

A model evaluation protocol for Computational Fluid Dynamics (CFD) models used in safety analyses for hydrogen and fuel cell technologies

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Hydrogen and fuel cell technologies are seen as an increasingly important means of energy conversion and energy storage as European energy policies encourage transition to renewable sources, reduction of greenhouse gas emissions, and an increase in energy efficiency. This brings a corresponding move of these technologies out of the industrial domain, which is characterised by large quantities and a controlled environment, to the public domain which is characterised by a more diverse range of applications in typically less well controlled environments. The increase in demand brings an increasing need to carry out safety analyses and will therefore result in a more widespread deployment of modern numerical tools such as Computational Fluid Dynamics (CFD). This in turn has led to a requirement for a better understanding of the suitability of CFD models for each specific application.

Model Evaluation Protocols have been in existence for many years as a means of testing the quality of simulation tools mainly in the area of pollutant dispersion modelling. There have been several European initiatives for model evaluation covering dispersion, as well as fire and explosion modelling. The "SUpport to SAfety ANalysis of Hydrogen and Fuel Cell Technologies" (SUSANA) project aims to support stakeholders using CFD for safety engineering design and assessment of fuel cells and hydrogen (FCH) systems and infrastructure through the development of a new model evaluation protocol. The protocol covers all aspects of safety assessment modelling using CFD, from release, through dispersion to combustion and not only aims to enable users to evaluate models but to inform them of the state of the art and best practices in numerical modelling.

To achieve the aims, the project has seven work packages which are based upon a support strategy of collecting information from outside the project and disseminating this information to the user community. There are seven partners in the SUSANA consortium and each is responsible for a particular work package and coordinating the work of the other partners in that area. This paper gives an overview of the SUSANA project, the work packages and the main stages of the model evaluation protocol.

Keywords: Computational Fluid Dynamics, Model Evaluation Protocol, Hydrogen

Introduction

Strategic documents on European energy policies support a transition to renewable energy sources and diversification of the energy supply. The use of fuel cell and hydrogen (FCH) technologies would form an important part of this transition, as a means of flexible and efficient energy conversion. To date the main use of FCH systems and infrastructure has been in industrial applications, but with wider use, as part of a transition, they will move into the public domain and increasing numbers of the population will interact with FCH systems. Concerns about the level of safety of FCH installations could affect public acceptance of the technology. Already increasing numbers of FCH early market projects require a growing number of hydrogen safety experts who are able to make efficient use of available tools for safety engineering design, for example, Computational Fluid Dynamics (CFD). CFD can be used as a compliment to experimental studies and testing of FCH systems, and it is often the only affordable way to develop engineering solutions and safe strategies for their use. However, CFD users may not have experience of the hydrogen industry and its safety issues, while those in the hydrogen industry may not have knowledge of performing numerical simulations for analysis of the safety of FCH systems. While computing power is increasing and the interfaces for CFD tools are becoming more user friendly, the knowledge and skills to use them in the hydrogen industry is still limited. These limitations include knowledge of the state-of-the-art in the physical and numerical aspects of the models, and best practice in the application of CFD for safety engineering design of FCH systems. Failure to apply this powerful technology properly could have serious consequences for safety and for the future of FCH technologies. The European "SUpport to SAfety ANalysis of Hydrogen and Fuel Cell Technologies"

(SUSANA) project aims to support all stakeholders using CFD for safety engineering design and assessment of FCH systems and infrastructure, especially those who have no specialised knowledge in hydrogen safety and associated CFD modelling/simulations practice, through the development of a Model Evaluation Protocol (MEP). The project is supported by the Fuel Cells and Hydrogen Joint Undertaking (FCH JU) a European initiative supporting research and development activities in fuel cell and hydrogen energy technologies. The three members of the FCH JU are the European Commission, fuel cell and hydrogen industries represented by the new Industry Grouping and the research community represented by Research Grouping N.ERGHY

A Model Evaluation Protocol for hydrogen Safety simulations

Model evaluation can be seen as a framework that encompasses several activities. A Model Evaluation Group (MEG) was set up by the European Community in the early 1990s. The group was set up to develop methods for the evaluation of models in the major industrial hazards area. It had become apparent that models used in industrial hazard assessment had never been formally validated, but were used as the basis for decisions that directly affected public safety and the environment. In 1994 the group published guidance on model evaluation protocols (MEG, 1994). This provides a framework for the key activities needed to evaluate models: model description, scientific assessment including limits of applicability, user-oriented assessment including ease of use, verification and validation. The purpose of the scientific assessment is to establish the scientific credibility of a model. Verification is used to ensure that models produce output as described by their specification, i.e. solving the equations correctly and with sufficient accuracy. In validation model outputs are compared with measurements of physical parameters to demonstrate that the model captures “real world” behaviour across its intended range of applicability.

Testing the results of model predictions against experimental data, Kakko et al. (1994) highlighted the need for suitable databases of model validation data as it was often difficult to obtain or not presented in a way which was suitable for model validation. A classic example of a model validation database is the modeller’s data archive (MDA) of Hanna et al. (1991) which recognised the need to collate data in a suitable form in a way that could be accessed by model developers. Since then, some other datasets have been produced, such as the Rediphem database (Nielsen and Ott, 1996).

The SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models) project (Carissimo et al, 2001) brought together the concept of a model evaluation protocol and specialised database. Its main aim was to provide a methodology not only for validation but also scientific review of models. The project focussed on situations in which complex effects such as aerosols, topography and obstacles were important, as well as simple situations. Ivings et al. (2007, 2013) set out a Model Evaluation Protocol for models used to predict the dispersion of vapours from Liquefied Natural Gas (LNG) installations. The protocol is based upon the SMEDIS project but is not confined to the modelling of LNG spills as other, simpler cases should also be taken into account in model evaluation. One of the recommendations of the MEP by Ivings et al. (2007, 2013) was that validation should be performed by running models against an experimental database. Such a validation database was constructed for this purpose (see Coldrick et al., 2009).

In 2011, a report titled “Prioritisation of Research and Development for modelling the safe production, storage, delivery and use of hydrogen” (Baraldi et al, 2011) was produced for FCH JU. The report was based on the outcomes of a literature review and a workshop attended by recognised experts in the field of hydrogen safety. A hydrogen accident usually follows a typical sequence of events and for each stage of the accident, the critical CFD modelling issues were identified and prioritised. This gap analysis found that a model evaluation framework and associated database (such as the LNG MEP of Ivings et al., 2007) did not exist for hydrogen safety modelling. The SUSANA project aims to meet this need by producing a Model Evaluation Protocol, in addition to a support infrastructure achieved through the following objectives:

- A review of the state-of-the-art in CFD, physical and numerical modelling applied to safety analysis in FCH technologies.
- Updating and enhancing the verification and validation procedures for CFD models/codes/simulations.
- Compiling a best practice guide in numerical simulations of problems specific to safety of FCH technologies.
- Developing a CFD Model Evaluation Protocol for assessment of the capability of the CFD models to accurately describe the relevant physical phenomena and the capability of the CFD users to follow the correct modelling strategy.
- Creating the infrastructure for implementation of the CFD Model Evaluation Protocol, which includes:
    - A database of problems for verification of codes and models against analytical solutions, designed to demonstrate capability of CFD codes to numerically solve the governing equations.
    - Model Evaluation Database of experiments for validation of simulations covering a range of phenomena relevant to FCH safety.
    - A benchmarking exercise for codes and models, further advanced during the project and to be continued beyond the project.

- A project website[1] to provide open access to the databases, the best practice document, benchmark exercise specifications, available benchmark results, etc. to all stakeholders through a public access area.

- Establishing an experts' group at an early stage of the project. The experts' group will complement the knowledge of the project partners and provide external feedback on the development of the project, and the implementation of the Model Evaluation Protocol.
- Provide cross-fertilisation of expertise and experience in the field available in Europe and globally.
- Dissemination of project results to stakeholders through different channels, including the project website, an expert workshop, a dissemination seminar, publications and conference presentations.

The project brings together partners with an established track-record in hydrogen safety, along with fundamental and industry-driven CFD research, from across Europe. The partners include stakeholders from research organisations (KIT-G, NCSRD, JRC), universities (UU), industry (AREVA/HELION, Element Energy), and regulators (HSE/HSL). This will maintain a proper balance between academic and practical aspects of the project outcomes, and will ensure that the project results are relevant to achieve the expected impacts on safety of emerging FCH systems and infrastructure. All project partners are actively involved in national programmes relevant to hydrogen safety, both at an academic level and in the practical use of CFD for the emerging hydrogen sector.

The project started in September 2013 and runs for three years. A draft of the review of the state of the art in CFD has been written, with input from all partners. An experts' workshop on "Computational Hydrogen Safety", was held in September 2014 to provide feedback on the proposed development of the project and benchmarking is in progress. Further information on these activities is given below.

The objectives for the project outlined above have been divided into seven work packages and each of the project partners is responsible for the delivery of one or more of the work packages. Each work package (WP) is divided into a number of tasks having a partner acting as a task coordinator, who manages the input from the other partners. Figure 1 is a graphical representation of the work packages showing their interdependencies. A description of each work package is given below.

Work packages in the SUSANA project

WP1 - Management

WP1 consists of two tasks; general project management and providing the project website. Project management is led by the coordinator (KIT-G) and the management committee. They are responsible for detailed planning and day-to-day operations, financial management, and preparation of reports for the FCH JU. The management committee is composed of work package leaders and includes at least one representative from each partner. General project management also includes the organisation of regular meetings to monitor the progress of the project. The project website is used to support internal project activities such as serving as a repository and exchange area for documents, reports, deliverables, etc. The project website also has an external aspect, acting as a tool for outreach and communication between stakeholders and for dissemination of the project outcomes during and beyond the life of the project.

WP2 - Critical analysis and requirements of physical and mathematical models

In WP2 models of physical phenomena related to safety in FCH technologies will be reviewed, and their strengths and weaknesses will be explored. A critical survey will be carried out of physical models and associated mathematical models for CFD modelling, including governing equations and source terms. This will cover the following phenomena: gaseous and liquid hydrogen releases, dispersion of permeated hydrogen, dispersion of hydrogen in the open atmosphere and ventilated enclosures, spontaneous ignition, jet fires and microflames, deflagrations and detonations. The survey will also outline knowledge gaps and bottlenecks of existing models. WP2, along with WP4 and WP5, addresses the capability of CFD models to accurately describe the physical phenomena relevant to FCH technologies. WP2 underpins activities in WP3, WP4, WP5 and the ultimate project outcome in WP6, i.e. the CFD Model Evaluation Protocol.

The results of WP2 are presented in the form of two deliverables. The first is a "Review of the state of the art in physical and mathematical modelling of safety phenomena relevant to FCH technologies", in which physical phenomena relevant to hydrogen safety are introduced, their physical and mathematical description is provided and commonly used numerical approaches used for their modelling are formulated and described, a draft of this document has been written. The second, "Critical analysis and requirements of models" will be dedicated to a comparison of the numerical models described in the review, formulation of their requirements and limitations, and comparative analysis of their strengths and weaknesses. Both deliverables are structured into four chapters, corresponding to the main groups of phenomena important for hydrogen safety engineering: release and dispersion, ignition and fire, deflagration, and detonation.

The first chapter covers the physical and mathematical modelling of hydrogen releases and dispersion. In simulating hydrogen releases, one will often encounter all three major types of fluid flow – laminar, transitional and turbulent. Each type of flow requires a different modelling approach in order to obtain accurate results and it is therefore critical to use appropriate models. The physical difference between flow types is discussed and the Reynolds number characterizing flow type is introduced. The equations governing flow behaviour are introduced and different types of turbulence closure model

[1] http://www.support-cfd.eu/

and the concept of turbulence scales are described and their comparative qualities are discussed. An accurate account of turbulence is essential for an accurate prediction of fluid flow. It is, however, one of the most challenging and computationally expensive areas of fluid dynamics modelling. Advanced models require very large computational resources, which can become prohibitive in many cases of practical importance. Selection of an appropriate approach to turbulence modelling is, therefore, of paramount importance in achieving success in CFD simulations. Three major types of turbulence modelling are discussed. Direct Numerical Simulation (DNS) is the most precise since it resolves turbulence down to the smallest scales. DNS is prohibitively expensive in terms of computational requirements for larger Reynolds number flows and all but simplest of geometries. Reynolds-Averaged Navier Stokes (RANS) approaches, on the other hand, are widely used for engineering modelling of large scale, high Reynolds numbers flows, including flows around complex geometries. In theory it is the least accurate, since it uses modelling rather than simulation of turbulence at all scales, and it often requires tuning of several parameters to reach adequate results. Large Eddy Simulation (LES) occupies a middle ground, simulating large scale turbulence and modelling small, or sub-grid scale (SGS) turbulence. Hence it can provide high accuracy for problems of practical interest while remaining within the acceptable range of computation power requirements. Application of DNS, RANS and LES approaches to different problems is discussed and different numerical models used in RANS (k-ε, k-ω) and LES (MILES, Smagorinsky, Dynamic Smagorinsky-Lilly, etc.) are described. Accounting for compressibility is another flow characteristic which needs to be taken into account in CFD simulations and the difference between equation sets describing compressible and incompressible flow is outlined. After introducing the fundamental physics underlying CFD modelling and providing a set of governing equations, the chapter continues with the description of a number of common physical phenomena encountered in safety related modelling and their numerical treatment. These include; the effect of wind, jet associated phenomena, release and dispersion indoors, diffusion and permeation, fast filling of storage tanks, and phenomena associated with liquid hydrogen releases and dispersion.

The second chapter describes hydrogen ignition and jet fires and the models used in their simulation. The ability to accurately calculate ignition conditions is of particular importance for the field of hydrogen safety since it allows one to predict if released hydrogen will ignite and determines if the subsequent hydrogen combustion will take the form of a jet fire or deflagration/detonation with obvious safety implications. A detailed list of various ignition mechanisms is provided. Particular attention is paid to the phenomenon of hydrogen spontaneous (diffusion) ignition and the models used to simulate it. Two dimensional DNS and three dimensional LES models are described along with requirements and limitations imposed on them by the physical characteristics of the phenomenon. The review of the phenomenon of jet fires starts with a description of the physical phenomena associated with jet fires. Different jet fire types, including buoyancy controlled, momentum dominated (under-expanded) and fully expanded momentum dominated jet fires are described. A novel dimensionless correlation for the flame length is described, which clearly identifies three jet fire types. The second part of the chapter covers fire modelling techniques and begins with an introduction to the governing equations for the reacting flow. Various combustion modelling approaches and their area of applicability are described. The choice of appropriate combustion model should be based on the phenomena to be modelled and available computational resources. Simplified models, such as Eddy Break-Up (EBU) and Eddy Dissipation Model (EDM) are computationally inexpensive and can be applied for modelling large scale fires. At the same time, due to their underlying assumption, they are incapable of capturing some phenomena such as flame lift-off and blow-down. If detailed modelling including such phenomena is required, more sophisticated models, such as Magnussen's Eddy Dissipation Concept (EDC) model are required. They allow more accurate modelling of combustion processes at the expense of increased computational requirements. EBU, EDM and EDC models, along with Flamelet, Linear Eddy and Arrhenius (finite chemistry) approaches are described and the examples of their application to fire modelling are provided.

The third chapter is dedicated to a description of deflagration phenomenon and its modelling. Predication of deflagration consequences is a topic of very high importance in hydrogen safety field due to a deflagrations potential for causing extensive property damage and threat to life. The chapter begins with an introduction to the physical phenomena encountered in deflagration modelling and their mathematical description. Deflagrations in closed vessels and in the open atmosphere are described, along with the problem of vented deflagration, including a description of coherent deflagration phenomenon and the effect of inertial vent covers. Deflagrations in obstructed environments and in enclosures with lean and non-uniform mixtures are considered and the physical and mathematical description of associated phenomena is provided. Deflagration to detonation transition (DDT) phenomena is described and required conditions are outlined. The second part of the chapter lists numerical models used for deflagration modelling and a set of governing equation is introduced.

In the fourth chapter detonation phenomena are described. Detonation propagation, reflection and curvature are described and the differences between one and three dimensional detonation propagation are explained. Detonation modelling using the Arrhenius reaction rate approach and gradient method are described. Examples of gradient method application are provided and its advantages and requirements are discussed.

WP3 - Guide to best practices in numerical simulations

WP3 gathers together the SUSANA partners' state-of-the-art knowledge on best practice in the application of CFD to safety engineering design of FCH systems. WP3 complements the survey of physical and mathematical models in WP2 and serves as a "user guide" for their implementation. The best practice guide addresses the issue of users' capability of correctly applying CFD codes through four chapters for each particular phenomenon. A further chapter covers user education and training. The chapters have been written by project partners who are specialists in each area of numerical simulation. The CFD Model Evaluation Protocol will refer to the guide as a knowledge base beneficial to all CFD users, and provide a learning tool for newcomers in the area of safety of FCH technologies.

The first chapter of the guide provides best practice guidelines for hydrogen release and dispersion simulations. As discussed in WP2, a wide variety of flow types can exist and turbulence modelling is very important, therefore both RANS modelling and LES approaches are discussed. Two phase flow modelling is also presented, because liquid hydrogen vaporises by absorbing heat from its surroundings and complex phenomena are involved, such as the condensation and freezing of the ambient air and moisture. Modelling approaches for dealing with such complicated scenarios are introduced. Guidelines for the domain size and mesh design considerations are also presented, such as expansion ratios, aspect ratio, density of the grid and refinement regions. Under-expanded jets may result from gas releases from a high pressure storage tank and their simulation can be challenging. The length of the resulting jet can be several orders of magnitude larger than the characteristic scales defining physical processes in the immediate vicinity of the nozzle. Consequently, numerical modelling of the entire jet in a single computational domain makes simulations prohibitively computer intensive. Therefore, to model under-expanded jet releases three different modelling approaches are presented: the two stage approach, the effective nozzle approach and the volumetric source model. Proper boundary and initial conditions are also suggested and initial conditions for simulations in an open environment with the presence of wind are discussed.

In the second chapter, best practice guidelines for ignition and jet fire simulations are given. Numerical modelling of hydrogen autoignition presents significant computational challenges. Shock heating seems to be the primary cause of hydrogen spontaneous ignition, which means that numerical methods seeking to model autoignition have to be able to simulate shocks, small scale turbulent mixing and shock wave/vortex interactions. As a result ignition models require a combination of a highly resolved mesh with a highly accurate numerical method. Problem setup, domain design, meshing, boundary and initial conditions of representative problems are given for both ignition and jet fire simulations. Finally numerical options such as solver type and discretization schemes are discussed.

Chapter three of the guide is dedicated to deflagrations, the modelling of which is a challenge. There is no modelling approach which is clearly superior to the others and applicable to all circumstances. This is due to the complex interactions between the turbulent flow field and combustion chemistry, together with the very wide-range of applications for which models are required. The modelling of the combustion rate has a strong effect on the deflagration process development. The key physics of hydrogen deflagrations in both open and enclosed spaces are reviewed providing the foundation for the best practice guide. Guidelines for the choice of the turbulence model are given first. Then combustion modelling is discussed focusing on open-air deflagrations, vented deflagrations and combustion with the presence of obstacles. Rayleigh-Taylor instability modelling is also discussed in the case of vented deflagrations. Guides for problem setup and numerical options are also provided.

In the fourth chapter best practice guidelines for detonations are given. The conservation equations in Euler formulation are usually used along with a model for the chemical interaction. The correct selection of the chemical interaction model often plays a key role in the successful implementation and utilization of a detonation model. In more complex cases such as transient regimes of detonation, deflagration-to-detonation transition, interaction with obstacles and shock reflections, utilization of the Navier-Stokes equations as well as modelling of turbulence appear to be necessary for adequate reproduction of the process details. A review of the main detonation models is made. Compression effects are the dominate factor in the propagation of a detonation wave, so high resolution is important. Two domain settings are described in detail, the computational domain with adaptive local mesh refinement and the dynamic computational domain. Local mesh refinement can largely reduce the total computational effort especially in simulation of detonation cellular structure. Practical guides about how the refined region should be generated in the computational domain are given and meshing requirements for different chemical mechanisms are also presented. The problem of detonation initialization is discussed and solver type and discretization schemes are also suggested.

In the fifth chapter of the best practices guide, recommendations for user education and training are given. Progress in development of user-friendly interfaces in commercial CFD tools can give the impression of easy and simple generation of engineering results, and mask the need for deep understanding of CFD tools. Recommendations to develop, hone and examine user skills are reviewed and formulated in relation to CFD techniques.

Finally simulations, following the best practices guidelines, will be performed of sample cases for each physical phenomenon related to safety of FCH technologies, i.e. hydrogen release indoors and outdoors, ignition, fire, deflagration and detonation. The simulations and the application of the best practice guidelines will be reported in detail.

WP4 - Verification and validation procedures

WP4 aims to develop organisational and technical frameworks for demonstration of the credibility of models and codes, to ensure they provide correct results from the perspective of their intended use. One output of WP4 will be the specification of processes to ensure that the models identified in WP2 and the best practices outlined in WP3 do provide meaningful results. Another important output of this WP is the compilation of a database of suitable verification problems and validation data applicable to FCH technologies. The database will be freely available to all stakeholders through the SUSANA website. A comprehensive analysis of simulation uncertainties arising due to our lack in understanding of physical phenomena is the third component of the WP4 output to be referenced by the CFD Model Evaluation Protocol.

Verification of models and codes

The objective of this task is to provide where appropriate, practical guidance on the verification of computer models of FCH systems. Verification is the process of determining that a model implementation accurately represents the conceptual description of the model (AIAA, 1998). The four predominant elements of a computer model which would typically give rise to errors and hence require verification are: the spatial discretisation; temporal discretisation, the iteration procedure for minimising residuals; and error checking of models (i.e. incorrect implementation of models in the code).

The accuracy of the computational procedure will be measured with respect to benchmark solutions. Benchmark solutions can mean analytical solutions or alternative approaches such as the Method of Manufactured Solutions (MMS), ASME (2009).

Validation against "real world" data

Once a model is correctly solved and verified, a "validation process will determine the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model" (AIAA, 1998). CFD simulations are compared with experimental data to measure the level of accuracy with which they represent the real world. The end objective of validation is to establish whether a model replicates reality to an acceptable degree.

The main goal of this task is therefore to define a validation assessment process for CFD in hydrogen safety engineering following the approach adopted and developed during the SMEDIS project (Daish et al., 2000, Carissimo et al., 2001) and further explained in Duijm and Carissimo (2002). The validation procedure will first specify, for each particular hydrogen phenomena (release, dispersion, ignition, fire, deflagration, detonation, etc.), the objectives to reach in term of quantification and assessment of the model performance. The key physics and variables involved in the different hydrogen phenomena and target scenarios will then be identified and described in detail in the literature review.

This task will also define the specific structure, content, and the format of the validation database to be created in WP5. This will include selection of datasets to cover the range of required phenomena. Furthermore, physical comparison parameters that are used to compare measurements with model predictions will be defined for each particular phenomenon e.g. overpressure for deflagrations.

Statistical Performance Measures (SPM) provide a measure of the error and bias in the predictions, i.e. the spread in the predictions such as the level of scatter from the mean and the tendency of a model to over/under-predict. Quantitative assessment criteria define acceptable numerical ranges for the SPM which result from applying the validation procedure. This task will identify appropriate SPM and associated quantitative assessment criteria values for each particular phenomenon.

Sensitivity analysis guidance will be defined to show how changes in model parameters affect the results generated by the model. Model predictions may be sensitive to uncertainties in input data, to the level of rigour employed in modelling relevant physics and chemistry, and to the adequacy of numerical treatments. The sensitivity analysis guidance will allow highlighting the dominant variables in the models, defining the acceptable range of values for each input variable and therefore informing and cautioning any potential users about the degree and level of care to be taken in selecting inputs and running model.

Simulation and experimental uncertainty

Verification and validation require consideration of the effects of errors and uncertainty when using models. This is recognised in AIAA (1998) where modelling uncertainty is described as "a potential deficiency in any phase or activity of the modelling process that is due to lack of knowledge". While it may be possible to minimise uncertainties by ensuring good practice, it will not be possible to eliminate them. ASME (2009) presents a series of calculation approaches to evaluate the effects of uncertainty from verification to validation, including accounting for experimental uncertainty when evaluating models. More widely, variability due to stochastic processes, for example wind speed and direction, may also affect the results of simulations.

Uncertainty quantification for computer models is a field in which the development of both methods and applications continues. Complex models, that are expensive to run, are an area of particular interest as can be seen in research projects, for example, the ASME Verification and Validation Symposium[2] and the recent formation by ERCOFTAC (European Research Community on Flow Turbulence and Combustion) of a special interest group in "Uncertainty Quantification in Industrial Analysis and Design"[3]. The aim of this task is to provide a practical guide to understanding simulation uncertainties when applying models to FCH applications.

WP5 – Model validation database and simulation benchmarking

WP5 implements two aspects of the CFD Model Evaluation Protocol: a Model Validation Database (MVD) and a benchmarking exercise. WP5 aims to make use of the best practice guidance and other findings from WP3 and the validation procedures identified in WP4. The database of experiments for different relevant phenomena will be created and partners' codes will be assessed across a series of benchmarks for each phenomenon, i.e. releases and dispersion, ignition and jet fires, deflagrations and detonations, etc. Partners' simulation results for a series of benchmarks will be analysed against experimental data to quantify predictive capabilities of models/codes and results will be available for future reference through the project website by anyone wishing to benchmark their own code, e.g. a CFD consulting engineer seeking an example of typical model and code evaluation.

[2] http://www.asmeconferences.org/VVS2015/

[3] http://www.ercoftac.org/special_interest_groups/uncertainty_quantification_in_industrial_analysis_and_design/

Model Validation Database

A large part of the MVD is already available on the project website and includes 38 experiments presented in groups based on the relevant phenomena. Each experiment is accompanied by a brief description including the experimental set-up and procedure (illustrated by images and drawings where appropriate), the objective of the experiment, the experimental data and references for each experiment. The results from the CFD benchmarking exercise, when completed, will be also available. The following paragraphs briefly discuss the currently available experiments in the MVD for each physical phenomenon.

In the releases and dispersion section, 11 different experiments are included. The experiments involve hydrogen (or helium as surrogate for hydrogen) release and dispersion indoors and outdoors. There are a set of experiments related to release and dispersion in a closed compartment, in a partially closed box such as the GAMELAN experiments (Cariteau 2010, Cariteau & Tkatschenko 2011) and in an open environment (Shirvill et al. 2006). Both liquid and gaseous hydrogen (at atmospheric pressure or compressed at high pressure) releases are included.

In the ignition and fires section one set of experiments is currently available. These experiments involve the investigation of the auto ignition of gaseous hydrogen in a pressurized tube with a T shaped pressure relief device (Golub et al. 2010, Bragin et al. 2013). Different pressures were tested in order to investigate the relationship between pressure and ignition.

In the deflagration section 14 experiments are included involving hydrogen deflagration. The set of deflagration experiments can be subdivided into groups dependent on the hydrogen concentration, on whether the deflagration takes place in an open environment, in a closed or vented box and on the presence of obstacles. For example, there are deflagration experiments on lean hydrogen-air mixture in closed or partially closed obstructed compartment (HYCOM series), on a stoichiometric mixture in open unobstructed environment (Schneider & Pförtner 1983, Becker & Ebert 1985) and in an open obstructed environment such as the experiment in a mock-up of a hydrogen refuelling station (Shirvill & Roberts 2006).

In the detonation section there are three experiments available. They involve detonation of uniform hydrogen-air mixture in open environment (Pförtner 1991) and in confined complex geometries (Breitung et al. 1995). Different concentrations of hydrogen in the mixture have been tested (from lean to stoichiometric mixtures).

Finally, two sets of experiments concerning deflagration to detonation transition (DDT) are in the database. The first set of experiments involves explosion experiments with hydrogen in straight pipes of three different diameters and with different gas concentrations (Chatrathi et al. 2001). The second involves combustion experiments in an obstructed tube with a lean hydrogen-air mixture.

Benchmarking exercise

The project partners have selected a number of experiments from the database to perform the benchmarking exercise. The experiments have been selected with a view to cover the whole range of the indicated phenomena and the partners will perform the simulations with their own methodologies using different numerical tools. The CFD benchmark will provide an indication of the accuracy and the range of applicability of each approach and it will assess the performance of each model for each kind of phenomena. The benchmarking exercise also offers the opportunity to suggest values for the statistical performance measures introduced in WP4. Historically, values have been suggested (for example, Ivings et al., 2007, 2013), and often it is recommended that the values are revisited in light of experience.

Thus far, for the benchmarking exercise in release and dispersion, JRC has simulated one of the GAMELAN experiments (5mm, 180 NL/min) related to helium release in a partially closed box of 1 m^3 volume. JRC and HSL have also simulated the Standard Benchmark Exercise Problem (SBEP) V21 of HySafe Network of Excellence (NoE) of a helium release in a full scale single car garage using the commercial code ANSYS CFX. NCSRD and UU have simulated the GAMELAN (5mm, 180 NL/min) experiment using the in-house code ADREA-HF and the commercial code ANSYS Fluent respectively. For the ignition benchmark, UU has simulated the spontaneous ignition experiment conducted by Golub et al. (2010). For the deflagration benchmark KIT has simulated a vented deflagration experiment (HIWP3-28_29_30) of 18% hydrogen-air mixture in a small (1 m^3) enclosure, while both NCSRD and UU have simulated a deflagration experiment of a large-scale hemispherical stoichoimetric hydrogen-air mixture in the open atmosphere. For the detonation benchmark, KIT has simulated the uniform hydrogen-air mixture experiments which were carried out at the RUT tunnel facilities in Russia (KI-RUT Hyd05 and KI-RUT Hyd05) using their in-house code COM-3D.

WP6 - The CFD Model Evaluation Protocol

In WP6 the main results and documents from work packages WP2 to WP5 will be collected and elaborated to develop the main output of the project; the CFD Model Evaluation Protocol. The development of the protocol structure and drafting of a detailed table of content started early in the project to allow timely modifications and adjustment of the content taking into account the inputs developed in WP2 to WP5, and the involvement of the experts' group (WP7). The table of contents and the main structure of a draft version of the Protocol were presented to the experts' group through different channels, including the workshop "Computational Hydrogen Safety" that was held in Athens in September 2014. This was to obtain critical and constructive feedback and is described with more detail in Section WP7. The final version of the Protocol prepared at the end of the project will be presented and discussed at the dissemination seminar for stakeholders at the end of the project.

The MEP aims to be the reference document for the following communities:

- For CFD code developers (universities, research institutes, R&D departments of industry). The MEP will provide the procedures for verification and validation both of existing and newly developed models, including the list of experiments that are suitable for validation and the relevant quantitative assessment criteria.
- For CFD code users (industry, consultancy companies). The MEP will provide guidelines, recommendations and modelling strategies for the correct use of CFD codes for simulations of typical physical phenomena that occur in hydrogen related accident scenarios.
- For regulatory/certifying bodies. The MEP will be an essential reference tool in assessing the quality of numerical simulations that may be provided as supporting evidence when gaining approval for the deployment of hydrogen and fuel cell technologies and infrastructure. The applicant may be required to show the validation results and their level of compliance with the evaluation criteria and whether the user's modelling strategy follows the best practice and recommendations in the MEP.

The following physical phenomena are addressed in the MEP: release and mixing with air of gaseous and liquid hydrogen, ignition, fires, deflagrations, detonations, and deflagration to detonation transition (DDT). Six main stages are included in the MEP: scientific assessment, verification, validation, sensitivity studies, quantitative assessment, and assessment report. In the initial scientific assessment, one has to describe all the details of the CFD model and to evaluate it according to currently available knowledge and literature, including the known strengths and weaknesses of the approach, the limit of applicability, and the completeness of the model e.g. if all the relevant physical mechanisms are represented in the model. In the same chapter, the key-parameters which affect each phenomenon (e.g. flow rate, source size, weather conditions, and others for hydrogen release) will be identified.

In the verification and validation chapter, the procedure for the verification and validation will be defined together with a matrix of cases for verification and a matrix for validation. The methodology for the sensitivity analysis for several parameters (e.g. time step, computational mesh, boundary conditions) will be described in detail.

In the quantitative assessment chapter, the target variables which have to be considered for the comparison between experimental data and simulation results for each phenomenon will be identified (e.g. concentration, velocity, and flammable mass for hydrogen release). The statistical analysis methodology, along with the statistical performance parameters and the quantitative criteria will be also defined.

WP6 will make a template available for a model evaluation report (MER). This should allow detailed description of each stage of the evaluation and should be sufficiently detailed to allow the repetition of the calculations by a third party.

WP7 – Experts' workshop and outreach

WP7 aims to make the project deliverables available to the hydrogen safety and wider community using various dissemination routes and to gather feedback early in the project to ensure that the outcome is fit for purpose. The two main outcomes of this project are the production of a detailed Model Evaluation Protocol and CFD Best Practice Guide that can be used by the FCH community for evaluating and applying CFD models. Careful consideration therefore needs to be given to ensuring that the outputs are of practical relevance and will be useable by the FCH community. In particular, the users of the protocol may not be experts in CFD and/or model evaluation and so ensuring that the protocol is practical for the intended user is very important. Feedback from the FCH and wider community was therefore sought at an early stage through an experts' workshop and the outcome of the project will be disseminated through an international seminar. Other dissemination routes also exist, such as the project website described in WP1, and conference and journal publications.

Experts' workshop

The workshop "Computational Hydrogen Safety" was held in Athens in September 2014 to which a number of experts were invited. These experts were from a diverse range of backgrounds including: hydrogen safety engineering, nuclear engineering, academia, code development and evaluation, and regulation. There were two main aims of the workshop; to present an overview of the SUSANA project and to gain feedback based upon the experience of the experts. Presentations were given by the SUSANA participants and the invited experts on the following topics:

- Model Evaluation Protocols.
- Best Practices in Numerical Modelling.
- Validation and Verification techniques, methodology and databases.
- Industrial and commercial perspective.

Prior to the workshop, the invited experts were also given access to the validation database and asked to comment on its structure, content and usability. Following each presentation session, there was a roundtable discussion period. An important outcome of this was to identify what industrial organisations, involved in CFD simulations on safety critical applications, routinely do to ensure quality of their results. Consideration also needs to be given to what might be required of CFD results from a regulatory point of view as this currently depends on jurisdiction. In some fields in Europe, for example, CFD studies are more commonly seen as a performance based proof of safety, while in others, more emphasis is placed on results from simpler integral or lumped-parameter models. These simpler consequence models, available as complete packages have often been validated for the scenarios they are used to model. Conversely, a complete CFD model is a collection of sub models assembled by a user for a particular purpose. Demonstrating the integrity of the results therefore requires effort by the user in addition to the developer and can raise questions in terms of what has actually been validated.

Dissemination seminar

The dedicated dissemination seminar will be organised at the end of the project to present the detailed project outcomes to the FCH safety community. The audience for this event is expected to comprise mainly those that are likely to use the outputs of this project. The seminar will present the Best Practice Guide (WP3) and Model Evaluation Protocol (WP6) in detail including their scientific basis and a practical guide on how they should be used. Dissemination of the Best Practice Guide and Model Evaluation Protocol will also be carried out through journal publications, conference presentations and developing the detailed project website. An important aspect of the Model Evaluation Protocol is that the validation and verification datasets continue to be available to users following completion of the project.

Conclusion

This paper has presented a collaborative project to develop a new Model Evaluation Protocol for CFD models used in safety analyses of hydrogen and fuel cell technologies. The project arose from a recognised need for a framework to support users and developers of CFD software undertaking simulations for the analysis of the safety of FCH systems. The structure of the project is based on seven distinct work packages arranged to collect and review information (WP2 to WP5), assemble the protocol (WP6) then to disseminate it through various different channels (WP7). The project aims to benefit from the wide ranging skills and experience of the seven project partners and its review by external experts to ensure it remains practical and relevant.

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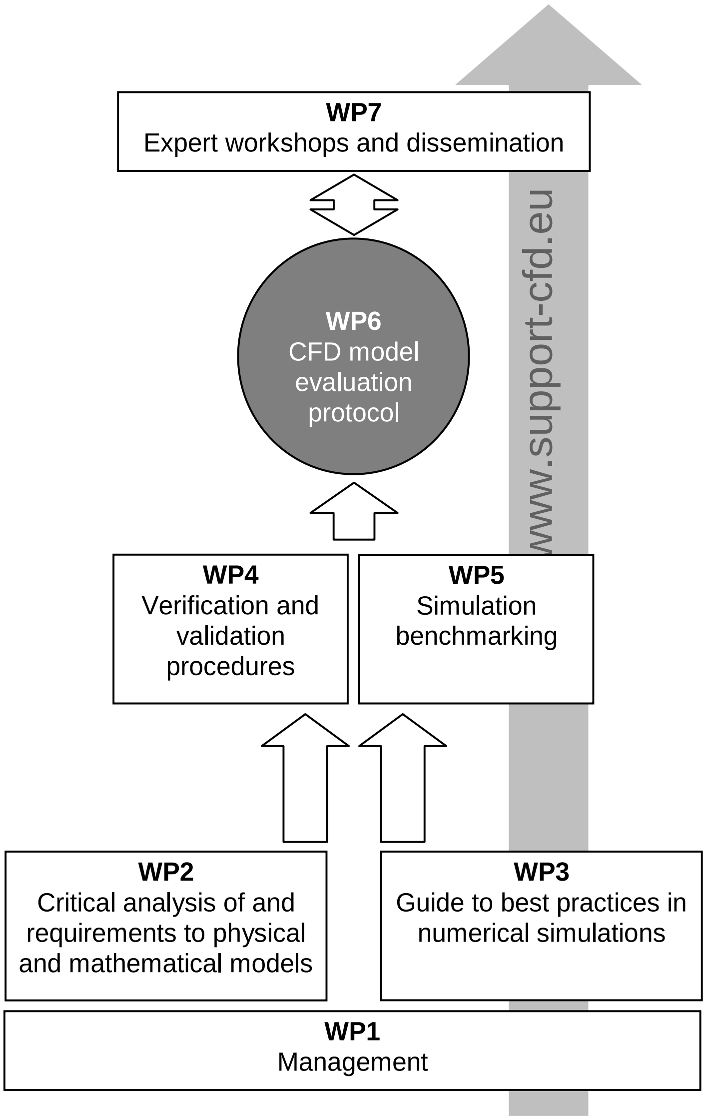

Figure 1 Graphical representation of the work packages and their dependencies. The grey arrow represents collection and dissemination of information on the project website.