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Support to Safety Analysis of Hydrogen and Fuel Cell Technologies

The CFD Model Evaluation Protocol

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1. Introduction (JRC)

1.1 Context/Background (JRC)

Computational Fluid Dynamics (CFD) is increasingly used to perform safety analyses of potential incident/accident scenarios related to the production, storage, distribution and use of fuel cell and hydrogen (FCH) technologies. CFD is a powerful numerical tool for hydrogen safety science and engineering that can provide useful data and insights, but it also requires a high level of competence and knowledge for the technique to be applied in a meaningful way. In order to apply CFD with a high level of confidence in the accuracy of the simulation results, two main issues have to be addressed: the capability of the CFD models to accurately describe the relevant physical phenomena and the capability of CFD users to follow a robust modelling and simulation strategy in developing the CFD analysis.

In this context, an international workshop with recognised world experts in the field of hydrogen safety and CFD was held at the Institute for Energy and Transport of the Joint Research Centre in The Netherlands in order to identify the gaps in CFD modelling and simulation of hydrogen release, dispersion, ignition and combustion. The main outcomes of the workshop were included in a report entitled “Prioritisation of Research and Development for modelling the safe production, storage, delivery and use of hydrogen” (Baraldi et al. 2011). One of the main gaps identified was the lack of a Model Evaluation Protocol (MEP) for hydrogen technologies; such as the MEP for liquefied natural gas (LNG) dispersion models (Ivings et al. 2013).

In the SUSANA project, which is co-funded by the Fuel Cell and Hydrogen Joint Undertaking, that gap was addressed and the Model Evaluation Protocol for hydrogen technologies safety was produced. The objective is that the CFD Model Evaluation Protocol will be the reference document for all users of CFD for hydrogen safety. It will allow users to assess their own capability of correctly using CFD codes, and help them evaluate the accuracy and limitations of the CFD models themselves. The Protocol is pertinent to all CFD developers (academia and research institutes) and users (such as industry and engineering consultancy companies) but also for regulatory/certifying bodies that have to permit hydrogen and fuel cell systems and/or hydrogen infrastructure/facilities. Through the hydrogen model evaluation protocol (hereafter referred to as ‘HYMEP’), regulatory/certifying bodies have a reference document that helps them to evaluate whether the CFD analysis supporting permission requests is of sufficient fidelity.

In many previous model evaluation studies (Daish et al. 2000.; Ivings et al. 2007; MEGGE 1996.), a definition of “model” was not given. This was partly because models were recognised as a single entity containing the mathematical model and its numerical solution. Integral models for gas dispersion are typical examples. These previous model evaluation studies often divided types of models into different categories, for example correlations, integral models and CFD models.

Various terms exist in connection with CFD modelling, such as code, model and simulation. Definitions of these terms are examined in detail in references such as (Oberkampf and Roy 2010; Roache 1998, 2009). Generally, the “model” is seen as the representation of a physical process (e.g. turbulence), a “code” may be used to implement models in software and a “simulation” is the use of the code and models to produce a result, i.e. the overall computational procedure. The above definitions are linked with verification, validation and scientific assessment which are described elsewhere in this document and in supporting document, Deliverable 4.2 “Final report on verification and validation procedures” (SUSANA D4.2 2016).

In the SUSANA project, for simplicity, the term “model” encompasses the physical and mathematical models implemented in code and used in a simulation to make a prediction. When undertaking an evaluation, the component considered should be made clear in context.

1.2 Other protocols: LNG, SMEDIS (JRC/HSL)

The development of the HYMEP was based also on previous experience and projects that were performed for technologies and applications outside of the hydrogen and fuel cell safety sector.

A Model Evaluation Group was established by the European Community in the early 1990s (MEGGE 1996). The group was set up to develop methods for the evaluation of models in major industrial hazards areas as it had become apparent that models used in industrial hazard assessment had never been formally assessed for their fidelity. Nevertheless those models 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 (MEGGE 1996) which provides a framework for the key activities needed to evaluate models.

Testing the results of model predictions against experimental data, Kakko et al. (Kakko et al. 1994) highlighted the need for suitable experimentally derived databases for model validation, as these were often difficult to obtain or not presented in a way suitable for model validation. A classic example of a model validation database is the modeller’s data archive (MDA) of Hanna et al. (Hanna, Strimaitis, and Chang 1989) who identified the need to collate data in a form that could be accessed by model developers. Since then, some other datasets have been produced, such as the Rediphem database (Nielsen and Ott 1996). Hanna and Chang also developed a model performance evaluation methodology for gas dispersion models and for air quality models (Hanna and Chang 2012), (Chang and Hanna 2004).

The SMEDIS (Scientific Model Evaluation of Dense Gas Dispersion Models) project (Daish et al. 2000), (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 a scientific review of models. As well as evaluating simple scenarios, the project focused on situations in which complex effects such as aerosols, topography and obstacles were important. Ivings et al. (Ivings et al. 2007) 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 could also be taken into account in model evaluation. One of the recommendations of the MEP (Ivings et al. 2007), (Ivings et al. 2013) was that validation should be performed by running models against experiments from a validation database that was constructed specifically for this purpose (Coldrick, Lea, and Ivings 2009).

1.3 HYMEP supporting documents (JRC)

In order to support CFD practitioners in the use of the HYMEP, the SUSANA consortium prepared four complementary documents:

- a review of the state-of-the-art in CFD modelling of hydrogen safety issues, "The state-of-the-art in physical and mathematical modelling of safety phenomena relevant to FCH technologies" (SUSANA consortium, D2.1 2014)
- a critical analysis of CFD modelling for hydrogen safety issues where the suitability of CFD approaches for real-scale applications, existing bottlenecks and model deficiencies are

identified and described, "Critical analysis and requirements to physical and mathematical models" (SUSANA consortium, D2.2 2015)

- a guide to best practice in numerical simulations with the purpose of supporting CFD users in the correct application of CFD methods to each relevant phenomenon, " Best practice in numerical simulation" (SUSANA consortium, D3.2 2016)
- a report on verification and validation procedures to help practitioners in the hydrogen safety CFD area to determine the fidelity of modelling and simulation processes, "Final report on verification and validation procedures " (SUSANA consortium, D3.2 2016)

An illustration of how these documents support the HYMEP is shown in Figure 1.

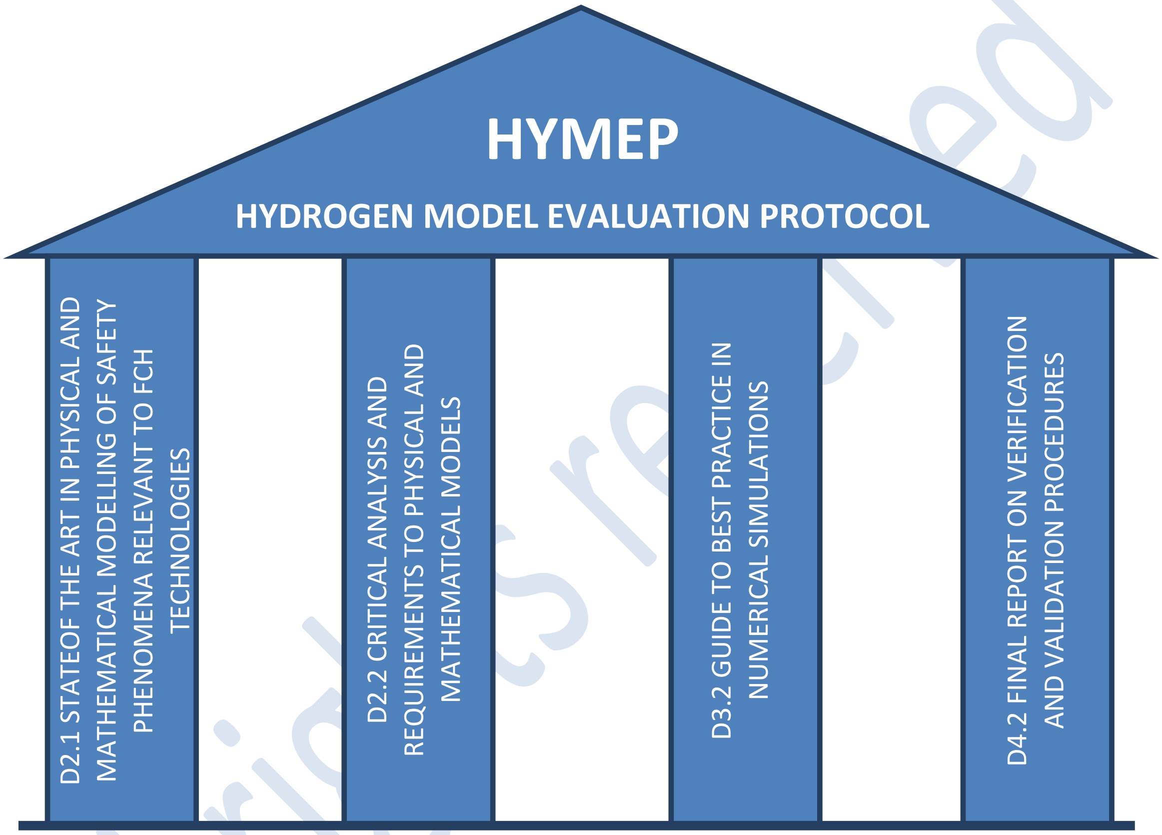

Figure 1: The HYMEP and supporting documents.

1.4 Structure of the Protocol (JRC)

The structure of the HYMEP is illustrated in Figure 2.

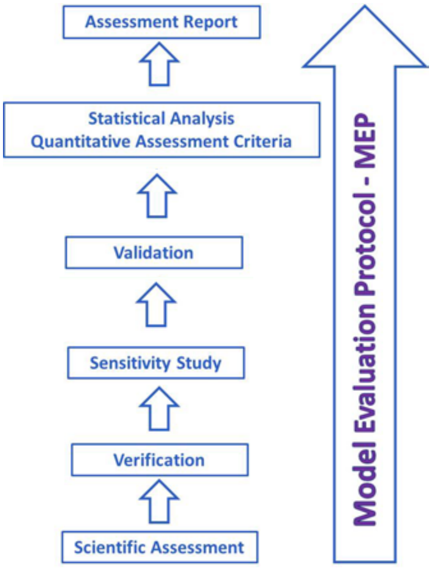

Figure 2: The structure of the Hydrogen Model Evaluation Protocol (HYMEP).

The initial stage of the HYMEP is a scientific assessment whose purpose is to establish the scientific credibility of the model. In that stage a preliminary qualitative assessment of the model is performed, by comparing the features of the model (both the physical model and the numerical model) with the current state-of-the-art available in the scientific and technical literature. The suitability of the model and of the numerical approach to completely capture the desired phenomena should be addressed at that stage. The range of applicability of the model, the limitations and advantages of the approach, and any special features of the model should be identified according to the available literature and the current knowledge of the scientific community in the relevant fields.

The next step is verification. Verification is used to ensure that the equations are correctly solved; whereas validation is used to determine the degree to which a model is an accurate representation of the “real world”. In validation, model outputs are compared with measurements of physical parameters to demonstrate that the model captures “real world” behaviour. A review of verification and validation procedures was carried out, and two databases were built which cover a range of phenomena relevant to FCH safety: a database of problems for verification of codes and models against analytical solutions and a validation database of experiments for validation of simulations. Both databases are available at the SUSANA project website (www.support-cfd.eu).

How changes in model parameters affect the results are evaluated via a sensitivity study. 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 methodology allows the dominant variables in the models to be highlighted, 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 models. For some relevant model parameters like the computational mesh, the time step, the numerical scheme, the initial and boundary conditions, and the domain size for semi-confined, vented and open configurations, sensitivity studies should be performed before or during the validation process. For input parameters like the mass flow rate or the leak size during the hydrogen release in a garage, the sensitivity study should be performed after the validation.

In the statistical analysis step, key target variables are identified for each phenomenon that is relevant for hydrogen safety: release, mixing and dispersion, self-ignition, fire, deflagration, deflagration to detonation transition, detonation, etc. As an example, the hydrogen concentration distribution, flammable mass, and velocity fields can be considered as primary target variables for the release and dispersion of hydrogen leaking from a tank of a vehicle in a garage. In the statistical analysis of the comparison between experimental data and simulation results, 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. In the validation procedure acceptable numerical ranges for the SPM are defined as quantitative assessment criteria.

The final step outlined in the HYMEP is a guide to the preparation of an assessment report that includes information and data about each stage of the protocol for the specific model i.e. CFD procedure that has to be evaluated.

1.5 Model Assessment Report (UU)

The Model Assessment Report (MAR) is the key output, which is produced following the acceptance and utilisation of the HYMEP. The report contains full details of all the stages of the evaluation protocol including the Scientific Assessment (see Section 2), which is based on the information provided through the distributed Questionnaire (an example is provided in Section 9.1). Supporting information may be included as required.

1.5.1 Model Assessment Report (MAR) structure (UU)

To act as a guide there are commonly eight main sections to the MAR:

1) General model description;
2) Scientific basis of the model;
3) User orientated aspects of the model and assessment;
4) Verification performed;
5) Sensitivity study;
6) Validation performed;
7) Statistical analysis and evaluation;
8) Conclusions.

The MAR may also contain appendices: A1) data arising from the assessment, e.g. summary of validation results, and A2) comments from model supplier/developer/expert. Typically, each of these sections is part description and part analysis.

The principal part of the assessment focuses on the general description, scientific basis and user-orientated aspects of the model (section 1 to 3). Each of these sections is then divided into the required specific subject headings. Where possible the essential information is presented using a ‘check-box’ format, which allows for a fast overview of the model. Section 4) to Section 7) summarise the previous verification, validation and evaluation work performed on the model. Finally, Section 8) concludes the MAR with a summary of the main findings of the report. In addition, three appendices are also included which contain the supplementary comments from the developer, as well as a summary of the new actively-generated results obtained from the validation exercise. The information must also be presented in a manner that does not require an unreasonable amount of time for analysis (Cambridge Environmental Research Consultants Ltd 2002).

2. Scientific assessment (UU)

The scientific assessment is carried out by critically reviewing the physical, mathematical and numerical basis of the model. This assessment can be undertaken using the information made available for this specific purpose (i.e. from the questionnaire created), from supplementary comments from the developer, from published literature if available, or from other appropriate sources. When the required information has been obtained, the scientific assessment can be completed. The findings from this assessment are summarised and presented in the MAR.

The scientific assessment consists of a comprehensive description of the model, an assessment of the scientific content, the applicability domain, the limitations and advantages of the model, a description of any further features and also areas for possible improvement. The description is based on the documentation provided by the model developer and should include but is not be limited to, a description of the dominant underlying scientific processes and should also explicitly state the values of any empirical constants. All important phenomena within the model's range of application should be included. The scientific content should address whether the mathematical modelling of important phenomena and any associated simplifications and parameterisations are well justified. This assessment should list the positive and negative aspects of the model and critically review the suitability (or not) of the model for the specific application (MEGGE 1996).

To appropriately undertake the scientific assessment the reviewer must have an in-depth understanding of the behaviour of each of the physical phenomena under consideration. Ideally, the reviewer should also be independent of the model developer; however it is accepted that the developer may be required to properly perform the validation exercise.

Additionally, it should be noted that, for the scientific assessment to most effectively meet its purpose it is preferable that models are addressed in a uniform manner wherever possible (Britter and Schatzmann 2007). To achieve this, a uniformly designed questionnaire may be the least resource demanding approach to undertake.

2.1 Questionnaire (UU)

The purpose of the questionnaire is to request and obtain the relevant information, which is required for the completion of the scientific assessment. This information is obtained from the model developer or alternatively from an expert user. The supplier of this information must therefore have a comprehensive knowledge and understanding of the model being assessed. An example of a questionnaire, which could be provided to such experts, is presented in Appendix 9.1.

Once completed, the questionnaire should be returned along with relevant documentation, containing other pertinent information including, but not limited to, user manuals, published papers, reports, etc. Peer reviewed applications of the model and validation exercises (published or confidential) are of particular relevance to this process. It should be noted that any confidential material supplied will ***not*** be included in the Model Assessment Report.

The questionnaire includes guidance on how it should be properly completed. This guidance must be followed. The questionnaire is based on the layout supplied by the European Commission's SMEDIS project (Carissimo et al. 2001), (Daish et al. 2000). It should be noted that the information supplied must refer to a ***single well-defined version*** of the model i.e. a complete description of the physical situation, comprising sub-models of turbulence, combustion, etc. implemented within a CFD code. This version must be unambiguously identified (on the cover sheet).

2.2 Scientific Assessment Procedure (UU)

The scientific assessment procedure will be based on the information contained in the completed questionnaire, which is returned by the model developer or the expert user. An example of a suitable questionnaire is provided in Section 9.1 of this document. The approach taken is to clearly specify the purpose of the model, produce a consensus of what 'science' is required for the model to meet its application(s) and to determine whether the 'science' is present in an adequate form in the model.

To carry out a scientific assessment of a given model, detailed information is required regarding the physical, mathematical and numerical basis of the model under consideration. At the most fundamental level, the results produced by the model must (broadly) adhere to theoretical expectations and be reproducible. For example, if two different groups investigate an identical scenario using two different methods of analysis (different models or a different application of the same model) and obtain significantly different results, then the details of both models must be available for scrutiny. This is essential in order to scientifically resolve the reason(s) for the differences.

The model must be based on sound physical principles which build on or use modelling techniques that have been accepted, and are therefore well understood, through publication in high quality peer reviewed journals or appropriate industrial reports or reports to clients. It may in fact be more appropriate for an innovative model, which has not been through extensive peer review and testing, to be published in an industrial context as it may not contain the new or innovative developments or ideas suitable for publication in a peer reviewed journal. Any innovative modelling aspects included in the model should be appropriately highlighted and their use justified through appropriate scientific argument, verification and validation.

A source term in a model is one which is not normally accommodated in the unsteady, convective or diffusive terms. They are meant primarily for internal generation processes such as heat generation in a fluid, production of a chemical species in a reaction, the generation of turbulent kinetic energy, etc. However when the corresponding physical quantity is destroyed rather than produced, the source term becomes negative and may be known as a sink term. As CFD models for the safety analysis of FCH technologies are associated with numerous physical phenomena, different models will utilise different source terms. It is essential therefore that a given model uses a credible source term.

The numerical methods employed should follow current best practice to ensure that the results produced are of the highest accuracy possible and also that erroneous solutions are avoided. Extensive guidelines exist for CFD models (Casey and Wintergate 2000). However, there may be cases where authors have implemented their own methods. In such cases appropriate justification, including the error control processes implemented should be provided.

The outputs produced by the model must be suitable for assessment and ideally should cover a wide variety of parameters including for example concentrations at different points and times, temperature, density, pressure, etc. The selection of particular parameters for assessment will vary depending on the particular model under consideration. Details of the target variables specific to each of the physical phenomena within the scope of the HYMEP are specified in Section 5.2.

Finally, the model description should include features specific to the type of model and the scenarios to which it will be applied. Such information should include: a short description of the model, key details of the model, evidence that the model is based on accepted/published science, evidence that the numerical methods employed are based on accepted/published good practices, the equations solved (including the fundamental equation system and any simplifications or approximations introduced), spatial (micro, meso, macro) and temporal (minutes, hours, days, …) scales, turbulence parameterisation, computation domain, grid design and resolution, numerical solution approach, near surface treatment, boundary and initial conditions, processing of input and output data, the specification of the source and applicability or not to specific scenarios (such as time varying input, complex terrain, wind conditions, heat and mass transfer, chemistry and how the model accounts for particular phenomena, etc.). This list should not be considered as exhaustive, other information could be added if required and depending on the particular physical phenomena under analysis (Britter and Schatzmann 2010), (Di Sabatino et al. 2011).

2.3 Physical problems addressed by the models (UU)

The assessment criteria identified for each of the physical phenomena defined within the scope of this protocol (i.e. release, mixing and dispersion, permeation, ignition, fire, deflagration, DDT and detonation) are presented below. The scientific criteria discussed give the current state-of-the-art model features and most recent model advancements. For each model assessment undertaken the key details of the physical model should be provided, along with confirmation that the model, and the set of numerical methods employed, is based on accepted/published science. Additionally, the outputs from each model should be suitable for assessment against the HYMEP statistical performance measures. The scientific criteria specific to each of the physical phenomena, provided in Section 2.3.1 to Section 2.3.7, should act as a guide during the assessment process.

It should be noted that the qualitative criteria provided in Section 2.3.1 to Section 2.3.7 do not represent an exhaustive list of all necessary model features for each model. Additionally, some of the criteria listed may not be applicable to a particular model when associated with a specific physical phenomenon. If the omission of various factors from the model can be appropriately justified, then omitting such factors should not necessarily lead to the exclusion of the model.

As a general principle, if a model does not take into account a given factor such as an obstacle, atmospheric conditions, heat transfer or chemistry, then it should be demonstrated that, nevertheless, the results are conservative. In the current context, a conservative result is one where the extent and scale of hazards are overestimated by the procedure. The inclusion of such factors will ultimately influence the choice if model, depending on the scenario being investigated and factors which a given model may or may not account for, is appropriate for use or not.

The sections below represent a brief overview of the physical problems addressed by the models. A more comprehensive review was performed by the SUSANA consortium (SUSANA consortium, D2.1 2014).

2.3.1 Release, mixing and dispersion of gaseous hydrogen, including permeation (UU)

The scientific criteria associated with models appropriate to the release, mixing and dispersion of gaseous hydrogen should include confirmation that the model accounts for or is applicable to: laminar, transitional and turbulent flows or combination of them; compressible and/or incompressible flows; wind speed and atmospheric stability/instability; impinging jets, including heat and mass transfer; passive/forced ventilation scenarios; buoyancy-controlled/momentum-dominated expanded/under-expanded jets; blowdown and variable boundary conditions; obstacles; release along a surface (attached jets); indoor releases and dispersion; and also “release” by diffusion/permeation and following dispersion.

The accuracy of the simulation of hydrogen concentration decay along the jet axis in an expanded jet is expected to depend on the grid resolution at the exit of the leak and in the near-field, as well as on flow parameters such as velocity distribution, hydrogen temperature and flow turbulence in the release source and surroundings.

The dispersion of a quasi-steady under-expanded jet is usually simulated using either a notional nozzle concept or a two-stage approach (SUSANA consortium, D3.2 n.d.). The notional nozzle concept considers that the release occurs from an imaginary source with flow parameters calculated using an under-expanded jet model. By comparison, the first stage of the two-stage approach requires a highly resolved simulation of the shock structure and flow in the near-to-nozzle-field. The flow parameters at the external boundary of this simulation are then used as the internal boundary for the simulation of the “far-field” at the second stage.

Implementation of the notional nozzle concept can be achieved depending on software/code either with the ‘area source’ approach or with the ‘volumetric source’ approach. In both cases, source terms are added into the mass, species, momentum and energy conservation and turbulence equations.

For unsteady under-expanded releases, e.g. blowdown of a high-pressure hydrogen storage tank, the notional nozzle exit size is reduced with time. Implementation of a time varying notional nozzle size can be done with a ‘transient area source’ approach or a ‘transient volumetric source’ approach described in (SUSANA consortium, D3.2 n.d.).

For the determination of hazard distances it is important that the model is able to produce the transition from a momentum-dominated jet to the buoyancy-controlled plume regime.

2.3.2 Release, mixing and dispersion of liquid hydrogen (NCSRD)

Models appropriate to the release, mixing and dispersion of liquefied hydrogen should satisfy the criteria for gaseous hydrogen (Section 2.3.1). Additionally, it should include confirmation that the model, depending on its complexity, accounts for vapour, liquid, solid physical properties, two-phase jet flashing, phase changes (evaporation/condensation), air/humidity solidification, underground heat transfer, film boiling conditions, liquid pool formation, spreading and evaporation, hydrodynamic non-equilibrium, thermal non-equilibrium, droplet size distribution and dynamics etc.

Source modelling in liquid hydrogen (LH2) releases is more complex than for gaseous hydrogen GH2 releases. The flashing that occurs at the nozzle adds the void fraction as an additional parameter to be calculated. Two-phase jets can be under-expanded or expanded. Simulation of the expansion process is performed under either isentropic or isenthalpic assumptions. In under-expanded two-phase jets, flow is choked (Mach = 1) at nozzle exit and a notional nozzle approach is required for further dispersion calculations. Source simulation must be performed using accurate physical properties which cover the liquid, vapour and possibly supercritical range.

Near a jet source two-phase conditions pertain where hydrogen liquid and vapour coexist. Even if liquid hydrogen has completely evaporated, temperatures may be so low that nitrogen, oxygen and humidity will change phase (become liquid or solid). Dispersion in such two-phase regions requires modelling of phase changes of multi-component mixtures as well as accounting for the possibility of slip between phases (different velocity between liquid/solid and vapour). Under the thermodynamic equilibrium approach (species share same temperature and pressure) one can obtain the phase distribution of species using Raoult’s law. If thermodynamic non-equilibrium is assumed between phases then evaporation/condensation should be explicitly modelled with source terms in the respective conservation equations for mass, momentum and energy. Slip will exist if droplets/particles are large enough. Accounting for slip (hydrodynamic non-equilibrium assumption) can be implemented either with algebraic slip models or by solving momentum equations for liquid/solid phase (either in Eulerian or Lagrangian form). Dispersion simulations at ambient pressure conditions can be performed with ideal gas assumption for vapour phase and adequate correlations for liquid/solid phase. Sensitivity analysis with more accurate equation of state (EoS) models could be performed.

When release is close to the ground (or water) a liquid hydrogen pool can be formed. Under such conditions dispersion calculations can be performed in single-phase (only vapour), using the pool evaporation rate as source term. Modelling of pool formation, spreading and evaporation (or boiling) is required to provide the source conditions as function of time. This approach is computationally faster than the two-phase approach described above.

An alternative to the above two approaches is to apply two-phase dispersion coupled with a pool model in cases when a pool is formed.

Ground heat transfer is very important in LH2 dispersion. This should be accounted for by solving the energy equation inside the ground. For dispersion over water a simple approach (provided that the water mass is large enough and well mixed) is to assume that the water interface temperature remains constant (ambient). Film boiling phenomena occur due to large temperature differences between substrate (ground or water) and an LH2 pool above. For release over ground the film boiling duration is usually small compared to the dispersion phase (ground gets cold very fast) and could be neglected as first approach. For release over water film boiling should be accounted for.

2.3.3 Ignition (UU)

Ignition can occur through various mechanisms/reasons including, but not limited to: ignition by a hot surface, mechanical spark, frictional ignition, impact, electrical ignition source, electrostatic discharge, electromagnetic waves, radiation, ionizing radiation, ultrasonic, the spontaneous ignition of sudden hydrogen releases into air by the so-called ”diffusion mechanism”, explosives, open flame, etc. Therefore, the scientific criteria related to a model appropriate to simulate particular ignition case should include the details of the ignition mechanism envisaged.

Spontaneous ignition following a sudden release of hydrogen into a pipe filled with air is a specific issue within hydrogen safety engineering. A model should be able to reproduce available experimental data, specifically referring to pressure transients and distances, where ignition by the diffusion mechanism is observed. In the majority of realistic cases, the application of 1D simulations is not appropriate, as the areas with the highest temperatures due to shock reflection may not coincide with the areas where the most reactive flammable hydrogen-air mixture is present. The authors are not aware of any publications reporting a successful quantitative comparison of 2D simulations with experimental results. There are, however, a limited number of journal publications which describe 3D simulations in which the spontaneous ignition observed in experiments was successfully reproduced. Due to limitations of computing power and thus restrictions on a mesh size, such 3D simulations currently require sub-grid scale (SGS) modelling of turbulence and combustion.

In experiments (Bragin and Molkov 2011) and in simulations in straight pipes, ignition by diffusion is observed to begin at the wall of the pipe where the temperature is a little higher, due to stagnation conditions and the presence of air.

It was demonstrated in a number of publications that simulation of rupture disk opening is essential for reproducing the underlying physical processes as was reported in (SUSANA D.2.2, 2015).

2.3.4 Fires (UU)

The scientific criteria associated with fire models are dependent on the model application domain under consideration such as : microflames; free, impinging and attached jet fires; indoor jet fires, etc.

Microflame models are associated with extremely small flow rates and are used to simulate laminar flows. These models include chemistry, which identifies the reaction zone not only by temperature but also through the presence of radicals at particular concentrations. Microflame models should reproduce the available experimental data detailing the quenching, i.e. at lower flow rates, and the blow-off, i.e. at higher flow rates, and limits of combustion for different nozzles. The flame lift-off and blow-off phenomena remain an active area of combustion research. The effect of heat losses from a microflame to the solid material of a “burner” could be of importance for the quantitative reproduction of experimental data.

Free jet flame models are expected to reproduce flame length for different regimes, including subsonic, sonic and supersonic flows, expanded and under-expanded jets, buoyancy-controlled and momentum-dominated releases, etc. In order to achieve a reasonable calculation time, especially when considering a large-scale problem, it may be useful under certain circumstances to neglect compressibility effects and start simulations from a notional nozzle as a boundary source (SUSANA consortium, D2.2 n.d.).

A notional nozzle concept in conjunction with an appropriate choice of turbulence intensity and length scale in the notional nozzle exit could be applied to simulate under-expanded jet fires. The ‘volumetric source’ method could be applied to simulate jet fires emanating from the blowdown of high-pressure storage tanks.

Indoor fire models are expected to include chemistry to reproduce both well-ventilated and under-ventilated fires, including regimes of self-extinction of a flame and formation of an external flame attached to the vent. In the latter regime there is no combustion within the enclosure. However, when considering scenarios such as open atmosphere jet fires the inclusion of chemistry may not be necessary. Indoor or impinging jet fire models should also include wall treatment strategies such as the standard log-law wall function. The quality of a grid and the inclusion of an external domain have to be considered and appropriately implemented in order to reproduce, when applicable, a two-way flow in the vent(s) which is necessary for reasonable simulation of indoor jet fires.

2.3.5 Deflagrations (UU)

Deflagrations can occur at various conditions including: closed vessels, open atmospheres, vented enclosures, inertial vent covers, obstructed environments, non-uniform mixtures, layered and localised mixtures, delayed ignition of the jet or flammable cloud, etc. Therefore models applicable to deflagration scenarios, depending on their applicability, may be required to account for different phenomena including the effect of: flow turbulence in the flammable mixture; turbulence generated by the flame front itself; fractal increase of flame front area; leading point concept (preferential diffusion in curved flames); critical stretch rate; and various combustion instabilities, including those promoted by confinement and obstacles. Other instabilities that may be included into models as separate entities that can be implemented when applicable are Landau-Darrieus, Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz instabilities. Therefore the scientific criteria associated with models appropriate to deflagrations should include an assessment of the relevant scenarios to which the model is applicable to, including the phenomena accounted for by the model.

For **deflagrations in a closed vessel**, where the entire volume is occupied by the flammable mixture, the model is expected to reproduce the Mache effect, i.e. higher temperature at the point of ignition, due to the compression of the initially burnt gases as compared to those burnt towards the end of the deflagration. If the deflagration of localised mixtures inside a closed vessel is considered, e.g. in a large warehouse or nuclear plant containment building, the model would be expected to reproduce the blast wave, which could form a shock during propagation. That could affect the structural integrity of the enclosure. In elongated pipes and tubes, models are also expected to reproduce the correct shape of the flame front, e.g. so-called ‘tulip flames’, and associated pressure transients.

In **open atmosphere deflagrations** a pressure wave is produced. The decay of this pressure wave with distance, along with flame front propagation, i.e. flame front position as a function of time, is expected to be reproduced by simulations. The effect of buoyancy could be significant for lean mixtures having low burning velocity; therefore, models are expected to reproduce pressure wave decay, and dynamics of flames distorted by buoyancy.

Various phenomena can occur in **vented deflagrations**. Therefore an assessment should be made on the applicability of the model to the scenario under investigation. For example, whether the model accounts for the generation of instabilities, including Rayleigh-Taylor instability, and (where applicable) also the interaction of acoustic waves generated by the deflagration occurring with a semi-enclosed structure.

Models applicable to **obstructed environments** should account for different obstacle configurations (including varying distance between obstacles, thickness, height, surface roughness, etc.). The challenge remains to make predictive forecasts of combustion regimes at conditions which mimic real industrial environments. Models which attempt to characterise obstructions are usually implemented following a non-standardised or not described in detail methods, e.g. porosity density models. This implementation procedure must be clear and transparent if it is to be assessed scientifically.

Models which are expected to simulate **deflagrations in non-uniform mixtures**, e.g. by using polynomial approximations, should account for variation of combustion rate with hydrogen concentration (volumetric mole fraction) e.g. treat burning velocity and the expansion coefficient of combustion products as functions of hydrogen fraction in a mixture (volumetric mole fraction). If the scenarios being modelled also include layered mixtures it must be recognised that concentration gradients can lead to faster deflagration dynamics due to the increase of flame surface area in the presence of fast burning part of a layer.

For scenarios involving the **delayed ignition of jets** deflagration may take place before the quasi-steady jet fire is established. In delayed ignition deflagration turbulence is known to have a greater effect on overpressure than the total amount of leakage or the premixed volume. Time and location of ignition, storage pressure, leak diameter and barrier employment are all known to play a critical role in the determination of the delayed deflagration overpressure. The initial turbulence in a flammable mixture must be accounted for in the initial conditions of the simulations, as it will affect both the pressure dynamics and maximum pressure obtained.

It should be demonstrated that a deflagration model is capable of reproducing deflagrations in a wide range of scenarios and conditions without any adjustment or “tuning” of the model constants/parameters (after the model constants/parameters have been fixed by means of the calibration process during the validation).

2.3.6 Detonations (KIT)

A detonation wave is a supersonic combustion wave across which the thermodynamic states vary sharply. Detonation is one type of a self-propagating combustion wave coupled with a leading shock wave. Ignition of the reactants is affected by the adiabatic compression of the leading shock front that precedes the reaction zone of the detonation wave.

Through analysis of conservation laws for detonation, it was shown that the chemical combustion reaction is the key to the propagation of the detonation wave. Further analysis shows that important parameters of a detonation wave such as speed of detonation wave, von Neumann pressure peak, Chapman-Jouguet (CJ) pressure and von Neumann density mainly depend on the chemical energy released by the reactants (Zeldovich et al. 1985). The capability of a numerical model to correctly reproduce detonation may be measured via simulation variables such as the detonation propagation speed, maximum pressure and peak density.

Cellular structure is another important characteristic of a detonation wave. The size of the cellular structure can be used as a key parameter for code validation. Through experiments, it has been found that the width of detonation cells is constant for certain concentrations (Shepherd 2005).

Therefore, the scientific criteria associated with models appropriate to detonations should include confirmation that the model accounts for detonation (coupled shock and combustion wave propagation), propagation (1D, 2D and 3D) with velocity close to CJ velocity (some velocity deficit could be observed for propagation in an obstructed environment) and detonation curvature. Referring to detonation propagation, models should be applicable to:

- different types of detonations, with regular/irregular and multi-dimensional structures; Rankine-Jouguet jump conditions, for steady, one-dimensional flows;
- Chapman-Jouguet (CJ) one-dimensional detonation pressure and velocity in unobstructed geometries, with the inclusion of an additional energy term;
- the dependence of detonation limits on composition, temperature, pressure of the mixture, geometry and roughness of the vessel.

Models resolving detonation structure should allow for:

- the estimation of detonation cell size, recognizing that cell size reaches its minimum at stoichiometric composition conditions and grows for leaner and richer mixtures, high activation energy asymptotic;
- the distinctiveness of length scales;
- Rankine-Hugoniot jump conditions for the flow field;
- detonation shock dynamics (DSD) theory to analyse the initiation, propagation and failure of the detonation;
- the influence of curvature on detonation;
- the limit of high activation energy where the critical curvature represents a limit after which the extinction of detonation may occur;
- unsteady corrections.

Detonation models should also account for pressure wave reflection and curvature. Large-scale detonation models may not resolve detailed detonation structures, but use conditions obtained from

CJ theory (e.g. CJ detonation velocity). Nevertheless they should reproduce the coupling of the leading shock and the combustion wave with the CJ detonation velocity.

2.3.7 Deflagration-to-detonation transition (UU)

Deflagration-to-detonation transition (DDT) refers to the phenomenon where the critical conditions for the onset of detonation are established during the combustion process itself, without an external energy source, through flame acceleration caused by various mechanisms and instabilities, reaching some critical conditions when the leading shock and combustion wave couple. DDT modelling remains an active subject of research up to now and no ‘applied’ models available for commercial applications exist.

Ideally, a robust deflagration model should be able to reproduce DDT without any modification or artificially implemented additional criteria. The accepted criterion for DDT is the coupling of the flame front with the shock, and subsequent propagation with a velocity close to the CJ velocity. Suitable models should also account for losses due to the presence of obstacles and heat losses to walls. The pressure in the detonation wave is expected to be at least equal to CJ pressure. It can be a problem to achieve good agreement between simulations and experimental results due to the difficulties involved in taking appropriate measurements, particularly considering that pressure in the detonation front is highly non-uniform and that pressure at triple points is much higher than in other areas. This difficultly is compounded due to the size of the triple point being much smaller than the pressure sensor taking the measurements.

However models would be expected to reproduce the location and timing of DDT, with reasonable deviation from the experiment. For such scenarios it is clear that information referring to the reproducibility of the experiment would be useful in order to appropriately assess the expected uncertainty in the predictions obtained from the CFD model.

3. Verification (EE)

3.1 Introduction (EE)

As computers become more powerful, the outputs of a simulation can *seem* highly realistic. For example, with the use of Large Eddy Scale models of turbulence, fine resolution of temporal and length scale phenomena can produce *realistic looking* behaviour. The simulation *may* have high fidelity to the activity being researched, or it may be complete nonsense. All models (and their simulation outputs) are abstractions from reality, and are based on a series of approximations. In all cases, a practitioner will:

a. Create a conceptual model which reflects the physical phenomena that pertain (for example, using the Navier Stokes Equations with a specific turbulence model for closure).
b. Programme that model into a computer.
c. Solve it via an iterative simulation.

During all of these steps, errors can be introduced or arise which cause the computational outputs to deviate – potentially significantly – from reality. Identifying and improving the fidelity and quality of modelling and simulation processes is vital.

This and the next chapter are a summary of the guidance provided in a companion document produced by the SUSANA project, Deliverable 4.2 “Final report on verification and validation procedures” (SUSANA D4.2, 2016).

3.2 Definitions (EE)

Verification and *Validation* are distinct and complimentary procedures that are both required to determine the fidelity of simulation outputs.

Verification:

The process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model

Validation:

The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended use of the model.

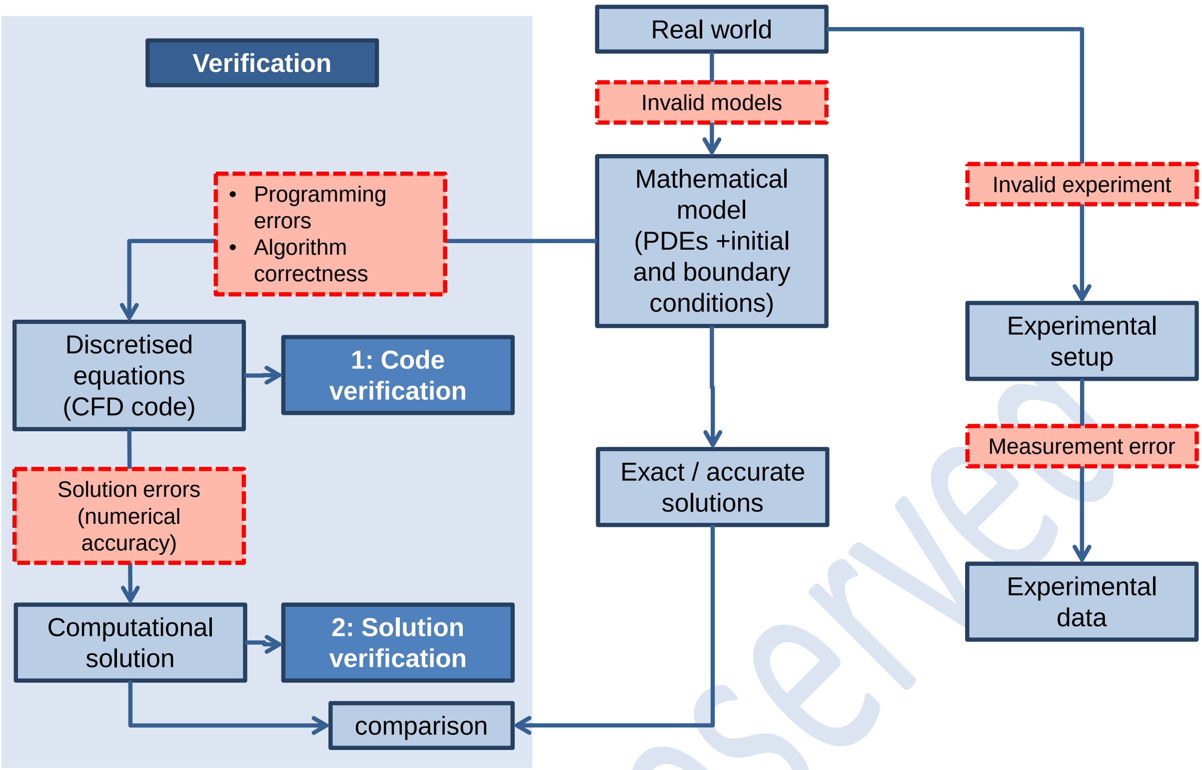

Figure 3: The objectives of verification in relation to the "real world" and experimental data. The red boxes indicate stages where errors are introduced.

The purpose of verification is to identify and reduce numerical errors, and to prove the numerical equations are solved correctly (or with sufficient accuracy for the intended application).

On the other hand, the objective of validation is to identify and reduce conceptual modelling errors, and addresses the relevance of the physics model by comparing computational results with experimental data.

As indicated in the diagram above, verification processes seek to identify and reduce errors when a model is programmed into a computer, and also when that computer code produces a numerical output. Some examples that distinguish verification and validation are shown below.

Table 3.1. The examples to distinguish verification and validation.

Step	**Verification**	**Validation**	**Example**
Check that the conceptual model (mathematical model) reflects reality		✓	Comparing experimental data with numerical results from various turbulence models to identify which is most appropriate to the specific application. Using a simplified "notional nozzle" to represent an inlet of hydrogen.
Model Calibration		✓	Calibration is the process of adjusting physical modelling parameters in the computational

			model to improve agreement with experimental data[1]
Check that the conceptual model has been implemented correctly in computer code (i.e. bug checking)	✓		Conservation tests. Invariance tests (symmetry, translation, rotation).
Check the order of accuracy of the solution	✓		Grid independence testing, identifying how error norms change as a function of grid size.
Check the numerical solution against a known result	✓		Compare numerical result against analytical solutions (Couette flow, Sod's Shock tube, etc) Compare result against highly accurate numerical benchmark solutions (e.g. NASA turbulence model verification http://turbmodels.larc.nasa.gov/).

3.3 Summary of Verification procedures (EE)

Deliverable 4.2 "Final report on verification and validation procedures" (SUSANA D4.2, 2016) sets out further detail on the procedures summarised below.

3.3.1 Code Verification

Code verification ensures that the computer program is a faithful representation of the original mathematical model. Errors can be introduced when implementing the conceptual models on a computer, via coding mistakes. Code verification procedures include:

- Software engineering: monitoring and controlling the software development processes and software products to ensure reliability. A formal quality procedure such as ISO 9001 is a positive indicator; publication of a comprehensive set of verification tests is recommended.
- Invariance tests: checking for consistency of outputs following simple operations such as translating or rotating the domain, mirroring the domain.
- Conservation tests – ensuring that mass and/or energy are conserved.
- Formal order of accuracy assessment. This examines whether the discretization error reduces at the theoretical rate expected as the mesh and/or time step are refined. Achieved via a grid refinement study and comparison of error norms for each result.

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[1] Definition from ASME guide 2006

- Convergence tests. A general recommendation is that iterative convergence is demonstrated by showing at least 3 orders of magnitude degrease in the normalized residuals for each equation solved.
- Discretisation tests: includes systematic mesh refinement to ensure the results are in the asymptotic region. Care is also required to identify and isolate grid dependent model terms, such as wall boundary conditions and turbulence models (for example, a Large Eddy Simulation gradually approaches a Direct Numerical Simulation when the grid is refined).

3.3.2 Solution Verification

The objective of solution verification is to improve confidence in the fidelity of the numerical simulations in relation to the application at hand. Code verification (which is focused on identifying mistakes in code implementation) is a prerequisite to solution verification.

Solution verification commonly takes the form of a series of test cases, each focussing on part of the code features or governing terms, each adding to the evidence that the implementation and use is correct. Taken together, the set of test cases would ideally cover the main features of the computation (physical terms, grid topology, discretisation etc.), providing confidence that its use is verified for the case under study. Solution verification tests include:

- Analytical Solutions: where the accuracy of numerical outputs from a code can be assessed against an analytical solution to the same equations.
- Numerical Solutions: where the accuracy of numerical outputs from a code can be assessed against the outputs from other codes which have been well tested and are of known high quality.
- Parameter sensitivity studies – extrapolating the above tests to more generalised conditions to ensure that expected results occur, improving confidence that the application domain is within that of the verified domain.

3.4 Verification Database

The above mentioned SUSANA document “D4.2 Verification and Validation Procedures” provides a number of practical worked verification examples all related to hydrogen simulation.

In addition, an extensive hydrogen safety specific verification database has been assembled by the SUSANA project to demonstrate procedures, techniques and worked examples to inform practitioners. The verification database entries are grouped according to the primary verification process they refer to. These are:

- Analytical solutions:
- Code verification:
- Manufactured solutions:
- Methodology:
- Numerical solutions:
- Sensitivity studies (grid and parameter sensitivity):

In addition, to aid the identification of useful references, the table given in the reference below has keywords on the main topic/application area for the reference, and the physical phenomena tested in that reference. The database can be found at: http://www.support-cfd.eu/index.php/verification-database

4. Sensitivity study (NCSRD)

The user should ensure that the simulation results are unaffected by numerical errors due to for example, insufficient grid resolution or implementation of unphysical boundary conditions. Therefore, several sensitivity studies should be performed before or during the validation. The most significant sensitivity studies are presented in the next sections. For more details about the numerical options and the sensitivity study procedures, the reader can refer to the "Guide to Best Practice in numerical simulations" (SUSANA D3.2, 2016). Apart from the above uncertainties there are also experimental uncertainties which influence the input data of the simulation. These kind of uncertainties are thoroughly discussed in (SUSANA D4.2, 2016). A sensitivity study for the experimental uncertainties can be performed during the validation.

Finally, in case the user carries out sensitivity analysis for input parameters such as hydrogen mass flow rate, this should be performed after the validation.

4.1 Grid independency (NCSRD/JRC)

The resolution of the computational mesh can affect the results. Therefore it is crucial that in the initial stages of any numerical investigation, including the validation, simulations with increasingly finer mesh resolution are performed until negligible differences in the target variables are reached (if computing power permits performing such simulations on a finer grid in a reasonable time). Usually at least three meshes (coarse, intermediate, and fine) are required in a mesh sensitivity analysis as this allows for the quantification of the numerical errors. The grid convergence index based on the Richardson extrapolation (Richardson 1911), (Richardson and Gaunt 1927) provides an estimate of the grid convergence error (Roache 1994). The relative error between results from different grids is a good indicator of grid independence (SUSANA consortium, D3.2 2016).

Ideally, the average length of the computational cells should be halved in each grid refinement. If this systematic refinement of the mesh is unfeasible because of the subsequent excessive simulation times, it is then recommended to refine the mesh according to the experience of the user, through an evaluation of the convergence of the simulations using the trends in the target variables (Andreani et al. 2008). The grid could be refined primarily in the regions where high gradients and complex phenomena are expected to appear. These regions are for example the area around the hydrogen source and around vents.

When a full grid sensitivity study is not possible because of the large size of the mesh, an alternative partial indication of the quality of the grid can be estimated by using the same mesh with different order numerical schemes. If the results with the higher order schemes are similar to those with the first order scheme, the numerical diffusion due to the coarse grid can be said to be minimal (SUSANA consortium, D3.2 2016).

Grid sensitivity studies with Large Eddy Simulation models require a special treatment. As explained by (Gullbrand, 2002), when explicit filtering is used, the explicit filter width has to be kept constant while the computational grid is refined to obtain a grid-independent solution. With implicit filtering, since the filter is directly connected to the mesh resolution, the solution converges towards a direct numerical simulation (DNS) as the grid is refined, and not towards the filtered Navier-Stokes equations (Gullbrand, 2002). It must also be emphasized that for a rigorous application of LES at least 80% of turbulence kinetic energy should be resolved on the numerical grid.

4.2 Time-step/CFL sensitivity (NCSRD/UU)

An important criterion which controls the stability and accuracy of numerical simulations is the time step. In explicit schemes, time step is usually controlled by the Courant-Friedrichs-Lewy (CFL) number (Courant, Friedrichs, and Lewy 1967). The CFL is very important for explicit schemes and should be below unity for numerical stability. For fully-implicit schemes the choice of the time step (and thus CFL number) also plays an important role as it may affect the solver convergence and the accuracy of transient phenomena predictions.

Large time steps might not be able to capture the physics of the problem. Therefore, a time-step (or equivalently CFL) sensitivity study should be performed in order to obtain the time step independent solution. An initial time step can be determined for a specific simulation based on the experience of the user and using the best practice guidelines (SUSANA consortium, D3.2 2016). The simulation then needs to be repeated using a smaller time-step or CFL number (ideally reducing the time step at least by half). If the difference in the target variables between simulations is significant, simulations with an even smaller time step need to be carried out until a time-step independent solution is obtained. A time-step independent solution is closely tied with the choice of the temporal numerical scheme. The choice of the temporal numerical scheme is important in order to achieve a time-step independent solution without the need to use extremely small time step (see also Section 4.4).

4.3 Numerical scheme (NCSRD/HSL)

For the discretization of the partial differential equations, an appropriate method (numerical scheme) to discretize the spatial and the temporal derivatives needs to be chosen. Regarding spatial discretization, the choice of the numerical scheme is of great importance for the convective terms of the equations. The order of accuracy of the numerical scheme is a crucial factor in CFD simulations. First-order accurate schemes, such as the upwind scheme, can introduce numerical diffusion into the solution leading to artificial mixing and reduction in the spatial gradients of flow variables. High-order schemes are prerequisite in Large Eddy Simulation (LES) in order to avoid the numerical dissipation of resolved vortices/turbulence. In transient simulations - which are usually the case in hydrogen safety applications – a temporal discretisation scheme is also required. High-order discretization schemes may be necessary in order to capture accurately the transient phenomena.

The proper selection of the numerical scheme should be made based on best practice guidelines (SUSANA consortium, D3.2 2016).

However, a sensitivity study of the numerical scheme selection should be undertaken in order to demonstrate that numerical diffusion does not influence the results. This also allows the user to estimate the magnitude of numerical diffusion when using lower order schemes.

4.4 Boundary conditions (NCSRD/KIT)

The choice of boundary conditions is of great significance to the accuracy of the computational results. There are several options available for boundary conditions and a user must decide the most appropriate boundary conditions for a particular application. The proper selection of the boundary condition should be made based on the best practice guidelines (SUSANA consortium, D3.2 2016). A sensitivity study of the boundary conditions could be performed in order to evaluate their impact on the results, e.g. to assess the performance of the notional nozzle approaches at the hydrogen inlet boundary.

4.5 Domain size (for unconfined / semi-confined / vented configurations) (NCSRD/JRC)

The size of the computational domain should be carefully chosen. Domain boundaries should be located far enough from the area of interest in order to minimize the impact of the boundary conditions on the simulation results. An example of the effect of changing computational domain size was shown in the benchmark problem SBEP-V20 (Papanikolaou et al. 2010) where an increase in the size of the computational domain produced a significant improvement in the agreement between simulation results and the experimental measurements. Therefore, it is always essential to investigate the effect of the size of the computational domain on the simulation results, performing the same simulation with an increasingly larger domain until the effect upon the relevant variables becomes negligible. Such sensitivity tests on the extent of the computational domain should be undertaken unless there is supporting information from the literature. Domain extension examples and sensitivity studies of several representative problems are presented in the “Guide to best practice in numerical simulations” document (SUSANA consortium, D3.2 2016) and in (SUSANA D4.2, 2016).

5. Validation (KIT)

Validation can be defined as a comparison between the predictions of a model which has been run to simulate a given event and the observations made in connection with the same event (Duijm and Carissimo, 2002).

The objectives of a validation procedure are:

- to define the variables that are the most important for predictions;
- to define how the comparison between the model outputs and experimental observations should be undertaken.

The validation process involves several steps: firstly the selection of experimental data, then the selection of the variables which will be compared with the experimental measures, the definition of how those variables will be compared and finally the estimation of the uncertainties.

Indeed validation can be either qualitative by means of graphs/plots of observed versus modelled values or more quantitative by means of statistical comparison between the observed and modelled values. In the SUSANA project, quantitative validation - via the use of statistical measures performance – is used.

After verifying the model is correctly implemented and defining the set of experimental data that will serve as comparison with simulation results, the next step in the validation process is the definition of target parameters and statistical performance measures.

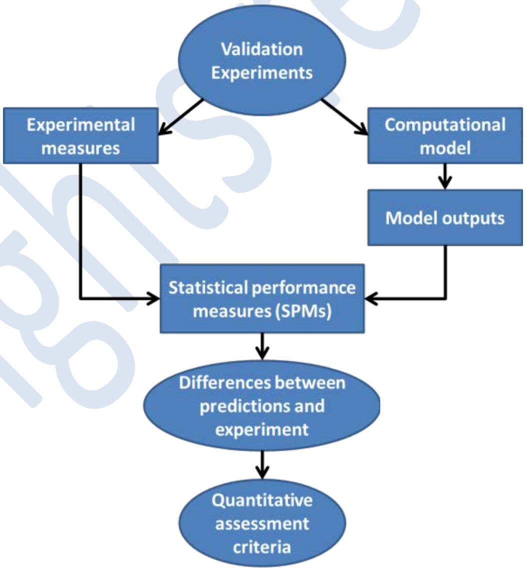

Figure 4: Diagram of validation procedure.

The main steps of the validation procedure are: (based on Ivings et al. (2007)):

a. Specification of the objective: this being the quantification and assessment of model performance in reproducing a selected phenomenon.
b. Identification and selection of suitable validation data sets.
c. Define the specific content and design the format of the validation database.
d. Selection of specific cases from these datasets so as to cover the range of target scenarios.

e. Definition of target variables that are measured or derived from measurements and which form the basis of comparisons with model predictions.
f. Selection of statistical performance measures (SPM) that allow quantitative comparison of predictions against measurements.
g. Review and definition of quantitative assessment criteria that define the acceptable numerical range of the SPM which result from applying this validation procedure.
h. Provide guidance on model application for the validation cases.
i. Apply the validation procedure and refine as necessary in the light of experience.

After the selection of various experimental data, the target variables can be selected. This indicates which parameters should be monitored during the CFD calculation. After running the model(s) the statistical performance measures are a set of formula that allows a comparison between the computed and measured variables. The quantitative assessment criteria can be defined as the ranges of values where the computed target variables are statistically considered to be correctly calculated.

5.1 Validation Database (KIT)

Model validation involves a comparison of model predictions with experimental measurements. Validation should be performed using several experiments that are within the model's range of applicability. For code validation high quality experimental data is important; a comparison between a numerical simulation and poor quality experimental data cannot reliably indicate that a numerical model reflects real physics. Building a high-quality validation database is the first step in a successful validation exercise.

To achieve the goal of successful validation applied to hydrogen safety analysis, a validation database containing high quality experiments and covering different physical phenomena has been established.

The validation database has been created using the following headings:

- Ignition and fires of hydrogen gas
- Release and distribution of gaseous and liquid hydrogen
- Deflagration of hydrogen gas
- Detonation of hydrogen gas
- Deflagration to detonation transition (DDT)

With each experiment, detailed information is given in a consistent format which is summarized as follows:

- Summary
- Author
- Experimental Setup
- Objective of experiment
- Applicable calculations
- Experimental procedure
- Experimental data
- Performed simulation
- Reference
- Comment

The above headings provide a detailed description of each experiment, including background, preparation, experimental procedure, results, the related numerical works and references.

In addition, to provide an acceptable level of quality assurance, an experimental evaluation procedure was introduced for the validation database. Following this process, each experiment should be evaluated by at least two experts who have experience in numerical simulation or experimentation. The experiments which are evaluated as high quality are included in the database, but the experiments which are regarded as lower quality should be revised, abandoned or used with caution.

In the validation database the experimental setup is presented and the experimental data and results are publicly available. A short description of each of the experiments included in the validation database is provided in Appendix 2 (Section 9.2). Details of each of these experiments, including the experimental setup and results, are provided in full in the validation database of SUSANA, which is available on the SUSANA website (www.support-cfd.eu).

5.2 Target variables (AREVA)

Target variables are the most relevant variables for each phenomenon that will be considered for comparison between the simulation results and the experimental data in the validation process. Target variables should be obtained from the outputs of the simulations. For each phenomenon, these selected variables allow for a greater understanding of the physics behind the phenomenon under consideration. Typically they will evolve in space and/or in time throughout the duration of the simulations.

All of the target variables are presented in detail in the Deliverable 4.2 “Final report on verification and validation procedures” (SUSANA D 4.2, 2016).

5.2.1 Release and mixing of gaseous hydrogen, including permeation (NCSRD/UU)

Table 5.1. Target variables for release and mixing of *gaseous* hydrogen.

	Direct target variable	**Comments**
Characterisation of the leak-source term	Pressure and temperature evolution inside hydrogen storage vessel and in pipe, and or pipe/nozzle exit	This will permit the flow rate to be calculated and affect flow rate and temperature of the released hydrogen. If the pressure in a vessel is above 7 MPa it is recommended to use the equation of state for real gases. A difference in temperature between the released hydrogen and surrounding air can affect mixing and dispersion.
	Flow rate (mass/volume)	From a flow rate, a velocity can be calculated using the known diameter and density
Jet/Plume	Hydrogen concentration evolution (distribution in space and time)	For all variables, the values should be provided both in the jet and/or outside the jet area.
	Sizes of jet (length and width), distance to the LFL and UFL (flammable envelope size)	
	Mass and volume of hydrogen in a flammable envelope	Derived from the concentration distribution field. Can give an idea of the total quantity of hydrogen released if the mass flow rate of the source is not known.
	Velocity flow field dynamics	At the nozzle exit. In different locations of the jet.
	Turbulent fluctuation velocity	Should include the turbulence intensity, *I*, and length scale, *Lt*, (turbulent flows only)
	Visualisation of jet shape	Schlieren and BOS techniques of visualisation of changes in gas density are useful for validation, e.g. for transition from momentum-dominated to buoyance-controlled jet.
Dispersion	Hydrogen concentration field	
	Flammable mass/volume	
	Velocity field	
	Pressure evolution inside the enclosure	Relevant to the pressure peaking phenomenon
	Flow rate through the opening vents	

5.2.2 Release and mixing of liquid hydrogen (JRC)

Table 5.2. Target variables for release and mixing of *liquid* hydrogen.

Direct target variable	Comments
Flow rate (velocity) at source	
Temperature	
Evaporation rate	
GH_2 fraction at the source	
LH2 pool radius	The vapour flashed fraction at the nozzle is significant input data for the simulation, as it affects greatly the exit velocity.
Hydrogen/oxygen/water vapour concentration	
Condensation rate of water and air components/species	
Flammable mass/volume	Derived from concentrations
Turbulence characteristics (such as turbulence kinetic energy)	
Pressure	For confined and closed spaces

5.2.3 Ignition (UU)

Table 5.3. Target variable for ignition.

Direct target variable	Comments
Location and shape of reacting zone	Reaction zone may be identified by OH radicals
Time of ignition initiation after the start of a rupture disk opening	Time of a rupture disk opening is proven to be extremely important to reproduce accurately the ignition location and time.
Location of ignition	
Rupture disk opening time	May be considered as a target variable in simulations with moving mesh
Pressure, temperature, and velocity field evolution	Give insights into underlying phenomena

5.2.4 Fires (UU)

Table 5.4. Target variables for fires.

Direct target variable	Comments
Hydrogen mass flow rate from the source	Affects flame length
Heat release rate	Radiation fraction of the total heat release rate should be addressed
Flame shape, length, and width	Development of flame in time and space is important for unsteady releases like blowdowns and fireballs
Temperature field	Distribution of temperature is important for validation and assessment of hazard distances
Species concentration field	Concentration of radicals, e.g. hydroxyl, may be used for reaction zone visualisation
Heat flux from fire	Important for assessment of hazard distances

5.2.5 Deflagrations (UU)

Table 5.5. Target variables for deflagrations.

Direct target variable	Comments
Pressure dynamics	Dynamics of positive and negative (when relevant) pressure phases, including maximum and minimum peak values. Pressure decay with distances from ignition source (inside and outside of a flammable cloud).
Flame propagation dynamics	Flame propagation velocity and acceleration may be obtained from flame propagation dynamics. Note: pressure in a blast wave is a function of both the flame propagation velocity and the flame acceleration.
Velocity and r.m.s. velocity field	Affects premixed flame propagation and deflagration dynamics.
Species concentration field	Shape of flammable cloud may be deduced from hydrogen concentration field. Location of reaction zones could be

	deduced from radicals' concentration, e.g. OH.
Dynamics of vent opening	In models allowing to model opening, and in simulations with moving mesh.

5.2.6 Detonations (KIT)

Table 5.6. Target variables for detonations.

Direct target variable	**Comments**
Detonation overpressure dynamics	Comparison of theoretical and experimental values of P_{CJ} and $P_{vN,}$ impulse, shape of pressure signal with simulated values.
Detonation cell size	Mainly for the codes which aim at reproducing the small scale detonations numerically. For large scale problems, validation through the comparison of detonation cell size is impossible.
Detonation wave propagation velocity	It can be derived from the sequence of the detonation wave (coupled shock and combustion wave) pressure dynamics records using a number of sensors. Deficit of coupled flame front/shock wave propagation velocity compared to the theoretical CJ value is observed due to losses in geometries with obstacles.
Velocity field	

5.2.7 Deflagration to detonation transition – DDT (KIT)

Table 5.7. Target variables for deflagration to detonation transition.

Direct target variable	**Comments**
Pressure dynamics	
Flame propagation dynamics	
Run up distance to DDT	Also called sometimes "the distance of pre-detonation"

5.3 Results analysis methodology (HSL)

The results of the validation exercise can be evaluated in two ways; either “qualitatively” or “quantitatively”. In either case, the target variables monitored during simulations are compared with target variables obtained from the experiments.

Qualitative evaluation of models can be undertaken by visual comparison of plots of the measured and predicted target variables.

Quantitative evaluation involves calculating Statistical Performance Measures (SPMs) which provide procedures for comparing measured and predicted target variables.

In a qualitative evaluation, one does not obtain measures that can be used to set performance criterion, and it can be hard to interpret results visually. On the other hand, only calculating quantitative measures may not give much insight into the overall behaviour, or why particular tests, or points, give the SPMs they do. Some form of qualitative analysis can help with a quantitative analysis.

The approach used in carrying out the evaluation will depend on the particular physics being modelled as well as the purpose of the evaluation. A general procedure for doing this is set out in the supporting document Deliverable 4.2 “Final report on verification and validation procedures” (SUSANA D4.2, 2016), which sets out the following tasks:

- Decide whether the evaluation is to be qualitative or quantitative, or both
- Select an appropriate set of SPMs, bearing in mind:
    - They should give an indication of the model’s ability, i.e. whether it under- or over-predicts values, such as the maximum concentration or overpressure.
    - They should give an indication of the level of scatter i.e. the deviation from the average.
    - Equal weight should be given to all measurements/predictions regardless of their absolute values.
- Decide on what basis the comparison is to be made, for example, whether it is to be:
    - In time only (measurements and predictions are spatially averaged).
    - In space only (measurements and predictions are time averaged at each spatial location).
    - In both time and space.
- If necessary, process the experimental and numerical data, giving consideration to the techniques used to average the data.
- Calculation of SPM and evaluation against quantitative criteria, including calculation of ranges of SPM based upon sensitivity and uncertainty analysis.

SPM can be computed for individual experiments and the results reported for each experimental basis. When several experiments have been simulated, a single score over all the experiments may help to answer the question of how good the model is on average. However, careful consideration needs to be given to how the average score is obtained so that individual results do not cancel each other out and result in what appears to be good model performance. An alternative is the approach adopted by Ivings et al. (2007) where the model performance over groups of experiments is assessed. These groups may be defined according to a particular physical aspect of the experiments, for example whether the experiment was undertaken in a wind tunnel. The advantage of this approach was that a distinction could be made between models able to account for these effects.

5.4 Quantitative Assessment Criteria (EE)

Being able to define what constitutes a “good” or “acceptable” model is not straightforward. Indeed, this decision should be based on a combination of different elements: firstly, the scientific assessment; secondly, the verification and finally, the validation. In the scientific assessment, the decision can be informed by the criteria set out in Section 2.3. Verification is discussed in Section 3 and this Section 5.4 is about quantitative values for validation.

Quantitative evaluation of the performance of a given model requires the definition of appropriate SPMs; presented in detail in the deliverable D4.2 (SUSANA D4.2, 2016) and described briefly in Section 5.3 above. Determining values of quantitative criteria is difficult because it relies to a certain extent on the results of previous model evaluations and of building up experience in a particular area. Atmospheric dispersion modelling is an area where there is a relatively large amount of experience as many of the evaluation studies report the results of statistical analyses. In other areas there is more limited experience of model evaluation and of setting appropriate quantitative criteria for validation of model performance. There is a danger that acceptance criteria for atmospheric dispersion models are adopted for other physical scenarios, but may not be appropriate for those scenarios which do not have the same level of inherent uncertainty.

An example would be in the assessment of dispersion indoors under mechanical ventilation, which is not governed by atmospheric wind or turbulence. For this case, it would be appropriate to adopt a much narrower range of acceptance for a model, to reflect the lower uncertainty of the process. However, selecting the range could be difficult depending on the evaluation data available.

Acceptance criteria will also depend on the quantity that is being predicted. Different criteria may therefore be used for the same problem if more than one parameter is being compared. For example, in an internal explosion in a sealed vessel, the maximum overpressure may be straightforward to predict but the arrival time less certain.

An alternative to using absolute values of quantitative criteria may occur when several models are being compared against each other. In this case, the “best performing” model for a particular scenario may be selected, but this is subjective.

Previous work on dense gas dispersion models made in the 90’s (Hanna et al. 1993) (Touma et al. 1995) or more generally on gas dispersion models (Hanna et al. 2004) gave some insights into and suggestions for the establishment of quantitative validation criteria.

SMEDIS (Carissimo et al. 2001), based on the works of (Duijm et al. 1996), suggested to use as statistical performance measures:

- MRB (Mean Relative Bias) and MG (Geometric Mean) for the bias in the mean
- MRSE (Mean Relative Square Error) and VG (Geometric Variance) for the scatter about the mean

SMEDIS also attempted to establish that a “good” model should have as quantitative criteria:

- A mean bias within ±50% of the mean (i.e. $-0.4<MRB<0.4$ and $0.67<MG<1.5$)
- A scatter of a factor of three of the mean (i.e. $MRSE<2.3$ and $VG<3.3$)
- A fraction of model observations within a factor of 2 of observations (FAC2) to be at least 50%

Most of these previous works used the maximum arc-wise concentration and plume width as target variables and highlighted the difficulty to apply SPMs on point-wise concentration.

Chang and Hanna (2004) recommend the use of the fractional bias (FB), the normalized mean square error (NMSE), MG, VG and FAC2. They consider that a “good” model would be expected to have mean bias ± 30% of the mean, i.e. $|FB|<0.3$ or $0.7<MG<1.3$, and random scatter about a factor of two to three, i.e. $NMSE<1.5$ or $VG<4$ (see the deliverable D5.2 (SUSANA D5.2 2015)). However, this depends on the physics involved and these quantitative assessment criteria are mostly adopted in atmospheric releases and they are not necessarily suitable for other phenomena.

Table 5.8 shows the ideal values of the most commonly used SPMs.

Table 5.8. Ideal value for the different SPMs

SPM	ideal value
FB/MRB	0
NMSE/MRSE	0
MG	1
VG	1

5.4.1 Presentation of the results

The results of a statistical analysis are usually presented in the form of scatter plots of FB against NMSE or MG against VG. Those plots are a useful indication of model performance and tendency to under/over predict. As reminder each SPM has an ideal or optimum value. For FB the optimum value is 0, consequently if FB has a negative value, the model is underpredictive while if FB has a positive value, the model is overpredictive. For MG, the optimum value is 1 and if $MG>1$, the model is underpredictive and if $MG<1$, the model is overpredictive.

Another point is that FB is symmetric about the ideal value; this allows an easier comparison between values due to an equal weight to under/over prediction while MG is not symmetric and is often plotted using a logarithmic scale.

Examples of SPM values and plots of MG against VG and FB against NMSE are available in the deliverable D4.2 (SUSANA D4.2 2016). Diagrams demonstrating SPM values and error percentage are presented in Section 9.3.

The SUSANA project consortium could not reach a consensus on the figures for the good/acceptable range of accuracy for all relevant phenomena and as a result no proper universal quantitative criteria could be determined.

Ultimately, identifying a model as “good” or “acceptable” may be via evaluating the SPMs which are as close as possible to their ideal values, irrespective of the phenomenon studied.

6. Model Assessment Report (UU)

6.1 Content of the report (UU)

The Model Assessment Report (MAR) represents the output from the assessment element of the scientific evaluation. This report is produced by analysing the information supplied by the model developer or expert user (the nominated organisation and is generally created from the information contained within the completed questionnaire; the questionnaire template is provided in the appendix) and/or from pre-existing model documentation. The MAR is split into seven sections described in Section 1.5.1.

A MAR is intended to be used by both the model developer and the model user. For the model developer, the MAR represents an independent model assessment, highlighting both the strengths and weaknesses of the model. For the model user, the MAR can be used to assist them in deciding whether (or not) a given model is suited to their particular task. As both the scientific and user-orientated aspects of a given model are addressed the user can make a well-informed choice as to how a model will meet their particular needs. Ultimately the MAR should form part of the standard documentation which accompanies the specific version of the model which was assessed.

6.2 Requirements for the detailed description of the model/code (UU)

This section of the MAR contains a general description of the model, including: name, version number and release date; physical problems and application areas addressed by the model; model type; model supplier; model history; model development; relationship to other models – interfacing to other models and software; current model usage; and hardware and software development and requirements.

6.3 Scientific assessment (UU)

This section of the MAR contains detailed information regarding the scientific basis of the model, along with a user-oriented assessment including: classification of the model, e.g. a zero- or one-dimensional integral model; specification of model inputs: source terms and method for accounting for environmental conditions; model physics and mathematical formulation; solution technique; model special features; and any future scientific developments being planned for inclusion in the model.

Focusing on the user-oriented aspects of the model: what user-orientated documentation/on-screen help exists; installation procedure; description of the user interface; internal databases; guidance in selecting model options and inputs; error messages and checks on data validity; resources – computational costs; results and outputs available from the model (providing clarity and flexibility); suitability of users – background, experience, support, model integration; and any planned user-orientated developments and improvements.

6.4 Sensitivity study (UU/NCSRD)

This section of the MAR includes details on the sources of uncertainty, limits of applicability and on the sensitivity studies undertaken. In order to quantify uncertainties in model outputs in relation to their comparison with experimental data and observations it is useful that an appropriate sensitivity study is undertaken, an example of such a study would be a group of simulations with a slight variation in input parameter(s). Presenting a single run of a model, or even a very limited number of runs, as the definitive solution is unsatisfactory. As wide a view of a particular phenomenon as possible should be presented, by testing the solution obtained against various inputs.

Details of such a study should include: the suitability of modelling assumptions made; suitability of numerical method employed; sensitivity to input parameters, domain size, boundary conditions, grid independency and time step/CFL sensitivity (see Section 5.4). It must be demonstrated that detailed sensitivity studies have been carried out which examine the sensitivity of the model to input, as well as confirming the robustness of the model.

A comprehensive sensitivity study should also include advantages, disadvantages and limits of applicability of the model as follows.

6.5 Verification and validation (UU)

6.5.1 Verification

This section of the MAR summarises the verification procedures that have been undertaken on the model. Have changes been made to the model following the completion of verification procedures? Has this led to improvements in model performance? For example, "The model has been verified against analytical solutions, correlations, other well-established models, etc." The steps undertaken towards verification of the model must be included in appropriate documentation and references. If applicable a quality assurance statement should be provided.

For further details on what information should be provided by the model developer/expert/user see Section 9.1.4.

6.5.2 Validation

This section of the MAR is associated with ascertaining what validation work has been performed on the model. This should include details of validations already performed and the conclusions drawn from this exercise.

When considering validation steps already performed the following should be considered for inclusion in this section of the MAR: statements such as "validation comparisons were made with…"; a description of each validation experiment, along with appropriate references; any assumptions made; a detailed discussion of the results obtained following statistical and graphical comparisons; details on whether the validation experiments cover a wide spread of phenomena (validation domain) and what data were compared?

Considering conclusions: overall, how did the model perform against the selected experiments? Can improvements be suggested following the validation procedure undertaken?

For further details on what information should be provided by the model developer/expert/user see Section 9.1.5.

6.6 Quantitative assessment (UU/EE)

An all-encompassing definition of what constitutes a 'good' or 'acceptable' model is not straightforward. This decision should be based on a combination of elements; firstly, based on the scientific assessment – which addresses whether the qualitative assessment criteria have been met; secondly, from the verification procedures that have been completed and finally, from the extent to which the pre-determined statistical performance measures (SPMs) assessment have been satisfied via the validation process.

The statistical analysis methodology developed for this study is presented in Section 5.3.

However, it must be recognised that there is only limited experience in conducting such in-depth model evaluations and therefore there will remain a degree of uncertainty as to what values of 'good' or 'acceptable' quantitative ranges should be selected as SPMs. This uncertainty can be reduced as models are evaluated against the protocol, leading to a refinement of the SPMs values that indicate a model as 'good' or 'acceptable'.

The target variables (as detailed in Section 5.2) are the physical quantities against which the performance of the model is evaluated. They can be directly measured or derived from measurements, and can be separated into parameters based on point-wise and arc-wise data. Point-wise parameters involve a comparison between model predictions and measurements that are paired at specific points, whereas arc-wise data involves comparisons made at specific distances (radius). The particularities of the scenario under investigation determine which of these two measures is most appropriate. For example, if steady releases are considered, the most commonly-used physical comparison parameter is the maximum concentration at a specific distance downstream of the release. Additionally, for this case, to gain a great understanding of the performance of a given model, the comparison of the maximum concentration should be combined with a comparison of the plume width, as described in (Hanna, Chang, and Strimaitis 1993), (Duijm, Ott, and Nielsen 1996) and (Duijm and Carissimo 2002). Point-wise time-averaged concentrations at specific locations can also be included as a physical comparison parameter for this scenario, referring to a continuous release, and as stated by (Carissimo et al. 2001), are known to provide a more stringent test of model performance than arc-wise comparisons.

Therefore, for each model under investigation recommended target variables should be identified (as per Table 5.1-Table 5.7) and experiments should be selected (specifically as per Table 9.1.-Table 9.6.), for comparison against model outputs. Continuing the above example of a steady release scenario, appropriate parameters would be:

- Maximum concentration across an arc at a given radius.
- Cloud width across this arc at the same radius.
- Concentration at specific sensor locations.

6.7 Conclusions (UU)

The conclusions section of the MAR forms a concise overview of the model under consideration, addressing each of the previous sections of the report in turn. The conclusions section should be no more than two or three pages and should include:

- general model description: short overview
- scientific basis of the model: short overview
- limits of applicability: list of limits and applicability range
- user-orientated aspects of the model e.g. the technical documentation is comprehensive, and also details of uncertainty, areas which require improvement, etc.
- verification performed e.g. the provided documentation describes the extensive verification work which has been completed, the verification work is focused, well-structured and clearly presented
- validation performed e.g. validation has been performed using (….), validation is clearly presented in the following documentation, etc.

- advantages and disadvantages of the model can be split into general usage and in context-of-use advantages and disadvantages;
- suitability of protocol for assessment of the model, a short statement for or against.

Considering *limits of applicability*, examples of applicable statements include: CFD models are applicable to the widest set of circumstances (….), however CFD models are not best suited to (….) due to time and effort involved in setting up, running and post processing; model is well suited to (….) with the following caveats (….); model cannot handle (….); pre-processing tools are only available for (….); all simulations must be run in transient mode; no obvious limitations, other than spatial resolution and (….); complex geometries may require a large number of mesh cells, etc.

Considering *advantages*, examples of applicable statements include: quick to run; complex features can be relatively straightforward to include; significant validation completed; model contains (….) which is missing from most other such models; based on previously tested and published numerical and physical sub-models; this model is specifically tailored to (….); user manual is available; model is capable of providing credible and acceptable predictions; model is flexible; model can handle complex geometries and terrain; model is based on an accepted 'state-of-the-art' commercial package; wide variety of output data obtained; technical support can be provided into the future; etc.

Considering *disadvantages*, examples of applicable statements include: assumptions employed require further testing; labour intensive; requiring significant computer resources; doubts regarding verification and validation processes previously completed; obstacles and rough terrain cannot be modelled; no user interface available; very limited error handling capabilities; typical run-times are lengthy; limited range of validation cases; limited amount of verification carried out; quality of results dependent on how model was applied; model required experience in the use of (….); limited amount of customisation possible; etc.

7. Conclusions (JRC)

In the SUSANA project the Hydrogen Model Evaluation Protocol (HYMEP) has been developed for the assessment of the accuracy and suitability of CFD models in the area of hydrogen safety. Previous experience related to the development of model evaluation protocols in other fields (MEG, MEGGE, SMEDIS and LNG protocol) have been taken into account. A Model Evaluation Group (MEG) was established by the European Commission in 1994 and produced a generic evaluation protocol for consequence models (MEGGE 1996). Following the generic evaluation protocol, expert groups were set up with the purpose of developing an evaluation protocol in specific areas like heavy gas dispersion (HGD) and gas explosions (MEGGE 1996). The HGD protocol was developed further by the project Scientific Model Evaluation Techniques Applied to Dense Gas Dispersion Models in Complex Situations (SMEDIS) (Daish et al. 2000). More recently a model evaluation protocol for LNG dispersion models was developed (Ivings et al. 2007).

The HYMEP includes 6 main stages: scientific assessment, verification, sensitivity study, validation, statistical analysis, and finally an assessment report. Practically all aspects of hydrogen safety phenomena have been considered in the document: release, mixing and dispersion of gaseous and liquid hydrogen, ignition, fire, deflagration, deflagration-to-detonation transition and detonation. HYMEP is applicable to other safety-related phenomena such as tank filling, consequences of catastrophic rupture of a high-pressure hydrogen tank in a fire (blast wave and fireball), etc.

The SUSANA consortium produced 4 complementary reports as supporting documents for the HYMEP:

- Review (SUSANA consortium, D2.1 2014) and
- Critical analysis (SUSANA consortium, D2.2 2015) of the state-of-the-art of the CFD modelling for safety analysis in fuel cell and hydrogen (FCH) technologies
- Guide to CFD best practice (SUSANA consortium, D3.2 2016)
- Report on verification and validation procedures (SUSANA consortium, D3.2 2016)

The HYMEP document is intended to be a reference document for all those groups that develop, apply and use CFD models in the area of FCH technologies and beyond: CFD model and tool developers (academia, research institute, commercial CFD code developers, etc.), CFD users (researchers in academia and industry, consultancy companies, etc.), regulation, codes and standards (RCS) developers, and regulatory/approval/certifying bodies that have to permit hydrogen systems and hydrogen infrastructure/facilities. Through the HYMEP, hydrogen safety engineers and regulatory/approval/certifying bodies have a reference document that helps them to evaluate whether the CFD analysis supporting their safety design and permission request respectively is scientifically sound.

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9. Appendix

9.1 Appendix 1: Questionnaire (UU)

Questionnaire foreword

This purpose of this questionnaire is to obtain the information which is required to assess each of the different types of models identified for safety analysis of hydrogen and fuel cell technologies. This information is supplied by the organisation responsible for its development or from an expert user.

The questionnaire is based on the form derived by the European Commission's SMEDIS project but has been adapted for the current purpose. As the questionnaire is aimed at all types of models: release, mixing, and dispersion, permeation and dispersion, ignition and fire, deflagration and detonation, etc some questions may not be applicable to all models and should be answered with N/A for "not applicable".

It is essential that the following guidelines are followed during completion:

Cover sheet: The angled brackets (<…>) should be replaced with the required appropriate information, including the specific model version under consideration (see directly below).

Model version: The information supplied in this questionnaire should relate only to a single well-defined version of the model, the ***reference version*** of the model. This version must be unambiguously identified.

Type of questions: There are two types of questions.

- Questions marked ***with*** an asterisk*: These questions require relatively concise, explicit information.
- Questions ***without*** an asterisk*: These questions require identification and the supply of documentation which describes a particular aspect of the model, for example using reports, manuals and papers. Only the reference to such documents needs to be provided. In the absence of such documentation the information supplier must add their own notes in the space provided.

Guidance on completing questions: These guidelines should be read before any of the questions contained in the questionnaire are answered, this guidance should be followed during the completion process.

Questionnaire
to obtain information on
<MODEL NAME>
<MODEL VERSION>

Information supplied by: <NAME, ORGANISATION>

Questionnaire completed on: <DD/MM/YYYY>

9.1.1 General Information

This section of the questionnaire is associated with requesting information on the general nature of the model. Each information request in this section should be answered explicitly, with a short concise response.

9.1.1.1 *Name of the model

9.1.1.2 *Model version (as per cover sheet) and date

9.1.1.3 *Year of original model origin and of the version under evaluation

9.1.1.4 *Heredity of the model

9.1.1.5 *Model developer(s) contact information

9.1.1.6 *Short description of the model

9.1.1.7 *Short description of the areas of application of the model

9.1.1.8 *List of supporting documents supplied

9.1.2 Information for scientific assessment

This section of the questionnaire is associated with requesting information on the physical and mathematical basis of the model. Therefore each of the information requests detailed below must be directly addressed with appropriate documentation, with as much detail as required, to describe the theoretical background of the model.

9.1.2.1 Physical problems addressed by the model

9.1.2.2 Physical processes modelled

9.1.2.3 Mathematical formulation of the problem

9.1.2.4 Solution method

9.1.2.5 What output variables are available from the model?

9.1.2.6 *Planned scientific developments

9.1.3 Information for user-orientated assessment

This section of the questionnaire is associated with requesting information on the practical characteristics of the model, referring to how the model is operated and used in order to solve specific problems. Some of the information requested is likely to be contained in the model's user manual or other existing documentation which outlines to the user how to set up and run the model. Information requests with an *asterisk must be answered with an explicit, concise response. All other information requests should be addressed with appropriate references and/or appropriate notes.

9.1.3.1 Computer environment

9.1.3.1.1 *Hardware

9.1.3.1.2 *Operating system(s)

9.1.3.1.3 *Auxiliary software

9.1.3.1.4 *programming language(s)

9.1.3.2 Installation procedure

9.1.3.3 User interface

9.1.3.4 Internal databases

9.1.3.5 Inputting data

9.1.3.5.1 Entering given input data

9.1.3.5.2 Guidance for selecting input data

9.1.3.5.3 Automatic checks on data validity

9.1.3.6 Running the model

9.1.3.6.1 *Modes for running the model

9.1.3.6.2 Error messages

9.1.3.7 Output from the model

9.1.3.7.1 Types and formats of output displayed

9.1.3.7.2 *Identification, organisation and accessibility of output from runs

9.1.3.7.3 Hard copy facilities

9.1.3.8 Interfacing to other models and software

9.1.3.8.1 *Part of program suite?

9.1.3.8.2 *Interfacing with software tools

9.1.3.8.3 *Source models

9.1.3.8.4 *Other models

9.1.3.8.5 *Customisation of software

9.1.3.9 Status and availability of the model

9.1.3.9.1 *Maturity of the model

9.1.3.9.2 *Availability of the model

9.1.3.9.3 *Peer review of the model

9.1.3.9.4 *Options for acquisition

9.1.3.9.5 *Contact information for obtaining model (if available)

9.1.3.10 Resources

9.1.3.10.1 *Financial cost of model (if applicable)

9.1.3.10.2 *Order of magnitude of run time on specified platform and for specified problem

9.1.3.11 Users

9.1.3.11.1 *Current users

9.1.3.11.2 *Knowledge requirements

9.1.3.11.3 *Set-up time

9.1.3.11.4 *Day-to-day support provided

9.1.3.11.5 *Training available in use of model

9.1.3.12 Planned user-orientated developments

9.1.4 Information on verification

This section of the questionnaire is associated with requesting information to demonstrate that the mathematical model being used has been accurately translated into computer code. This can be most practically demonstrated by:

- Comparing the model against:
  - Analytical solutions, relevant published correlations, other well-established models.
- Showing the accuracy of conservation relations, or

Additional issues to be addressed when completing this section of the questionnaire include:

- Has verification been applied to any internal databases utilised?
  - Verification of each database used is required to show that it has been accurately constructed.
  - It must be demonstrated that the information in any database utilised is being correctly used by the model.
- Have quality assurance procedures been adopted?
  - May be internal or from a more independent source.
  - Can a quality assurance statement be provided from the developer?

Information about how each of these issues has been addressed should be entered here, ideally using appropriate, cross-referenced documentation which describes the verification and quality assurance activities followed.

9.1.5 Information on sensitivity

This section of the questionnaire is associated with requesting information on previous sensitivity studies:

- Have any sensitivity studies been performed?
  - Have the results been documented?
  - How have changes to model parameters affected the output?

9.1.6 Information on validation

This section of the questionnaire is associated with requesting information on previous validation work:

- What validation work has been performed on the model in the past?
- Has the model been validated against experiments?
  - What experiments? (List these and provide references)
  - Do experiments cover a wide range/spread of phenomena (validation range)?
  - How/what data has been compared in these experiments?

These issues should be addressed using appropriate documentation describing any validation or sensitivity studies performed. Any supporting documentation must be appropriately cross-referenced.

If such studies were undertaken on a previous or different version of the model, then they should also be included here, however this should be noted and any differences between the models appropriately documented.

9.1.7 Administrative details

Following the completion of the questionnaire, contributor(s) should enter their details below. The principal contributor should enter their details first, followed by the next most significant contributor (if they exist) and so forth:

Name:

Organisation:

Position:

Status of organisation: Developer/Licensee/User/other_____________________________

Date:

Name:

Organisation:

Position:

Status of organisation: Developer/Licensee/User/other_____________________________

Date:

Name:

Organisation:

Position:

Status of organisation: Developer/Licensee/User/other_____________________________

Date:

Name:

Organisation:

Position:

Status of organisation: Developer/Licensee/User/other_____________________________

Date:

9.1.8 Guidance on completing the questionnaire

NB: In this guidance a number of suggestions on what information to supply to complete the questionnaire are provided in bullet points. These bullet point lists ***should not*** be considered as exhaustive, the information provider should add additional information if and where they see fit.

9.1.8.1 General information

9.1.8.1.1 *Name of model

Expand on any acronyms used in the name.

9.1.8.1.2 *Model version (as per cover sheet) and date

Give the number of the reference version under consideration. This is the only version of the model under evaluation. The date of the release of this version must also be included.

9.1.8.1.3 *Year of original model origin and of the version under evaluation

Give the year in which the model ***first*** became available.

Give the year in which the ***current*** version (under evaluation) became available.

9.1.8.1.4 *Heredity of the model

Briefly describe any historical relation to other models that exists (complete with N/A if not applicable).

- Model ancestors?

9.1.8.1.5 *Model developer(s) contact information

Give: name, work address, telephone number (fax number), and e-mail address of a contact associated with the model developer.

9.1.8.1.6 *Short description of the model

Appropriate information to provide may include:

- General type – empirical, integral, CFD (RANS/LES/DNS)
- Scenarios to which it may be applied – releases and dispersion, ignition, fire, deflagration, DDT, detonation, etc…
- Computer platform used (hardware, operating system)
- Output produced (what variables, resolution), etc…

(Please aim for no more than 100 words)

9.1.8.1.7 *Short description of the areas of application of the model

Appropriate information to provide may include:

- 1D/2D/3D
- Compressible and/or incompressible
- Laminar/turbulent/transitional

- Source characteristics
- Types of environment – indoors, outdoors, wind effects, obstacles, etc…
- Ignition sources, etc…

(Please aim for no more than 100 words)

9.1.8.1.8 *List of relevant supplied documents

- This list must include ***all documents*** referred to during the completion of the questionnaire.
- The numbering must match that of the copies supplied.
  - The filename of the documents should be changed in order to match the number of the list provided in this section.
  - The most dominant reference should be at the start of the list:
    - E.g. of filename format - 1_filename_CD.doc/pdf
    - See below for definition of 'CD'

Suggested format to follow when providing details of references:

1. Number of reference: No. 1 (most prominent reference), 2, 3, 4, 5…
2. Reference (using a consistent format)
3. CD/CI/U – Please add a note to indicate what documents / information must remain confidential (if any)
4. Outline scope – Describes the content of the document and also lists the questionnaire headings/number which the reference addresses and is relevant to.

If the information supplier wishes the documents / information supplied to remain confidential, this should be indicated in both the filename and in the suggested format.

- CD = Document confidential
- CI = Information confidential
- U = Not confidential (universal)

9.1.8.2 Information for scientific assessment

The information provided in this section of the questionnaire should include, where appropriate, statements and documentation referring to any assumptions that have been made to define a given aspect of the model.

9.1.8.2.1 Physical problems addressed by the model

Provide information regarding the capabilities of the model, for example:

- How does the model handle time dependent variables?
- Specification of the environment:
  - Frame of reference, atmosphere, turbulence, terrain, obstacles, etc…
- How are boundary layers modelled?
- How are source terms handled?
- Can the model recalculate source terms?

This information will vary depending on whether a release and dispersion, ignition, fires, deflagration or detonation model is under consideration.

9.1.8.2.2 Physical processes modelled

Provide information on the physical processes that are taken into account by the model. How have these processes been simplified, approximated or modified?

Such processes to be considered are:

- Fluid dynamics and mass transfer
  - Turbulence, diffusion, permeation, dispersion, impingement, interaction with obstacles, ventilation, reflection, etc…
- Mass transfer mechanisms
- Chemistry
  - Composition, reactions, etc…
- Thermodynamics,
  - What data are calculated by the thermodynamics model?
  - Heat transfer, sources of heat gain/loss, hot surfaces, etc…
  - Correlations for thermodynamics properties – perfect gas law, etc…

9.1.8.2.3 Mathematical formulation of the problem

Provide information on how the mathematical problem is formulated.

Information to be provided includes:

- Governing equations used/how are they set-up?
- Dependent and independent variables
- Boundary conditions specified
- Approximations made to the equations
- Final equation set solved
- Initial conditions specified
- Particularities of the different models involved in this study: releases and dispersion, ignition, fire, deflagration, DDT, detonation, etc…

9.1.8.2.4 Solution method

Provide information on how the mathematical problem is solved by the model.

Examples of appropriate points to consider include:

- What numerical methods are employed by the model?
- Discretisation methods
- Computational grids available (structured, unstructured, Tet, Hex, Poly…)
- Turbulence modelling – what turbulence models are available?
- How is accuracy of the solution achieved?
  - What is the time step value?
  - Modelling assumptions
  - Refinement / convergence study?
- Are there further steps required to process the solution?
  - Scaling?
  - Transformations?

9.1.8.2.5 What output variables are available from the model?

Provide information on what outputs (directly or indirectly) are available from the model. Points to consider include:

- Steady or time-varying situations
- Directly – dependent variables of the governing equations
- Indirectly – variables derived from the primary variables
- Point-wise, derived or fluctuating data?
- Are solutions averaged? How are averaged variables dealt with/incorporated into subsequent calculations?
- How can computed variables be compared to measurable quantities?

9.1.8.2.6 *Planned scientific developments

List any known scientific developments which are planned to be added to the model.

- What are the major items for further work?

9.1.8.3 Information for user-orientated assessment

9.1.8.3.1 Computer environment

9.1.8.3.1.1 *Hardware

List the hardware platform(s) on which the model runs

9.1.8.3.1.2 *Operating system(s)

List the operating systems supported on each of the hardware platform(s) listed in Section 9.1.3.1.1.

9.1.8.3.1.3 *Auxiliary software

List any additional software required in order to run the model

9.1.8.3.1.4 *Programming language(s)

List the programming language(s) used to write the computer code

9.1.8.3.2 Installation procedure

Describe the installation procedure that must be followed in order to install the model on a particular platform (i.e. on those listed in Section 9.1.3.1.2 and Section 9.1.3.1.3). If this procedure is outlined in an 'installation manual' or 'user manual', a reference to such documentation (if it exists) should be provided.

9.1.8.3.3 User interface

Describe how the model is used. If this information is detailed in a pre-existing 'user manual' or another document, providing a reference is sufficient.

- Comment on the user interface: Interactive, graphical, textual, etc…

9.1.8.3.4 Internal databases

If any databases are used in conjunction with the model, information on their content should be provided. This may include information such as properties of hydrogen, correlations utilised such as laminar burning velocity, adiabatic flame temperature, expansion ratio, etc…

- Material properties, can these databases be modified by expert users?

9.1.8.3.5 Inputting data

9.1.8.3.5.1 Entering given input data

Provide information on how the user interface is operated, in order to provide input and initial data to the model. If this information is appropriately detailed in a pre-existing 'user manual' providing a reference to this documentation is sufficient.

9.1.8.3.5.2 Guidance for selecting input data

Points to consider include:

- Does the model provide the user with any guidance on appropriate input data?

- Is the user requested to provide particular input data?
- Is appropriate input data recommended?
- Is appropriate information to guide the user provided in the ‘user manual’?

9.1.8.3.5.3 Automatic check on data validity

Points to consider include:

- Are there any checks carried out by the model on the data being input?
- Are range limits provided when choosing what data to input?
  - Sensitivity to inputs
  - What happens if data outside this range is entered?
- Is there a particular range of applicability for the model?

9.1.8.3.6 Running the model

9.1.8.3.6.1 *Modes for running the model

List the modes which are available for running the model: batch, interactive, bot

- Batch mode – run a group of commands
- Interactive mode – one at a time

9.1.8.3.6.2 Error messages

- Are there any error messages built into the model?
- Are these error message described in the user manual?
- Are they produced at the setting up stage and/or during running?

9.1.8.3.7 Output from the model

9.1.8.3.7.1 Types and formats of output displayed

- What variables are outputs from the model?
- How are they displayed?
- What format are they displayed in? Tabular / graphical / contour plots
- Can the output be easily imported, e.g. to MS Excel?

9.1.8.3.7.2 *Identification, organisation and accessibility of output from runs

- Can the output files produced be given identifiable/customisable names?
- How are case-runs organised?
- How can previous cases be accessed?
- Can case runs be easily compared?

9.1.8.3.7.3 Hard copy facilities

- Does the user have control over how often output files are produced?

9.1.8.3.8 Interfacing to other models and software

9.1.8.3.8.1 *Part of program suite?

- Is the model under consideration one of several models linked together or is it a standalone model?
- Is it self-contained?
- Can the model be used as one part of a suite?
- Is it inextricably bound to other models?

9.1.8.3.8.2 *Interfacing with software tools

- What other types of software tools can the model be interfaced with?

9.1.8.3.8.3 *Source models

- What source term models are available?
- Are they incorporated with or interfaced to the model under consideration?

9.1.8.3.8.4 *Other models

- What other models are available?
- Are they incorporated with or interfaced to the model under consideration?

9.1.8.3.8.5 *Customisation of software

- Is customisation possible? Addition of subroutines, additional calculations, development of sub-models, etc…

9.1.8.3.9 Status and availability of the model

9.1.8.3.9.1 *Maturity of the model

- Is the model a mature and tested technology?
- Is it used as a research tool?

9.1.8.3.9.2 *Availability of the model

- Is the model commercially available or only for ‘in-house’ use?
- Are there any specific/additional boundary conditions, sub-models etc… that need to also be supplied for the model to be used?

9.1.8.3.9.3 *Peer review of the model

- Has the model received any public exposure?
    - International conferences, workshops, seminars, etc…

9.1.8.3.9.4 *Options for acquisition

- Is the model free of charge? E.g. open source
- Licensed? (perpetual, time-limited or otherwise)
- Available for outright purchase?
- Not available? Proprietary?

9.1.8.3.9.5 *Contact information for obtaining model (if available)

Provide necessary contact details required to obtain the model.

9.1.8.3.10 Resources

Both financial and computational cost of running the model

9.1.8.3.10.1 *Financial cost of model (if applicable)

Indicate the order-of-magnitude (or cost at time of writing) of any options, as described in Section 9.1.3.9.4 incurred financially, for the model to be used.

9.1.8.3.10.2 *Order of magnitude of run time on specified platform and for specified problem

Provide an estimation of the typical run time required (indicate the specification of the machine on which the model was run on).

- Seconds / minutes / hours / days / weeks

9.1.8.3.11 Users

9.1.8.3.11.1 *Current users

- Enter the number of users
- Enter user distribution – USA, UK, Europe, Worldwide
- Background of the users – Engineer, Researcher, Developer, Consultant, Regulator, etc…
- Frequency of user – occasional, constant

9.1.8.3.11.2 *Knowledge requirements

Provide information of the type of experience of the users:

- Dispersion, fluid dynamics, thermodynamics, chemistry, mathematics, statistical methods, numerical methods, programming, risk analysis, consequence modelling, etc…

9.1.8.3.11.3 *Set-up time

Give an approximate time period required by a user to set up, run and if necessary indicate whether it is necessary to monitor the model during computation.

Give an indication of total time period from start to finish (including setup) for a typical scenario.

9.1.8.3.11.4 *Day-to-day support provided

Provide information on what assistance provisions are in place on a day-to-day basis:

- Telephone help desk
- Web-based support – website, frequently asked questions, user-forums
- Direct contact with developer
- Technical support
- Available documentation
- Is there an associated cost with any of these support options?

9.1.8.3.11.5 *Training available in use of model

- Is there any specific training available on the use of the model?

9.1.8.3.12 Planned user-orientated developments

List any further user-orientated developments of the model that are being planned by the model developer.

9.2 Appendix 2: Validation database: overview of experiments

The lists below include only some examples of the experiments which are available in the validation database. The complete and updated sets of experiments can be found in the database websites.

9.2.1 DDT experiments (KIT)

Table 9.1. Deflagration to detonation transition experiments contained in the model validation database.

id	Experiment name	Short description
17	FIKE Experiment	Explosion experiments with hydrogen in straight pipes of 3 different diameters (all with L/D = 98) were carried out, for the 6"/15 m pipe, 6 different gas concentrations were applied.
18	FZK-R 049809	Combustion experiments have been carried out in an obstructed tube of 350 mm diameter and 12 m in length. Repeatable obstacles with blockage ratio BR=0.3 at distances 500 mm. Hydrogen-air mixture with H2 concentration of 15% by volume was tested.
39	MiniRUT	Processes of fast deflagration and DDT were studied in an obstructed channel and in a chamber called MiniRUT using high-speed shadow photography, pressure transducers, and photodiodes. A regime of DDT was observed in the channel, which showed detonation origin in a zone between the lead shock and turbulent flame brush of propagating fast deflagration. Detonation onset in the chamber resulted either from Mach reflection of lead shocks, or shock focusing in a corner. Critical mixture compositions for onset of detonations were determined. The detonation cell size was confirmed as a reliable scaling parameter for characterization of detonation onset conditions.
42	GRS029	This DDT experiment was carried out in a semi confined volume of size 9x3x0.3m, inside the facility repeating 53% block ratio obstacles were installed for the flame acceleration. The experiment facility was filled with 23% hydrogen-air mixture, and the burnable gas was ignited by a 2m flame tube.
43	GRS037	This DDT experiment was carried out in a semi confined volume of size 9x3x0.6m, inside the facility repeating 50% block ratio obstacles are installed for the flame acceleration. The experiment facility was filled with 22% hydrogen-air mixture, and the burnable gas was ignited by a 2m flame tube.

44	GRS056	This DDT experiment was carried out in a semi confined volume of size 9x3x0.6m, inside the facility repeating 50% block ratio obstacles are installed for the flame acceleration. The experiment facility was filled with gradient hydrogen-air mixture (at the top the concentration of hydrogen is 21.8% and the concentration decreases by 0.3% per cm), and the burnable gas was ignited by a 2m flame tube.
45	GRS057	This DDT experiment was carried out in a semi confined volume with size of 9x3x0.6m, inside the facility repeating 50% block ratio obstacles are installed for the flame acceleration. The experiment facility was filled with gradient hydrogen-air mixture (at the top the concentration of hydrogen is 15.6% and the concentration decreases by 0.2% per cm), and the burnable gas was ignited by a 2m flame tube.

9.2.2 Deflagration experiments (UU)

Table 9.2. Deflagration experiments contained in the model validation database.

id	Experimental name	Short description
5	HYKA A2 experimental facility	A homogeneous mixture of hydrogen (10 vol.%), steam (25 vol.%) and air was formed in the vessel. The initial pressure was 1.49 bar, and the average initial temperature was about 90 ^{o}C. The mixture was ignited at the bottom of the vessel and the consequent flame propagation in axial and radial directions was observed. Pressure and temperature were measured at different locations.
6	HYCOM-HYC 14	Combustion experiment was carried out in a large scale multi-compartment geometry consisted of a curved channel and a canyon. Four obstacles with blockage ratio BR=0.3 were installed in the channel. The canyon was divided into four separate rooms connected by orifices. Uniform hydrogen-air mixture of 11.5 vol.% was tested.
8	HYCOM-HYC 01	Combustion experiment was carried out in a large scale multi-compartment geometry consisted of a curved channel and a canyon. Four obstacles with blockage ratio BR=0.3 were installed in the channel. The canyon was divided into four separate rooms connected by orifices. Uniform hydrogen-air mixture of 10 vol. % was tested.
9	HYCOM-HYC 12	Combustion experiment was carried out in a large scale multi-compartment geometry consisted of a curved channel and a canyon. Four obstacles with blockage ratio BR=0.3 were installed in the channel. The canyon was divided into four separate rooms connected by orifices. Uniform hydrogen-air mixture of 11.5 vol.% was tested.
10	HYCOM-HC 020	Combustion experiment was carried out in obstructed tube of 12.4 m length combined of two parts with diameter of 174 mm and 520 mm respectively. Uniform hydrogen-air mixture of 10 vol.% was tested.
12	HYCOM-MC 012	Combustion experiment was carried out in obstructed tube of 174 mm diameter and of 12.2 m length (DRIVER facility). Repeatable obstacles with blockage ratio BR=0.6 were placed at distances equal to diameter. Uniform hydrogen-air mixture of 13 vol.% was tested.
13	HYCOM-MC 003	Combustion experiment was carried out in obstructed tube of 174 mm diameter and of 12.2 m length (DRIVER facility). Repeatable obstacles with blockage ratio BR=0.6 were placed at distances equal to diameter. Uniform hydrogen-air mixture of 10 vol.% was tested.
14	HYCOM-MC 043	Combustion experiment was carried out in obstructed tube of 174 mm diameter and of 12.2 m length. Repeatable obstacles were placed at

		distances equal to diameter. The experimental tube was divided in two equal parts by thin polyethylene membrane with different blockage ratios and hydrogen concentrations.
15	Combustion experiments carried out in obstructed tube	Repeatable obstacles with 2 different blockage ratios at distances equal to diameter were installed. Two typical hydrogen-air mixtures with concentrations of 10 vol.% (for subsonic deflagration) and 13 vol.% (for sonic deflagration) were tested in a tube with different end venting. Ignition was at various distances from the open end of a tube.
16	Kumar 1983	Deflagration of 29.5 vol.% hydrogen-air quiescent mixture in the 6.37 m3 closed spherical vessel (diameter 2.3 m). Central point ignition source. Initial temperature 373 K, initial pressure 97 kPa.
19	Vented hydrogen explosions in a channel	Vented hydrogen explosions in a channel without or with 2 baffles; ignition centrally at the closed end; concentration variation provided for the empty channel.
20	Mock-up of a Hydrogen Refuelling Station	Mock-up Hydrogen Refuelling Station, including a brick wall, two dispensers and simplified steel structure representing a vehicle, was used. Polythene film was wrapped around the rig, which is then filled with a homogeneous stoichiometric hydrogen-air mixture. The ignition source is spark plug generating ignition energy of ca. 50 mJ.
25	HIWP3-28_29_30	Hydrogen combustion experiments were performed in 1 m3 facility. In the experiments, 18 vol.% hydrogen-air mixtures was prepared in the chamber, ignition points were installed on the rear plate and 50cmX50cm venting was made in the front plate of the cubic test facility.
30	Open Atmosphere Deflagration	Deflagration of large-scale (initial radius 10 m) hemispherical stoichiometric hydrogen-air mixture in open atmosphere ignited at the centre of hemisphere.
52	Blast wave and fireball generated by hydrogen fuel tank rupture during fire exposure	The effects of catastrophic failure of a 5.000-psig Type-IV hydrogen cylinder. The cylinder was filled at 34.5-MPa (1.64 kg) of hydrogen, 84 cm long, 41 cm diameter, with an inner volume of 72.4 L. The cylinder was placed over a propane bonfire source of 370 kW exposure. The cylinder was exposed to the fire for 6 min 27 sec when it lost its integrity and failed catastrophically.
46-51	Large scale (64 m3), lean hydrogen-air, vented deflagration	Uniform 18% vol. hydrogen-air mixture. 64 m3 test chamber. Back wall ignition. Wall mounted with different venting.

9.2.3 Detonation experiments (KIT)

Table 9.3. Detonation experiments contained in the model validation database.

id	Experimental name	Short description
21	Open environment detonation	Detonation of 29.05 vol.% hydrogen-air quiescent mixture in the 53 m3 hemispherical balloon (diameter 2.93 m). Central point ignition source.
22	KI-RUT Hyd 05	Detonation experiments were carried out in large scale confined complex geometry (263 m3). Uniform hydrogen-air mixture of 20 vol.% was tested. Ignition was at location (A).
27	KI-RUT Hyd 09	Detonation experiments were carried out in large scale confined complex geometry (263 m3). Uniform hydrogen-air mixture of 25.5 vol.% was tested. Ignition was in the channel at location (B).

9.2.4 Release and distribution of gaseous and liquid hydrogen tests (NCSRD)

Table 9.4. Release and dispersion of **gaseous** hydrogen experiments contained in the model validation database.

id	Experimental name	Short description
28	GAMELAN-300Nl-pipe20mm-ventA	Helium release experiments carried out at CEA in an enclosure with dimensions HxWxL=1.26x0.93x0.93 m with one vent located on a wall. The release was directed vertically upward from a pipe with internal diameter 20 mm located 21 cm above the centre of the floor.
29	HYSAFE_SBEP_V21	The GARAGE facility is representative of a realistic single vehicle private garage. The GARAGE facility is situated indoors to attenuate the variations in meteorological conditions. The internal volume of GARAGE is 40.92 m3. Continuous injection of helium is installed in this big volume GARAGE.
31	GAMELAN-180NL-pipe5mm-VentB	Helium release experiments carried out at CEA in an enclosure with dimensions HxWxL=1.26x0.93x0.93 m with one vent located on a wall. The release was directed vertically upward from a pipe with internal diameter 5 mm located 21 cm above the centre of the floor.
32	GEXCON	The experimental rig consists of a 1.20 m x 0.20 m x 0.90 m vessel, divided into compartments by the use of 4 baffle plates with dimensions 0.30 m x 0.20 m. There is one vent opening at the wall opposite the release location centrally located. Different installations of the plates and nozzle diameters are used in the test.
33	INERIS-6C	The experiment INERIS-TEST-6C, performed within the InsHyde project by INERIS, consisting of a 1 g/s vertical hydrogen release for 240 s from an orifice of 20mm diameter into a rectangular room (garage) of dimensions 3.78 X 7.2 X 2.88m in width, length and height respectively. Two small openings at the bottom of the front side of the room assured constant pressure conditions.
35	SBEP_1_WP8	A subsonic release of hydrogen in a closed vessel with height 5.5 m, diameter 2.2 m and volume 20 m3. Hydrogen concentrations are detected by 6 sensors installed at the central line of the vessel.
36	SWAIN_GARAGE	The experimental facility represents a full-scale single car garage with dimensions 6.4 X 3.7 X 2.8 m and two vents on the door. Vent openings with varying height were examined. A full-scale plywood model vehicle was placed inside the garage. The helium flow rate was 7200 l/h and the release lasted 2 h.

37	SWAIN_HALLWAY	In the vented hallway experiment, the hydrogen leaks from the floor at the left end of a hallway with the dimension of 2.9 m × 0.74 m ×1.22 m. At the right end of the hallway, there are a roof vent and a lower door vent for the gas ventilation. The hydrogen leak is at 2 SCFM (Standard Cubic Feet per Minute) and for a period of 20 minutes.
23	Release 1	Hydrogen distribution tests in horizontal free turbulent jet have been carried out in a compartment with an internal volume of 160 m3. Experimental facility consisted of high pressure gas system to provide hydrogen release at pressures in the range 20 – 260 bar through the nozzle. Experiments were made in order to evaluate amount of burnable hydrogen – air mixture (above the lower flammability limit) in free turbulent jet at different pressures.
24	Release 2	A set of experiments involving horizontal high-pressure hydrogen jet releases was conducted at HSL. Different release pressures and nozzle diameters were used.
86-92	Pressure peaking phenomena KIT HIWP4-001-006, 040	The series of experiments were performed to investigate and confirm the pressure peaking phenomena (PPP), discovered earlier analytically. Helium, hydrogen and air releases: 0.1-1.086 g/s in KIT enclosure of 1x1x1 m, vent: 1-3 cm^2.
95	HSL-Test 5	LH2 (liquid hydrogen) is released horizontally along ground through a 26.6 mm orifice. The ground is concrete. The spill rate is 60lt/min and the spill duration is 248 sec. Average wind speed at 2.5 m height is about 2.7 m/s and average wind direction is in line with the release.
96	HSL-Test 6	LH2 (liquid hydrogen) is released vertically 100 mm above the ground through a 26.6 mm orifice. The ground is concrete. The spill rate is 60lt/min and the spill duration is 556 sec. Average wind speed at 2.5 m height is 3.35 m/s and average wind direction is in line with the release.
98	HSL-Test 7	LH2 (liquid hydrogen) is released horizontally 860 mm above the ground through a 26.6 mm orifice. The ground is concrete. The spill rate is 60lt/min and the spill duration is 305 sec. Average wind speed at 2.5 m height is about 3 m/s and average wind direction is in line with the release.
99	GAMELAN-60Nl-pipe20mm-ventA	Validation experiments were carried out at CEA in the enclosure with sizes HxWxL=1.26x0.93x0.93 m with one vent located on a wall. The release of helium was directed vertically upwards from a pipe with internal diameter 20 mm located 21 cm above the centre of the floor.

100	GAMELAN-60Nl-pipe20mm-ventB	Validation experiments were carried out at CEA in the enclosure with sizes HxWxL=1.26x0.93x0.93 m with one vent located on a wall. The release of helium was directed vertically upwards from a pipe with internal diameter 20 mm located 21 cm above the centre of the floor.
101	GAMELAN-60Nl-pipe20mm-ventC	Validation experiments were carried out at CEA in the enclosure with sizes HxWxL=1.26x0.93x0.93 m with one vent located on a wall. The release of helium was directed vertically upwards from a pipe with internal diameter 20 mm located 21 cm above the centre of the floor.
103	GEXCON_27	The experimental rig consists of a 1.20 m x 0.20 m x 0.90 m vessel, divided into compartments by use of 4 baffle plates with dimensions 0.30 m x 0.20 m. There is one vent opening at the wall opposite the release location centrally located.
104	GEXCON_58	The experimental rig consists of a 1.20 m x 0.20 m x 0.90 m vessel, divided into compartments by use of 4 baffle plates with dimensions 0.30 m x 0.20 m. There is one vent opening at the wall opposite the release location centrally located.

Table 9.5. Release and dispersion of **liquid** hydrogen experiments contained in the model validation database.

id	Experimental name	Short description
A	Arthur D, Little Inc. Final report on an investigation of hazards associated with the storage and handling of liquid hydrogen. Report C-61092, Cambridge, USA; 1960	Spill experiments with L_{H2} quantities ranging between 5 l and 19m^3 (description from Verfondern 2007).
B	Witcofski, R.D., and Chirivella, J.E., Experimental and analytical analyses of the mechanisms governing the dispersion of flammable clouds formed by liquid hydrogen spill, Int. J. Hydrogen Energy, 9, No. 5, 1984, pp. 425-435. Witcofski, R.D dispersion of flammable clouds resulting from large spills of liquid hydrogen NASA technical memorandum 83131 May 1981 Chirivella, J.E., and Witcofski, R.D., Experimental results from fast 1500 gallon LH2 spills, Am. Inst. Chem. Eng. Symp. 82, No. 251, pp. 120-140, 1986.	Usually they are identified as the NASA experiments. Ground spills of L_{H2}. Experiments were simulated by Demokritos, Ulster Univ., Sklavounos. ONE EXPERIMENT IS ALREADY IN THE VALIDATION DATABASE
C	Schmidtchen, U., Marinescu-Pasoi, L., Verfondern, K., Nickel, V., Sturm, B., Dienhart, B., Simulation of accidental spills of cryogenic hydrogen in a residential area, Cryogenics 0883:23: (ICEC Suppl) 401-404, 1994. No data in this paper. Verfondern, K., Dienhart, B., Experimental and Theoretical Investigation of Liquid Hydrogen Pool Spreading and Vaporization, Int. J. Hydrogen Energy, 22, No. 7, 1997, pp. 649-660. Dienhart, B., Ausbreitung und Verdampfung von flüssigem Wasserstoff auf Wasser und festem Untergrund, Research Center Juelich Report No. Juel-3155, 1995. (KIWI test facility at the FZJ with LN2)	Series of L_{H2} spill experiments were conducted to investigate in detail pool spreading and vaporization on a liquid (water) and solid (aluminum) ground. (FZJ) Experiments were simulated in the last paper (2007)

	Verfondern, K., Dienhart, B., Pool spreading and vaporization of liquid hydrogen, International journal of hydrogen energy 32, 2007, 2106–2117.	
D	Nakamichi, K., Kihara, Y., Okamura, T., Observation of liquid hydrogen jet on flashing and evaporation characteristics. Cryogenics 48, 2008, 26–30.	The evaporation speed of liquid hydrogen jet were measured using high speed CCD camera
E	Proust, Ch., Lacome, J.M., Jamon, D., Perrette L., Process of the formation of large unconfined clouds following a massive spillage of liquid hydrogen on the ground, 2nd International Conference on Hydrogen Safety, San Sebastian, Spain, Sept. 11-13, 2007.	INERIS Because of safety reasons, liquid helium was used as replacement for liquid hydrogen. Maximum flow rate 1.5 and 2.1 kg/s.
F	Royle, M., Willoughby, D., The safety of the future hydrogen economy, Process Safety and Environmental Protection 89, 2011, 452–462 Hooker, P., Willoughby, D.B., Royle, M., Experimental releases of liquid hydrogen, 4th International Conference on Hydrogen Safety. September 12-14, 2011, San Francisco, CA, USA. HSL report "Releases of unignited liquid hydrogen RR986" HSL report " Ignited releases of liquid hydrogen RR987"	The work plan involved releasing liquid hydrogen at a fixed rate of 60 l/min for differing durations. This flow rate represents a release from the tanker pressurised at 1 bar, chosen to provide optimum pool spill conditions simulating a catastrophic failure of a filling hose. - Concentration of hydrogen in air, thermal gradient in the concrete substrate, liquid pool formation, and temperatures within the pool - Flame velocity within the cloud, thermal radiation, IR and visible spectrum video records. - Sound pressure measurements - An estimation of the extent of the flammable cloud was made from visual observation, video, IR camera footage and use of a variable position ignition source RR986: experiments performed to investigate spills of unignited liquid hydrogen at a rate of 60 litres per minute. Concentration of hydrogen in air, thermal gradient in the concrete substrate, liquid pool formation and temperatures within the pool were measured and assessed. RR987: hazards and severity of a realistic ignited spill of L_{H2} focussing on; flammability limits of an L_{H2} vapour cloud, flame speeds through an L_{H2} vapour cloud and subsequent radiative heat and

		overpressures after ignition.
G	Friedrich, A., Breitung, W., Stern, G., Veser, A., Kuznetsov, M., Fast, G., Oechsler, B., Kotchourko, N., Jordan, T., Travis, J.R., Ignition and heat radiation of cryogenic hydrogen jets, International Journal of Hydrogen Energy. 37, 2012, 17589-17598.	Release and ignition experiments with horizontal cryogenic hydrogen jets at temperatures of 35-65 K and pressures from 0.7 to 3.5 MPa were performed in the ICESAFE facility at KIT. In distribution experiments the temperature, velocity, turbulence and concentration distribution of hydrogen with different circular nozzle diameters and reservoir conditions was investigated for releases into stagnant ambient air. Subsequent combustion experiments of hydrogen jets included investigations on the stability of the flame and its propagation behaviour as function of the ignition position. Furthermore combustion pressures and heat radiation from the sonic jet flame during the combustion process were measured. Safety distances were evaluated. Note: hydrogen is liquid in the reservoir but it is not clear if at the exit the fluid is still liquid or cryogenic gas or a combination of both.

9.2.5 Ignition and fire experiments (UU)

Table 9.6. Ignition and fires experiments contained in the model validation database.

id	Experimental name	Short description
38	Auto Ignition in mock PRD	In order to investigate the spontaneous ignition of hydrogen, the pressurized tube with a T-shaped pressure relief devices were used. In the experiment, the tube was filled with different pressures to investigate the relation between the storage pressure and ignition.
53-63	Indoor jet fire dynamics HSL experiments WP4/1-WP4/12	These experiments have been carried out to investigate the behaviour of hydrogen jet fires within enclosures fitted with passive ventilation. Regimes investigated: well-ventilated and under-ventilated; Release types: subsonic and choked; Flow rates: 149-891 Nl/min; Orifice size: 0.55-10 mm; Vent configuration:1 upper vent, 1 upper and 1 lower, 2 upper and 1 lower, 3 upper and 1 lower, 25-50% 1 upper.
64-85	Indoor jet fire dynamics KIT experiments KIT HIWP4	The main focus in the experiments lies on conditions that lead to quenching of an ignited jet in an enclosure due to the reduction of the oxygen concentration during the combustion. Regimes investigated: well-ventilated and under-ventilated (self-extinction, re-ignition, external flame); Release type: subsonic; Flow rates: 0.1086-1.086 g/s; Orifice size: 5 mm; Vent configuration: upper horizontal, lower horizontal, upper vertical, 1 upper and 1 lower horizontal.

9.3 Appendix 3: Statistical Performance Measures

Figure 5 and Figure 6 show the graphical representation of four Statistical Performance Measures (SPMs) mentioned in section 5.3 and 5.4 for single values only. These graphs give visual illustration of how “good” or “bad” could be the performance of the particular model in terms of under-prediction or over-prediction.

MG and VG are defined as follows:

$$MG = exp\overline{\left(ln\left(\frac{C_o}{C_p}\right)\right)} \tag{1}$$

$$VG = exp\overline{\left(\left[ln\left(\frac{C_o}{C_p}\right)\right]^2\right)} \tag{2}$$

A perfect model would result in MG and VG of 1.

The MG varies between 0 and ∞, where the optimum value is 1. Values smaller than 1 indicating over-prediction by the model, and values larger than 1 under-prediction.

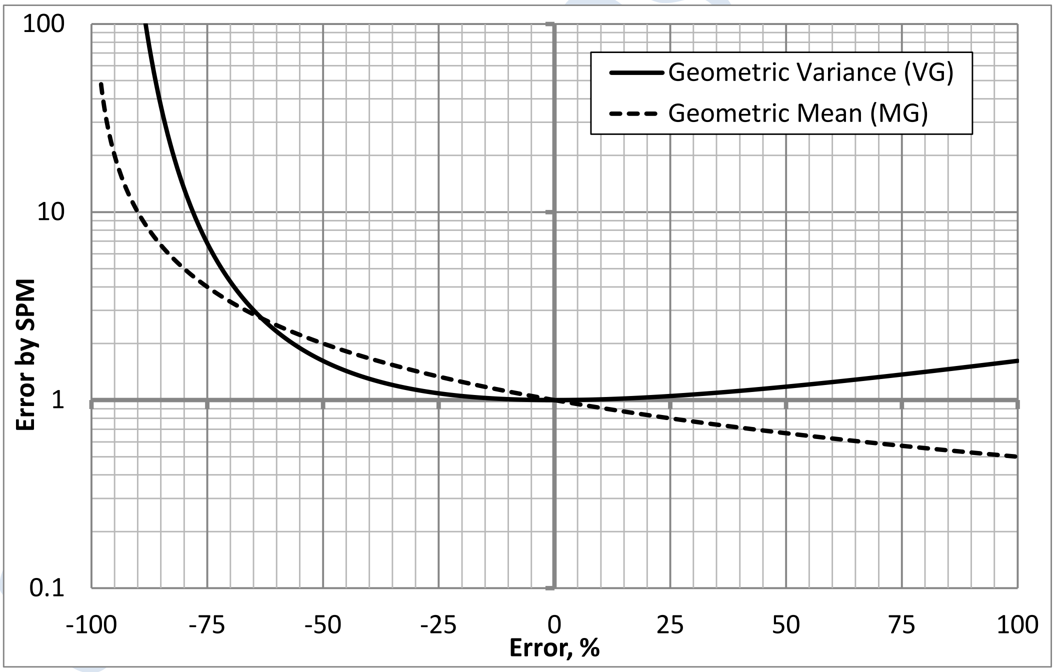

Figure 5. Geometric Mean (MG) and Geometric Variance (VG) for under and over-prediction.

MRB is based upon the difference between observed (C_o) and predicted (C_p) values, but to meet the requirement for equal weight given to all observed/predicted pairs, the values are normalised by the average of the two:

$$MRB = \overline{\left(2\frac{(C_o - C_p)}{(C_p + C_o)}\right)} \tag{3}$$

Where the overbar denotes an average over all the observed/predicted pairs. MRB gives an indication of a model's ability to predict the measured values on average, and its sign indicates whether the model is under- or over-predicting. A perfect model would result in an MRB of 0, but under- and over-predictions cancel each other out and a model may appear to perform well for the wrong reason. Therefore, MRB is paired with MRSE which sums the squares of the errors and therefore gives an indication of the scatter in the predictions:

$$MRSE = \overline{\left(4\frac{(C_o - C_p)^2}{(C_p + C_o)^2}\right)} \tag{4}$$

The MRB ranges from -2 to 2 with the optimal value of 0. Negative value indicates over-prediction and positive under-prediction.

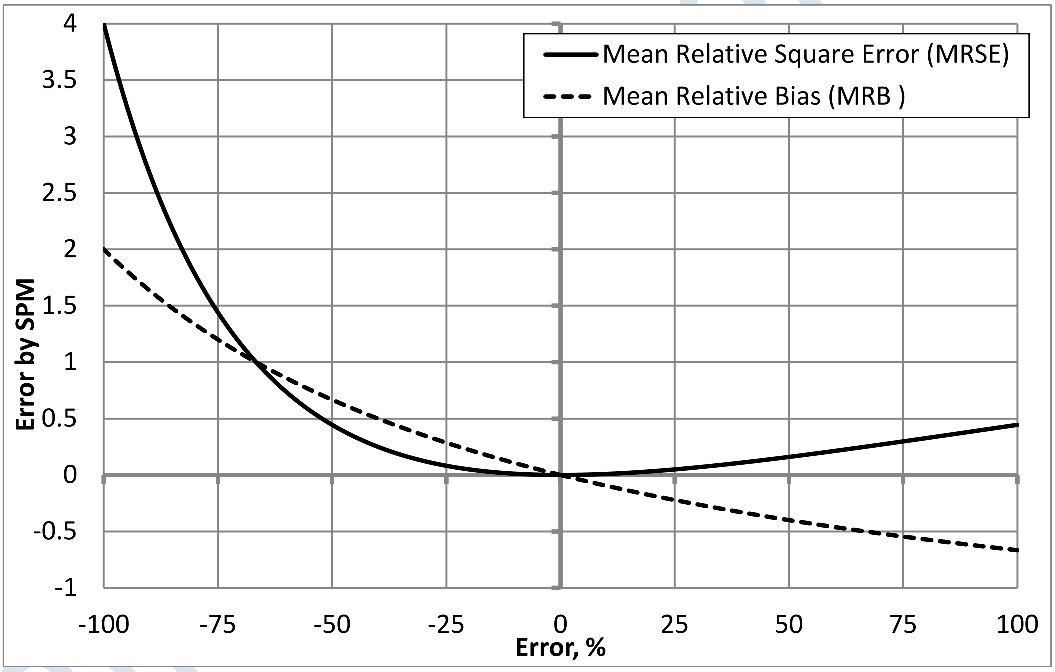

Figure 6. Mean Relative Bias (MRB) and Mean Relative Square Error (MRSE) for under and over-prediction.