenic storage tech	Limited number of CFD models. Need for more experiments for CFD validation.		Various issues with CFD modelling of accidental releases including physical properties, humidity effects, heat transfer from surroundings, phase changes, etc (see JRC reference report). Separation distance based on cold burns, burning velocity of hydrogen-air mixtures at low temperatures to calculate pressure effects of combustion. Lack of experimental data on concentration distribution and burning behaviour in cold jets and spills to evaluate CFD modelling	Cost of H2 must be competitive.	
Liquid H carriers (e.g. CH3OH, lig. NH3)					Flammability and ignitability of mixtures of hydrocarbons and hydrogen.		
Solids for storage (chemical & physical)	Gravimetric and volumetric capacity, conditions for hydrogen sorption, reversibility and kinetics, cyclability. Poor understanding of H2 sorption mechanisms (role of dopants/additives etc.), gas purity (side products such as NH3, B2H6)	Cost of elements (actually NOT: Na, Al, B, Li), but cost of materials production; cost of system (housing, heat management)	Hydrogen sorption properties are difficult to predict by modelling. Controversy over measured H2 storage capacities on different types of materials and need for improved and reliable performance assessment (including life cycle); in-situ characterization both in research and application (fuel gauge)	Heat management issues, gravimetric capacity at system level, long cycle life, system filling time, discharging flow rate	High reactivity of many hydrogen storage materials (e.g. pyrophoric in air). Lack of reliable safety assessment of materials and storage systems. Deflagration parameters of a cloud of particulates in air. Lack of international /European standards regulating solid-state or hybride hydrogen storage tanks for transport.	Not yet competitive to compressed H2 when weight is an issue	
Pressurized H2	Hydrogen quality	Production cost of high purity H2.	H2 ISO standard is very general and strict. The quantification limits required for QC requires use of 7-11 different analytical techniques. This is very cost driving. By differentiating the H2 based on feedstock, the QAVC could be greatly simplified. Different for CFD models producing different results. Need for harmonization. Need for more experiments for CFD validation and intercomparison.	Reliability of PRDs; risk of auto- ignition while closing; efficiency of ventilation of enclosures (mechanical, natural or a combination)	Various issues with CFD modelling of accidental releases including notional nozzle approaches, dispersion in enclosures, non-ideal gas behaviour at high pressures, etc (see JRC reference report). Plane jets and switch-of-axis phenomenon. Interaction of multiple jets. Underventilated fres, including phenomena of self-extinction and re-ignition. Extinction of hydrogen jet fires. PRD with reduced fiame length. Fire resistance of hydrogen storage vessels. Predictive simulation of coherent deflagrations (simultaneous internal and external deflagrations) and role of Rayleigh-Taylor instability. Deflagration-to- detonation transition modeling and simulations at large scale, including the role of Richtmeyer-Meshkov instability. Experimental data on H2 burning behaviour in mixtures) is needed, but methods for the generation of concentration gradients and concentration measurements have to be improved.	Cost of H2 must be competitive. QA is cost driving.	
Pressurised H2 tanks	Energy density low in comparison with the reference cases of gasoline and even methane. Lack of broad enough statistic on operation performances.	Production of the external shell, made by carbon fibre reinforced epoxy	For type IV tanks ageing/deterioration mechanism not yet clear.	3 minutes filling requires a very accurate filling protocol and the requirement of hydrogen pre- cooling, which contributes considerable to costs, system complexity and decrease of efficiency	International standard almost ready, Global Technical Regulation near approval stage, European regulations in place. Nevertheless safety margins are in some case very high and not based on real operative failure, deterioration experience and on knowledge of the materials used nowadays.		
Bulk H2 transport					Pressure relief devices with reduced flame length.		
Pipeline transport					Engineering design to reduce extremely large deterministic separation distances		
H2 fuelling station components		Reliability of individual components far worse than for gasoline RS.	Lack of comprehensive and harmonised sets of worse case scenarios to be simulated by CFD—It is not possible to ensure that one has identified the worst case		Large mass flow rates in case of rupture of equipment. Lack of harmonised regulatory framework in Europe, for example a "type-approval" of refuelling stations. Lack of harmonised RCS. Lack of failure rate data of equipment/systems hampers the QRA		Lack of field experiences (component availability, real efficiencies, etc.). Lack of failure modes and frequencies. Despite the many demonstration projects, data are confidential.
Other components - H2 safety sensors	Shortcomings of H2 detector arise from technology limitations (speed of response, lower detection limit, dependence on ambient environmental conditions) and incorrect use of such devices (incorrect placement, incorrect maintenance and calibration).	All H2 sensing devices will reduce in price as the demand increases. At present the H2 market is not extensive enough for economy of scale to reduce the price of H2 sensors.	Current H2 sensing technologies have known performance limitations. Emerging technologies may reduce this limitations but these need to be developed and verified		Reliable performance is an issue. Also selection of the most suitable sensors for a specific application requires good knowledge of the ambient conditions of the application - in other words some sensors are more suitable than others for a particular application. Correct location of the sensing device is also crucial - it does not matter how 'fast' a H2 sensor responds to H2, if the sensor is located far from a H2 leak then this is the bottleneck to rapid leak detection and hence safety. Other issues, such as cross ensitivity to other species, are specific to the application. Sensor drifting.	Lack of market means that insufficient sensors are being sold (some manufacturers considering withdrawing their products) which hinders further development of feasible products.	There is a need for guidelines on how H2 sensors should be optimally used (including choosing the right one and correct placement). This is being address for indoor applications in HyIndoor.
Metal Hydrides by SHS	Lower pressure storage, conformable shapes, reasonable volumetric storage efficiency and safe storage compared to gas and liquid state. Cost effective method.	High cost of the materials, in particular rare earths. Low volume production	No, not especially limited.	Control software allows monitoring and storing all the relevant data of the process (T, gas volume flow along the time, reaction pressure during the process, gas consumption during the		High weight. The temperature of dissociation is high and in the refill of the material, refrigeration is needed.	

		Identified bott	lenecks for HYDROGEN E	END-USE / SYST	EMS		
Sub-topic	What are the main materials challenges (i.e. performance, stability, lifetime)? Please specify.	List the limiting cost factors related to the technology.	Is the research limited by lack of characterization and/or modelling tools and techniques? Please specify.	What are the main system challenges related to this technology (i.e. BoP)? Please specify.	What are the main safety issues (incl regulations, codes, standards)? Please specify.	What are the main market challenges inhibiting further/early development of the technology? Please specify.	Are there other challenges regarding this technology? Please specify.
Engines (ICEs) and Turbines			Inadequate models for DDT, at least for realistic scale scenarios in 3D; detonation modelling (3D and realistic scale) still beyond the reach of current models and computers for routine simulations; how are the LFL and UFL altered by high pressure and/or high temperature?	How to deal with flame-outs and restarts; how to protect the GT and equipment from damage in		Distrust of hydrogen technology; fear of the safety implications of using hydrogen;	
PEMFC 1	Main materials challenge is to improve stability of all components and reduce costs. Long term stability of electrocatalysts, support corrosion. Reduce costs of bipolar plates and decrease contact resistance. Durability target of 5000 hours (transport) of operation far from reached. Transient operation causes rapid degradation of ionomer used in electrolyte and electrodes. Power density requirements has lowered electrolyte thickness and thereby reduced durability.	Coatings for bipolar plates. Noble metal catalysts. High cost perfluorinated membranes. Need to upscale production and assembly methods to reduce costs. Given mass production cost reduction estimates, noble metal catalyst is still main cost driving component, followed by bipolar plates and the perfluorinated ionomer used as electrolyte. Balance of plant/system engineering/manufacturing costs.	Models accurately describing two phases are scarce. This requires proper test setups to validate models especially to monitor water formation and built-up, e.g. by visualisation using transparent cells. Need for in situ measurement/modelling tools and standardised test methods to raise understanding of the phenomena and to validate mitigation means Dynamic non-isothermal porous flow models couple to mechanical models. The verification of such models should be by experimental validation.	Low operating temperatures makes large heat exchangers necessary (transportation). Water balance in transient operation is always a challenge for PEMFC systems with respect to performance and durability	Hydrogen refuelling, hydrogen leaks	Competing, already existing technology makes price level very low. Hydrogen Refuelling infrastructure must be established. High cost of raw materials, limited durability of real world systems.	Low operating temperature limits its use in CHP systems. Inherent limitation in the use of water- based proton conduction. Public perception - safety.
PEMFC 2	Catalyst: stability for load and start/stop cycles Catalyst: electrode structure for high current density Membranes: chemical and mechanical resistance Membranes: operation at higher temperatures (e.g. 100-120°C) - humidification and durability aspects Gas diffusion layers (GDL): need of material with good characteristics in both low temperature/high humidity and high temperature/low humidity conditions Bipolar plates: if metallic, need of proper coating	 Loading of noble metal catalysts. The necessary catalyst loading is not primarily determined by the beginning-of-life catalyst activity, but by durability issues and by mass transport limitations in the catalyst layer. Expensive PFSA membranes. Alternative membrane materials have good conductivity at high humidity but a stronger loss of conductivity than PFSA at low humidity. Cost of bipolar plates, in particular if non-metallic (carbon) 	 Lack of water transport (two phase flow) Models with convincing experimental validation. Recent advances in characterization techniques (e.g. neutron and synchrotron imaging) are expected to help filling this gap. For electrodes (catalyst layer), only limited characterization methods are available, in particular concerning the micro'nano structure of the different components (e.g. carbon and ionomer) 	 Reduction or complete removal of external humidification Size of heat exchangers due to the low temperature difference between stack and ambient Automobile applications: hydrogen storage 	- Better stack performance when pressurized (e.g. 2 bar abs.), but possible safety issues from leakage	- Automobile: very high performance/cost ratio of current ICE technologies.	- Need of hydrogen distribution infrastructure
мсғс	Poisoning resistant anodes and cathodes	MCFC have reached 40,000 hours operation, very good reliability, only the cost is still an issue even if is not too far from the target cost of 1000 $-$ 1500 \in /kW: mass production seems to be the solution	Poisoning and recovering mechanism should be further investigated mainly against Cl, F compounds and siloxanes	Inverter, clean up system, interaction with the grid, turbine for hybrid configuration. In general all components should be more reliable and cost effective	CE "stamp"	Incentives and or directives driving the market toward more efficient and cleaner CHP and decentralized power generation systems	Broaden its use for new applications such as hydrogen production, CO2 separation, coupling with biomass gasifier
SOFC 1	New ceramic powders (ScSZ) would lead to a of the electrolytes. These electrolytes would have better ionic conductivity. The deposition would be by High Frequency Pulse Detonation (HFPD) offers an electrolyte dense and with less volumetric defects reducing the working temperature: This technique would reduce the time of production so the manufacturing costs will be reduced. Materials for low temperature SOFC, Nano powders to improve status of the art performances	High cost of the powder material. Micro CHP: mass production; Hundreds kW/MW size systems: develop larger fuel cell geometry	No, not especially limited. Modelling (CFD and mechanistic) is still in its infancy; there might also be scarcity of experimental data suitable for model validation. Thermal cycling, redox, sealing, internal ohmic resistance : all these mechanism should be better investigated	The overheating of samples was avoided by cooling with compressed air at 5-6 bar. Inverter, clean up system, interaction with the grid, heat exchanger, catalytic burner, micro turbine for hybrid configuration. In general all components should be more reliable and cost effective	Hydrogen leaks. CE "stamp" for micro CHP already ready for the market entry	Thermal ageing of SOFC components. Incentives and or directives driving the market toward more efficient and cleaner CHP and decentralized power generation systems	Use of SOFC into the "waste to energy chain" and biomasses
SOFC 2	Materials challenges: (thermo-mechanical) stability and lifetime! gas-tightness of sealings; redox stability of anodes; stability and density of protective layer on steel (prevention of Chromium evaporation); stability and density of interdiffusion barrier layers (prevention of Strontium interdiffusion); thermo-mechanical stability of electrical contacts at (all) interfaces	Currently, since no mass production exists: all manufacturing costs, starting from cells, up to stack assembly! IC coating, material costs of ICs; fabrication techniques for cells;	Yes, stationary applications require lifetimes above 40,000 hours. Real-time durability tests should be accompanied (replaced?) by (still lacking) accellerated life-time tests. To design accellerated lifetimes tests detailed degradation models are required.	Highest efficiencies are reached with steam reforming of natural gas. This requires water supply and/or anode gas recycling. De-sulpherization of fuel.	fuel leaks, mostly at H2;	costs; competing / existing technologies can only be beaten with higher efficiencies at same or lower costs. redox stability; long term stability	
Portable and micro fuel cells						Inability to take FC-driven devices (for example laptops) on flights (not sure how train operators feel about FCs); this may be an non- issue if tablets (iPads and others) find more widespread use	
System integration (vehicles, vessels, etc.)					Safety characteristics, especially fire resistance, of a total system rather than components.		

			Identified	bottlenecks for	CROSS-CUTTING ISSUES		
		List the limiting cost factors related to the technology.	modelling tools and techniques?		What are the main safety issues (incl regulations, codes, standards)? Please specify.	What are the main market challenges inhibiting further/early development of the technology? Please specify.	Are there other challenges regarding this technology? Please specify.
Demonstration	resistance. Increase of fire resistance issue is practically ignored in current studies of tank 3 and 4. For example, cycling tests of tanks covered by	part of FCH system or infrastructure cost. Before introduction of new safety culture to public it has to be a constituent part of activities in each company that designs and/or manufacturers FCH	Bonfire testing protocols are either absent or not yet widely validated for different storage tanks. Modelling and simulation of fire resistance is at a rudimental level. There are scientific difficulties with application of full chemistry models for predictive simulation of large scale accident scenarios.	1	vehicles requires bonfire test. However, it does not require level or fire resistance or clear requirements for provision of life safety.	manufacturers of systems and infrastructure will demonstrate to	Lack of financial support from some national governments. Develop the concept of "big" demo projects integrating several different technologies: from renewable energies to hydrogen production/storage/distribution, FC cars, FC CHP. Or from waste treatment to tri-generation - CCHP systems . Lighthouse projects?
Education/ Outreach				at designer/regulator/managerial levels.	Practically absence in Europe of higher education in the field of FCH (both undergraduate and postgraduate level). Disbalance between large investment to training events like summer schools and no investment to higher education, e.g. through bursaries.		Lack of higher education on hydrogen safety at national level.
Standardization	systems.	Lack and/or absence of demonstration to public of safety performance of systems (e.g. vehicles) and infrastructure (e.g. refuelling stations), in particular in fire conditions.		Need to standardize most of conventional (blowers, valves, inverters,) BoP component to make them cheap and reliable		For industrial partners, lack of specific standards and regulations for marketing and installations	Lack in harmonization and standardization of safety issues (ongoing work).
Other (please specify)				safety issues" for their systems.	makes QRA difficult (in general, failure frequency data for NG is	Difficulty in gaining approval for building and operating stationary FC applications, especially in domestic or commercial settings.	Hazardous Area Classification; lack of interest from some regulatory authorities; lack of support from Governments in supporting R&D a belief that hydrogen economy will not happen; lack of infrastructure for hydrogen distribution