



H₂FC

Integrating European Infrastructure to support science and development of Hydrogen- and Fuel Cell Technologies towards European Strategy for Sustainable, Competitive and Secure Energy

Grant agreement no.: FP7-284522

Start date: 01/11/2011 Duration: 48 Months

The H₂FC project is co-funded by the European Commission within the 7th Framework Program

Deliverable

D10.4 Roadmap for addressing bottlenecks in the H2FC e-infrastructure

Due date of deliverable	M24 (October 2013)
Completion date of deliverable	M29 (March 2014)
Start date of H2FC project	1st November 2011
Duration of project	48 months
Version of deliverable	2.0
File name	D10.4_H2FC_vers.2.0.docx
Responsible partner for deliverable	JRC
Contributing partners (short names)	UU, JRC, CEA, NCSRD
Partners external to H2FC	Prof Froudakis (Crete University)

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1 INTRODUCTION

Three main areas for bottlenecks have been identified and described in separate chapters in the report:

- Hydrogen Safety
- Hydrogen (Solid State) Storage
- Hydrogen Fuel Cells

2 HYDROGEN SAFETY

The following kinds of bottlenecks have been identified in hydrogen safety:

- Technological safety issues
- Regulations, codes and standards
- Education and training
- Dissemination
- CFD modelling issues

2.1 TECHNOLOGICAL SAFETY ISSUES

Issue	Solution/Deliverable
Better estimate (and decrease when possible) of separation distances	Validation of simple methods/tools for estimate of separation distance
Increase fire resistance rating of hydrogen storage systems	Fire resistance rating to be increased from 10-20 minutes to 1 – 2 hours
Indoor release & dispersion of gas and liquid hydrogen: Development of indoor ventilation systems	Testing & validation of new systems facilitating indoor ventilation.
Development of best practice guidelines to reduce hazards & risks	Delivery of best practice guidelines for emerging FCH applications.
Mitigation of combustion & explosions consequences	Development & validation of techniques to mitigate the associated temperature & pressure effects
Safety at indoor car parks & tunnels	Safety strategies & guidelines to control indoor accidents, including indoor car parks & tunnels.
Safety of high pressure electrolysers & fuel cells, and onboard and stationary storage systems	Recommendations for increased safety procedures, including harmonisation of testing protocols.
Open source computational hydrogen safety engineering tool(s)	Following development and validation, hydrogen safety engineering tools and databases made publically available.
Development of incident / accident databases, e.g. HIAD	Linking to & expansion of already established incident/accident databases to support developers & regulators

2.2 REGULATIONS, CODES AND STANDARDS (RCS) ISSUES

Issue	Solution/Deliverable
Harmonization of hydrogen related standards	- Creation of new regulations. - Maintain & update existing, e.g. Global Technical Regulations for hydrogen-powered vehicles 2013.
Development of existing, & establishment of new, testing protocols	Development of existing, & establishment of new, testing protocols that are based on outputs from pre-normative research (PNR) projects.

2.3 EDUCATION AND TRAINING ISSUES

Issue	Solution/Deliverable
Establishment of tailored undergraduate & postgraduate courses	High quality teaching materials, books, lectures, etc...
Continuous professional development (CPD) & Life-long learning (LLL)	System of higher education: CPD & LLL systems.
Short courses	e.g. technical schools, training days, site visits,
Organization of conferences & workshops	Series of national and international conferences & workshops

2.4 DISSEMINATION ISSUES

Issue	Solution/Deliverable
Addressing public awareness and acceptance.	Demonstration of social, economic, environmental & energy impact of FCH technologies.
Engage internal & external stakeholders, to encourage increased RTD.	Series of conferences (national & pan-European), workshops, seminars, etc...

2.5 CFD MODELLING ISSUES

In hydrogen accident scenarios the physical phenomena occur following a typical sequence of events: release and dispersion, ignition, fire or/and explosion (deflagrations or detonations or deflagration to detonation transition DDT). The CFD modelling gaps are listed following the typical sequence of an unintended event. The lists of gaps in the following paragraph are based mainly on two documents (Baraldi et al., 2011) (Kotchourko et al., in Press).

As shown the list of modelling gaps is long and addressing those issues requires times and efforts that goes well beyond the H2FC projects. Nevertheless, a limited number of issues will be addressed within the project, as explained in the “Round-robin tests” paragraph.

2.5.1 RELEASE OF GAS HYDROGEN

- CFD simulation/validation of releases in real complex configurations such as with barriers, obstacles, confinement etc
- Hydrogen releases in enclosures with natural or forced ventilation (effect of mass flow rate and direction; location, number, shape, and area of vents; wind, etc.)
- Validation of notional nozzle models
- Effect of the wind on outdoor releases including areas with complex surroundings such as in urban streets
- Surface effects on jet release (attached or impinging jets)
- Effect of the shape of the nozzle on the release
- Interaction of multiple jets.
- Cryogenic jets (phase change i.e. vapour condensation)
- Turbulence modelling
- Mesh sensitivity
- CFD validation matrix
- Jets from flapping source
- Universal scaling law for the length of the flammable cloud
- Dynamics of unsteady jets e.g. blow downs, puff, bubbles

2.5.2 RELEASE OF LIQUID HYDROGEN

- Two-phase release source.
- Multi-phase jets.
- Dispersion of cryogenic and LH2 in enclosures with passive and forced ventilation
- The physical properties of liquid hydrogen and gaseous hydrogen at very low temperature (but also of O2 N2, H2O – close to saturation) including differences with the ideal gas law.
- Phase change issues such as the hydrogen evaporation and the condensation and solidification of nitrogen, oxygen, and water in the air.
- Effect of weather conditions on the release e.g. humidity, temperature, wind speed and direction, atmospheric stability class.
- Conductive, convective and radiative heat transfer between the cold hydrogen and the surrounding environment including air and the ground.
- Effect of buoyancy and turbulence on the above phenomena.
- The lack of experiments that can close the above open issues is a major obstacle to the development, validation, and application of numerical tools.

2.5.3 IGNITION

- Quantitative validation of CFD models. Experiments are required.
- CFD modelling and validation of the membrane/disk rupture and valve opening.
- CFD modelling of transition from spontaneous ignition to jet fires and/or the quenching of the spontaneous ignition.
- Development and validation of sub-grid scale models accounting for interaction of turbulence and chemistry. The required fine mesh resolutions that are used to simulate small scale experiments are not applicable yet in simulations of large real-scale configurations.
- Development of strategy for ignition delay time and position of ignition source for numerical simulations of hydrogen combustion.
- Ignition in complex geometry: with obstacles, confinement, pipe bends, non-circular openings
- Ignition of hydrogen/hydrocarbon mixture.
- Ignition propensity of hydrogen and hydrogen/hydrocarbons mixtures by different mechanisms (mechanically generated source, electrostatic and corona discharge) at different concentrations
- Ignition probability database generated by numerical simulations with validated tools for different parameters (geometry e.g. length and shape of nozzle, pressure of the vessel/pipe, etc)

2.5.4 FIRES

- A detailed and extensive CFD validation for large-scale H₂ jet fires is missing.
- CFD reproduction of flame length/width and temperature profiles for jet fires (even under conditions of decreasing notional nozzle and H₂ temperature during blowdown).
- Thermal and pressure effects of indoor hydrogen fires. The key issue to be addressed is the limit of mass flow rate from a pressure relief device that will not destroy the enclosure like garage.
- Impinging jet fires and heat transfer to structural elements, storage vessels and communication infrastructure.
- Effects of wind, surfaces, release direction, and obstacles on parameters of jet fires.
- Predictive simulations of blow-off, lift-off, and blow-out phenomena.
- Flames from plane jets (cracks).
- Combination of premixed and non-premixed cases requires further development and validation of partially-premixed models (validation of Takeno and Domingo index and of models within the Takeno/Domingo index approach)
- Self-extinction of hydrogen fires in enclosures and re-ignition.
- Dynamics of under-ventilated hydrogen jet fires in enclosures.
- Modelling and simulations of micro-flames which can potentially cause domino effects. Quantitative reproduction by numerical simulations of flow rate for quenching and blow-off of micro-flames.
- Radiation effects at various distances, including CFD and engineering methods.
- Simulation of fireballs, their cooling down and movement dynamics, especially for large clouds, where cooling occurs mainly by radiation.
- Investigation of the hydrogen release from various types of currently favored hydrogen storage materials and the effects of real storage containers, depending on loading status, operational state, ambient temperature etc.
- Investigation of accident/crash situation including hydride storage facilities.
- Use, improvement and validation of imaging spectroscopy (e.g. fast scanning) and BOS techniques.

2.5.5 DEFLAGRATIONS

- Currently a single physical model and numerical tool that can cover the entire range of phenomena in flame acceleration and propagation does not exist. There are many numerical combustion models but it seems that the range of applicability of many models is limited to a specific type of event/regime.
- More experimental research is needed on laminar burning velocity for all ranges of pressure, temperature and equivalence ratio.
- The effects of thermo-diffusive instabilities, flame stretch and curvature on the flame speed are not completely understood from the quantitative point of view and in connection with numerous mechanisms affecting burning rate of hydrogen-air mixtures.
- CFD modelling and predictive simulation of all flame acceleration mechanisms or mechanisms increasing mass burning rate, including the transition between different combustion regimes such as the transition from laminar flame to turbulent regime.
- Representation of unresolved small-scale geometries in the computational mesh by physical models.
- Development of multi-phenomena combustion models that take into account mechanisms beyond an interaction between flow turbulence (intensity and scale) and combustion, e.g. anisotropic effects, flame instabilities (acoustic, parametric, Rayleigh–Taylor, Kelvin–Helmholtz, Richtmyer-Meshkov, Landau-Darrieus) and their effect on the flame dynamics including scaling conditions
- Dynamics and physical mechanisms allowing to model coherent deflagrations in vented enclosures (parallel development of internal and external deflagrations). Effect of inertia of vent cover on explosion dynamics, including DDT.
- CFD validation of mitigation measures on deflagration strength e.g. appropriate use of water spray or water mist.
- CFD simulations/validation of explosions in real-scale configurations, such as complex geometry with multiple obstacles and different level of confinement.
- Model constants are often adjusted in order to describe different combustion events and to enlarge artificially the range of applicability of the model. This should be clearly stated and it is expected that “varying constants” should be finally understood and explained in the scientific literature.
- Development and validation of very large eddy simulation (VLES) models and LES models in conditions of limited computer resources
- Partially premixed flames, in particular triple flames in hydrogen-air layers and their pressure effects in enclosed space.
- Critical conditions for flame acceleration (and DDT) in cryogenic hydrogen-air mixtures
- Mechanisms of LH2 enrichment by oxygen and explosions after LH2 spills

2.5.6 DETONATIONS AND DDT

- Development of models and quantitative reproduction of experimental data by CFD.
- Very high mesh resolution requirements or reliable SGS models of DDT (similar issue in Ignition: Development and validation of sub-grid scale models accounting for interaction of turbulence and chemistry. The required fine mesh resolutions that are used to simulate small scale experiments are not applicable yet in simulations of large real-scale configurations)
- Simulations of pressure and impulse dynamics in real-scale complex geometries.
- Real gas properties and gas law for the high pressure and high temperature range.

2.6 HYDROGEN SAFETY ROADMAP

2.6.1 ROUND – ROBIN TESTS

As described in deliverable D10.5 (1st Report on round robin testing), some experiments were selected to perform CFD model benchmarking with the software packages that are used by the project partners. More specifically, experiments were selected to address some of the relevant issues in hydrogen dispersion and in combustion, as it is illustrated in the following paragraphs.

2.6.1.1 RELEASE AND DISPERSION

In the first set of experiments, helium was released in a 1 m³ enclosure with one opening. The CEA GAMELAN facility is illustrated in Figure 1. Helium was released with a flow rate is 300 NL/min through a 20mm diameter vertical nozzle that is located at 210 mm above the floor.

The second set of experiments was carried by HSL in a much larger facility (5m x 2.5 m x 2.5 m) as shown in Figure 2. Hydrogen was released with a flow rate of 169 NL/min through a 0.55mm diameter hole which is located at the center of the facility at 0.5m above the floor. The release velocity was sonic and its duration was 1400 sec. More details about the experiments can be found in deliverable D10.5.

By the dispersion round-robin tests, the consortium will address the following issues that are related to hydrogen release in enclosures with a vent:

- Hydrogen releases in enclosures with natural ventilation.
- Validation of notional nozzle models.
- Effect of the wind on outdoor releases, since the HSL facility is placed in an unconfined environment.
- Surface effects on jet release, in particular impinging jets.
- Turbulence modelling.
- Mesh sensitivity.
- CFD validation matrix.

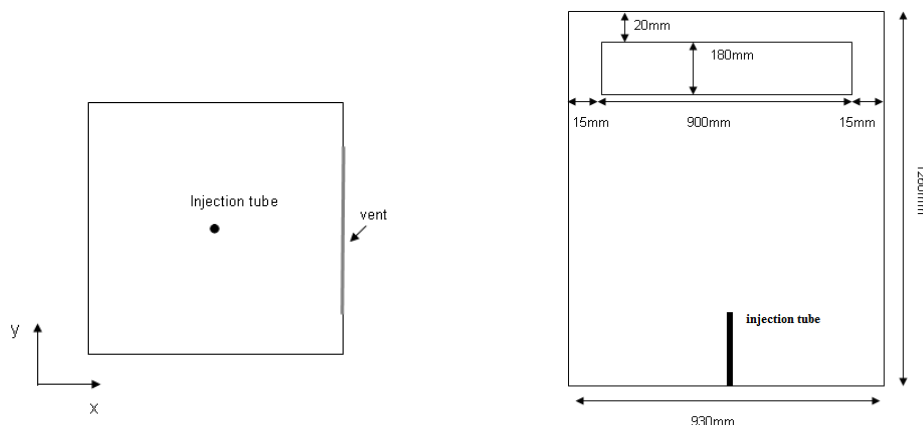


FIGURE 1: GAMELAN FACILITY

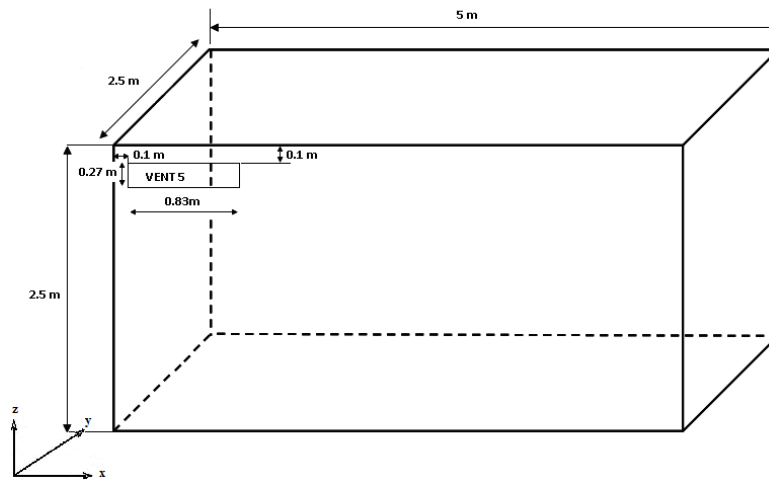


FIGURE 2: HSL FACILITY.

2.6.1.2 COMBUSTION

Following on from D10.5, D10.6 (2nd Report on Round Testing) will address CFD combustion benchmarking. After discussions with partners, one of the FM Global set of experiments was selected (Bauwens et al., 2011).

The details of this experiment are illustrated in Figure 3 and are summarised below.

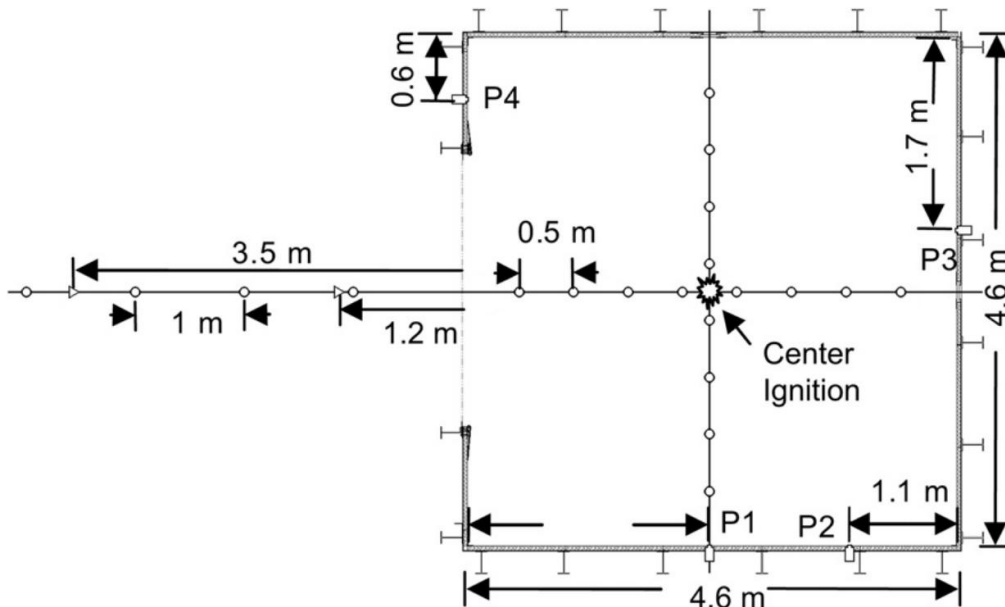


FIGURE 3: FM GLOBAL CHAMBER GEOMETRY AND INSTRUMENTATION.

The experiment as described in (Bauwens et al., 2011) was performed at the FM Global 63.7 m³ (4.6 m x 4.6 m x 3 m) large scale test chamber, with a square vent of 5.4 m² located on one of the vertical walls. In this experiment

hydrogen concentration was 18% by volume. Ignition occurred at the centre of the chamber. Four pressure transducers were mounted to the inside of the chamber. The initial mixture was supplied by injecting the pure fuel through an inlet at floor level while mixing fans within the chamber were used to create a uniform mixture. Prior to ignition, the unburned mixture was contained within the chamber using a 0.02 mm thin sheet of polypropylene. Ignition was supplied using a carbon rod igniter. Pressure-time histories were provided, recorded by transducer P1. This allowed detailed comparison with simulation results permitting model analysis.

2.6.2 ROADMAP BEYOND H2FC

Several issues have been identified and described in the previous chapters. A certain number of issues are addressed within the H2FC project e.g. in deliverable D9.1 (Harmonised Methodology for Testing of Pressure Relief Devices) and D9.2 (Fire Resistance of Hydrogen Storage Tanks and Bonfire Test Protocols) the issue of development of existing, and new testing protocols (in the RCS paragraph) are addressed.

Nevertheless as it was described in the previous paragraphs the number and the complexity of the issues are too large to be addressed and tackled within the H2FC project. In order to close the most relevant open issues, it is necessary to foresee an effort that goes well beyond the year 2015 as described in Figure 4.

Figure 4 outlines how the hydrogen safety deliverables achieved within H2FC1 will feed into the resolution of the outstanding safety issues going forward beyond H2FC1 (i.e. to fulfil the issues outlined in Section 2.1 to Section 2.5).

For example as outlined in Section 2.1 a technological safety issue which must be addressed is the increase of the fire resistance rating of hydrogen storage systems, from their current levels of 10 – 20 minutes. In order to resolve this issue there must be a harmonisation of test methods, test protocols and benchmarking for fire resistance of onboard pressurised hydrogen storage tanks, materials and components, fuel cell components degradation mechanisms and fuel quality measurements. This development of methods, protocols and benchmarking is the objective of WP9 (JRA3) within the H2FC project. Following the conclusion of H2FC1 this work will feed into the knowledge base required to resolve the technological safety issue of increasing the fire resistance rating to 1 – 2 hours (this is indicated by the dotted arrow shown in Figure 4).

Additionally the outcomes from H2FC1 will also facilitate the resolution of other hydrogen safety related issues including better estimation of separation distances, indoor release and dispersion of hydrogen, mitigation of combustion and explosion consequences, the development on open source computational hydrogen safety engineering tools, the continued need to address public awareness issues, the development of high quality teaching materials and the continued development of incident and accident databases, among others. These issues, along with the remaining issues identified in Section 2.1 to Section 2.5, will be addressed going forward into Horizon 2020 if they have not been resolved within H2FC1.

Finally, it should be noted that the development of the European e-Infrastructure for H2FC research, which is planned to be operational after the end of the H2FC1 project is reliant on the transfer of the distributed research infrastructure that exists into a Pan-European Research Infrastructure in H2FC after the end of the project.

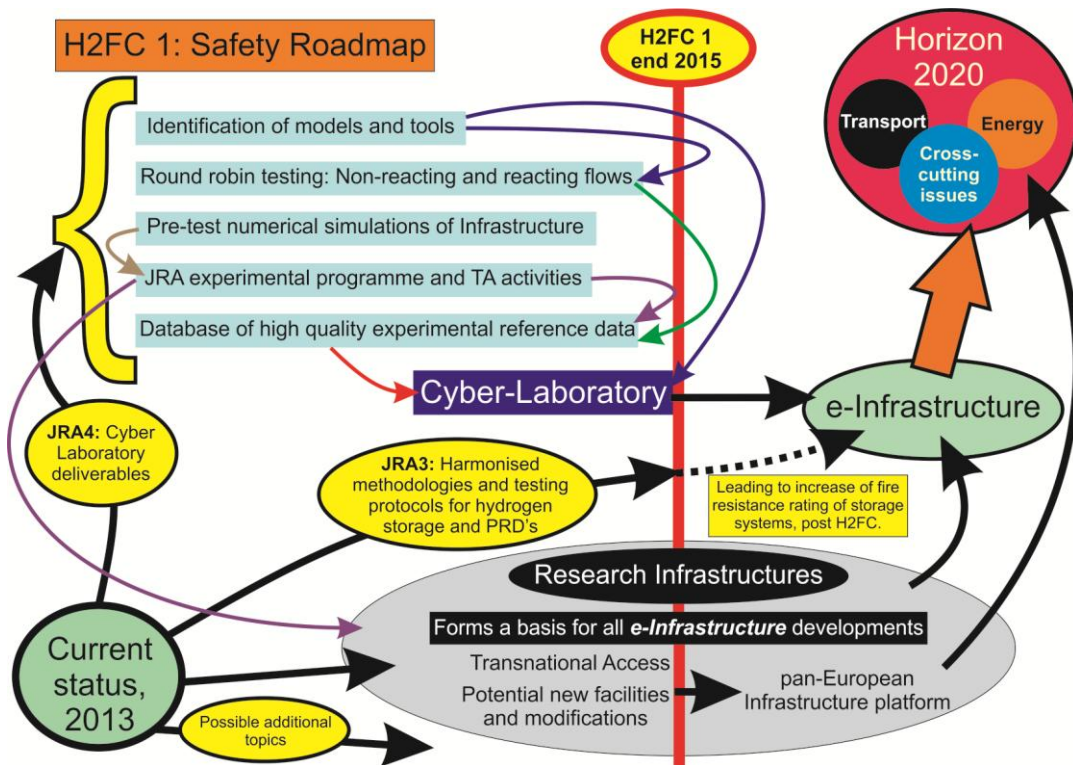


FIGURE 4: HYDROGEN SAFETY ROADMAP

3 HYDROGEN STORAGE AND BEHAVIOUR IN SOLIDS

In the case of hydrogen storage and behaviour in solids, the effective cooperation between microscopic, mesoscopic and macroscopic approaches and models is necessary for the efficient study of storage materials and systems from the small to the pilot scale. This requires a multi-scale approach that can be summarized in the following steps (the output of each step is used as input to the next):

- Modelling H₂-material interactions (Ab-initio calculations)
- Use effective potentials to calculate hydrogen adsorption / desorption capacities of the material (Monte Carlo methods, mesoscopic scale)
- Use material properties and capacities to design optimal storage tanks
- Integrated models encompassing the overall system (storage tank and fuel cell thermal coupling)

In addition, certain specific gaps were identified in D10.2 as mentioned below (the list is by no means meant to be exhaustive).

Limitations of current models / codes and existing gaps

- Reliability of material properties used as input to models and codes. A systematic evaluation of the respective data is needed.
- Understanding of the role of additives and dopants in various system configurations is missing.
- A systematic comparison among the different existing codes at the Density Functional Theory (DFT) level is necessary. Their findings for very similar configurations may vary considerably adding large uncertainties to the simulation results. In addition, the attained accuracy in the calculations vs. speed should be assessed.
- Evaluation of DFT functionals as well as evaluation of weak interaction & dispersion forces insertion in DFT-D should be carried out (in connection to the above item)
- Evaluation of different 'connections' & communication in the proposed Multi-Scale Scheme, e.g. how the uncertainties in the output of a model at micro- or meso-scale affect the predictions for material capacities and storage system (tank) performance and design optimization.

Three representative integrated case studies have been built to address such gaps and demonstrate the Multi-scale Approach and the respective models / codes:

- I. Hydrogen clathrates (Physisorbing materials);
- II. Carbon based structures / MOFs; (Physi- & weakly Chemisorbing, after doping)
- III. Metal hydrides; Metal hydride tanks (Chemisorbing)

Work has been initiated and is underway for the first two cases.

3.1 CASE 1 – STORAGE IN HYDRATES: FROM THE MOLECULAR TO THE CONTINUUM SCALE AND BEYOND

3.1.1 BACKGROUND

In hydrate-related studies multiple length scales can be identified, as very clearly pointed out in the figure below. The length scales span from the molecular level (i.e. characteristic lengths that are less than 1 nm), where distinct molecules are considered and their behaviour is examined, up to the continuum scale (characteristic lengths of the order of metres). Different problems need to be addressed at the different length scales as shown in Figure 5.

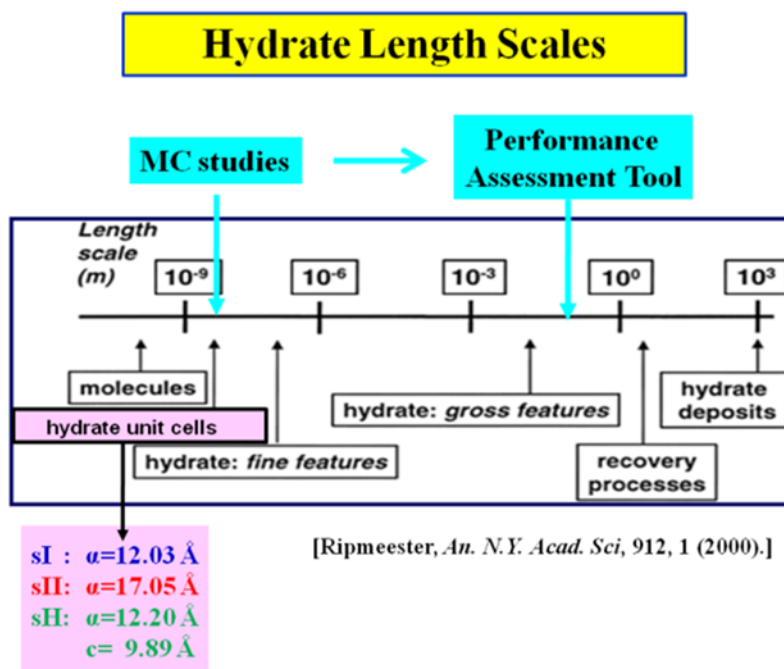


FIGURE 5: HYDRATES LENGTH SCALES

3.1.2 STUDY OBJECTIVE

The objective of this study is to demonstrate the applicability of a multi-scale approach to the case of a gas storage system. To fulfil this purpose the case of H₂ storage in clathrate hydrates will be considered as a demonstration paradigm. The proposed study consists of three distinct steps that address issues at different length scales. In particular:

- **Step 1:** We use molecular level simulations (Monte Carlo) to obtain the gas storage capacity of different hydrate structures.
- **Step 2:** We develop a macroscopic Performance Assessment Tool (PAT) using the mathematical expressions obtained in the previous step.

- **Step 3:** We use the developed PAT in order to identify attractive candidate systems for gas storage and recommend experimental work for confirmation.

3.1.3 CURRENT WORK PROGRESS

Step 1: An extensive series of Grand Canonical MC (GCMC) simulations is currently in progress at various temperatures, pressures, hydrate structures and examining the effect of different intermolecular potentials between the different molecules involved in the simulations. The GCMC simulations will provide the parameters for each hydrate structure that will enable us to calculate the gas-storage capacity for each structure.

Step 2: An on-line tool is currently under development based on Python language that performs the parametric calculations. With the use of PHP language the numerical calculations and the resulting figures (e.g., % wt of H₂ as a function of pressure for a given temperature) will be mounted on a web page. Both aspects of the current step are in progress.

Step 3: For validation and testing purposes of the python-based part of the work, a MATLAB code is also under development. This code can also be used for the parametric studies to identify attractive candidate systems for gas storage and recommend experimental work for confirmation.

3.2 CASE 2 – STORAGE IN CARBON STRUCTURES

This work was performed in cooperation with the task force member: Prof. Froudakis of Univ. Crete.

The main aim here is to address one important existing gap by comparing and evaluating several computational methods for the calculation of potential energy surface of the interaction between molecular hydrogen and benzene. According to bibliography, computational studies have shown that hydrogen can interact with a parallel or vertical formation above the centre of benzene ring. A series of calculations are performed to produce appropriate comparison charts and reach conclusions with regard to:

- DFT functionals with semi empirical correction to include dispersion forces such as BLYP, BP86, PBE, TPSS, B3LYP and B2PLYP.
- Comparison RI-MP2 and RI-SCS-MP2. All computations performed with the basis set def2-TZVPP and RI approximation by using the ORCA computational package.
- Comparison of DFT functionals with D3 dispersion correction. All computations performed with the basis set def2-TZVPP and RI approximation for GGA functionals and RIJOCS approximation for hybrid functionals by using the ORCA computational package.
- Comparison of ORCA and TURBOMOLE computational packages for the PES calculation using the same computational method and details. All calculations performed with DFT's functional PBE, D3 dispersion correction, def2-TZVPP basis set and RI approximation.
- Comparison of calculations that include BSSE correction and without it. All calculations performed with DFT's functional PBE, D3 dispersion correction and def2-TZVPP basis set with the TURBOMOLE package.

First results of the above approach are reported in D10.7.

4 HYDROGEN FUEL CELLS

The road map for fuel cell (PEMFC and SOFC) modelling for the horizon 2020 is focus on two main directions:

- To elaborate predictive models at different scales in order to both help new material designs for the different components of the cell (catalyst, membrane, Gas diffusion layer,...) and also to improve control command and energy management strategies with durability constraints
- To elaborate systemic Round Robin tests between partners, and start to share libraries and code in order to have an European database for fuel cell modelling (PEMFC & SOFC)

The main objectives for modelling and simulation are:

- Understanding of degradation mechanisms (with a bottom-up or top-down approach)
- Further development of existing kinetic models (multi-scale approaches) at the cell and stack level
- Prediction of complete system performances and lifetime (durability constraints function of the operating conditions)
- Models to improve design and optimized sizing of a system (with durability constraints)

The different activities of modelling (for both FC, EC and HT or LT) are defined below, and illustrated in Figure 6.

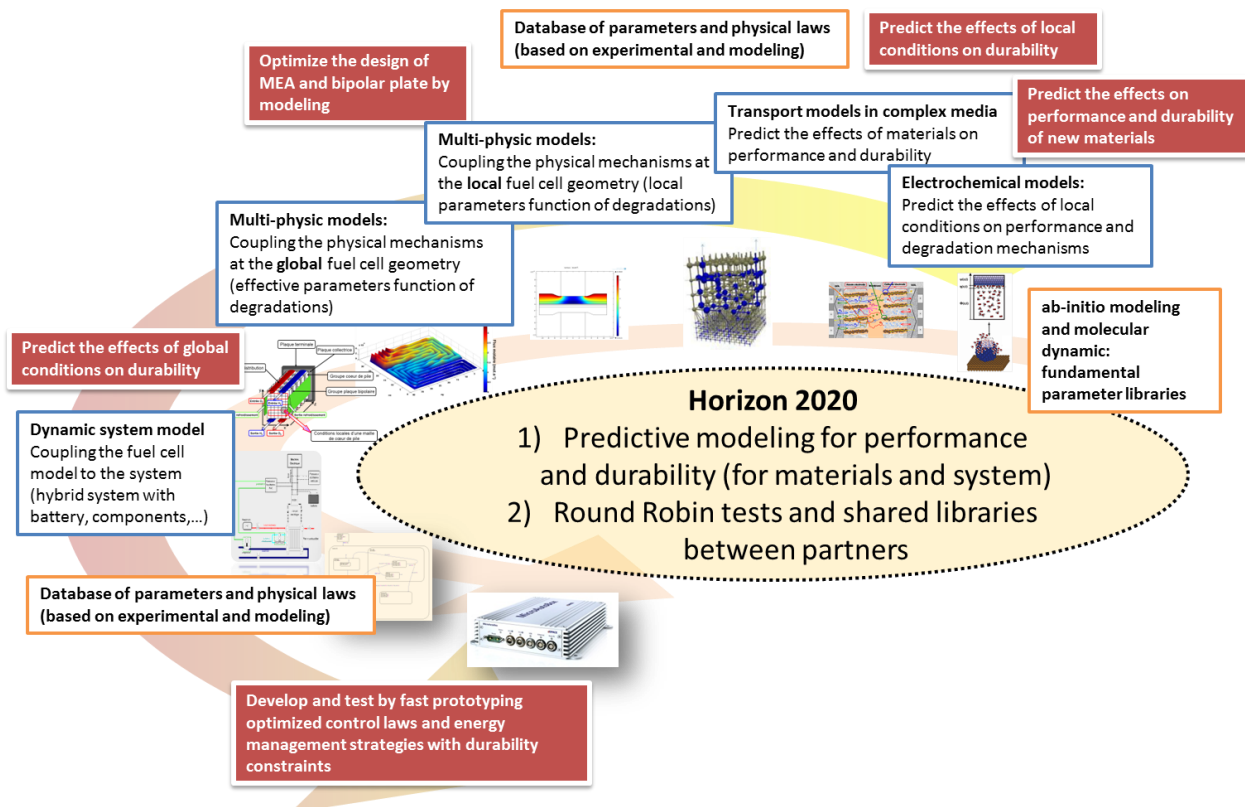


FIGURE 6: FC MODELLING ACTIVITIES

- ***ab-initio* modelling (DFT, kinetic Monte-Carlo, dynamic molecular)**
 - Increase the understanding of phenomena and their kinetics
 - Developed a common library with the fundamental parameters of different catalysts, catalyst supports, ionomer

- **Development of a predictive electrochemical model**
 - 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
 - Study the influence of material properties variation especially as caused by or leading to degradations
 - Propose relevant models simplifications in order to include them in a cell and stack models

- **Development of transport models in a complex media**
 - Develop anisotropic model of porous media
 - Predict the effects of a new porous media on performance and durability
 - Build a shared libraries of effective transport parameters for the continuous models

- **Development of multi-scale approach for the cell level**
 - Multi-scale modelling 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
 - Mapping of operating conditions which promote materials degradations
 - Round Robin tests of existent codes, co-development and sharing of libraries

- **Development of global multi-scale approach**
 - Multi-scale modelling approach able to combine predictive laws of degradation mechanisms (reversible and irreversible), taking into account the specific stack architectures and the dynamic operating conditions of the system
 - Methods and rules to improve thermal and water management and the overall stack performance; simplified thermal components in terms of design, manufacturing and maintenance
 - Round Robin tests of existent codes, co-development and sharing of libraries

- **Design models of bipolar plates and stack and system**
 - Further development of actual codes for the design of BP, stacks, flow distributions
 - Develop stack model useful to investigate stack performance during transients and dynamic interactions between system components; robust and accurate simulation tools that can reduce the time needed for stack design
 - Simulation tools to optimize cost, performance and durability as a function of the application and constraints of the system

- **Dynamic system models and diagnostic models**
 - Validated physical FC/EC system models at different operating range conditions and applications, with degradation mechanisms and validation
 - Link performance/lifetime to operating conditions, development of diagnostic tools able to follow degradation in performance/lifetime; SOH indicators and management, predictive commands for the improvement of the FC/EC durability
 - Signal analysis to detect first signals of degradation
 - Developed a common library with degradation rates function of the operating conditions

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

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