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Support to Safety Analysis of Hydrogen and Fuel Cell Technologies

Expert Workshop Athens Report

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

Content

1. Introduction

SUSANA WP7 has two objectives: to gather expert feedback early in the project to ensure that the planned outcomes will be fit for purpose; and to make the project deliverables available to the hydrogen safety and wider community using various dissemination routes. The two main outcomes of this project are the production of a detailed Model Evaluation Protocol and CFD Best Practice Guide that can be used by the FCH community for evaluating and applying CFD models. Consideration therefore needs to be given to ensuring that the outputs are of practical relevance and will be useable by the FCH community. In particular, the users of the protocol may not be experts in CFD and/or model evaluation and so ensuring that the protocol is practical for the intended user is very important.

One of the objectives of WP7 was to organise and host an international workshop to discuss the CFD model evaluation protocol and therefore obtain feedback from the FCH and wider community. IN recognition of the procedures developed by other safety critical industries, invitations were sought from within and outside of the FCH community (for example, Nuclear power). To ensure the relevance of the project, this feedback was therefore sought at an early stage. The workshop aimed to have two distinct themes: the first relevant to the CFD modelling in the FCH community and the second relevant to industrial users. This approach would mean that the quality of the work plan could be assessed and there would be feedback on the relevance of the project output to practical users.

The workshop “Computational Hydrogen Safety” was held in Athens in September 2014 (Figure 1), covering two days of presentations and discussion, which are described in the following Sections.

Figure 1 Attendants at the expert workshop

2. Workshop structure and invitees

To meet the objectives, the workshop was structured around five main themes:

- Introduction
  - Explanation of the project's aims and objectives
- Model Evaluation Protocols
  - Historical perspective on model evaluation
- Best practices in numerical modelling
  - Application of best practice to CFD simulation in FCH applications
- Validation and verification techniques, methodology and databases
  - Current practice in verification and validation methods in CFD
- Industrial and commercial perspective
  - Practical applications and challenges in CFD modelling for safety analyses in FCH

To provide feedback and an objective review of the project activities, a number of experts were identified who would be able to provide input on the above themes and attend and present at the workshop. The initially invited list of experts was selected from a broad range of academia, industry, consultancies and regulators, both in the area of FCH as well as CFD modelling and consequence assessment. The list included representatives from commercial software companies in addition to software users and applications specialists. Experts were drawn from a large number of countries, with one expert attending from the US. The initial contact list is given in Appendix 1. From the initial contact list, the group of eleven experts who participated is given in Table 1.

Table 1 Experts attending the SUSANA Workshop in Athens

Surname	**First Name**	**Institution /company**	**Expertise area**
Graham	Steve	NNL	Steve has experience of modelling of hydrogen and has been involved in developing guidelines for Sellafield. He has also taken part in CFD quality and best practice initiatives in the UK and Europe
Iudicello	Francesca	Xaar	Best practice/ NAFEMS
Prankhul	Middha	gexcon	CFD provider
Scheuerer	Martina	GRS	Nuclear safety
Oberkampf	William	Ex Sandia National Laboratories	Expert in verification processes
Truchot	Benjamin	INERIS	Head of the Unit Dispersion, Fire, Experiment and Modelling, Direction of Accidental Risks
Dimmelmeier	Harald	AREVA	Section Manager "Severe Accidents"PEPA-G Radiological, Severe Accident and Building Analyses

di Sarli	Valeria	Institute of Combustion, CNR	Hydrogen combustion theory, experimental research, and modelling, particularly - hydrogen deflagration modelling.
Puttock	Jonathan	Shell research	Explosion modelling
Wen	Jennifer	University of Warwick	CFD: releases, fires, detonations
Vyazmina	Elena	Air Liquide	CFD, candidate for user group

All arrangements needed to host the workshop and external experts were undertaken by the coordinator. To foster communication and discussion on the general topics of the workshop, all participants (external experts and project partners) were accommodated at the same hotel and the chosen hotel also hosted the workshop. The invited experts participated actively in the workshop with their own presentations on their own work and expertise on validation and verification of codes and models. Presentations were also made by the SUSANA consortium to introduce the project and the various work packages.

Prior to the workshop, the invited experts were asked to complete a questionnaire on the content of the validation database. These comments are included in Appendix 3.

3. Meeting Notes

Meeting notes were taken as a summary of the discussions that followed each of the presentations. The primary objectives with these were to capture attendees experience in their industries and academic area, and the expert response to SUSANA outlined work plan to ensure that this is structured to be relevant and valuable to Hydrogen Safety Practitioners using CFD as a daily computing tool.

3.1 Discussion: Model Evaluation Protocols (MEP)

There was a discussion about improving the confidence of simulation results via sensitivity studies.
It was highlighted that some sensitivities relate to boundary conditions, the correct value of which cannot be determined. An example might be atmospheric/wind conditions, which cannot be determined precisely but which can have a material effect on the outcome of a simulation.

Using the example of applying boundary conditions, Bill Oberkampf (BO) advised that the process should be split into:

- The physics side – i.e. which boundary condition is a "correct" representation of the underlying physics.
- The implementation of that boundary condition; i.e. the numerical implementation of the physics (e.g. for gradients, do you extrapolate, and what order of extrapolation do you use). This is a numerical issue.

Steve Graham also made a similar point, in the context of turbulence modelling, there is a need to distinguish between the choice of an appropriate model (physics) and how it is implemented (numerics).
BO advised that to help users, we should:

- Identify sources of modelling uncertainty.
- Identify what model output variables are of concern, and what factor of safety do we apply to these
- Ensure that when accounting for uncertainty, that the key outputs never lie within the factor of safety described above.

BO said there are areas where there are situations where the complexity of physics is so high that you cannot come up with "reliable" models and therefore would it be possible to come up with system response parameters. In other words, complexity prevents the model from being a realistic representation of reality, and so instead the overall system is treated as a single entity with inputs and outputs (system response parameters). Steve also identified that NAFEMS has guidance on usability but also limitations. The best that you can do is to discourage some errors from occurring.
Benjamin Truchot agreed with this point, that in his organisation the "user error" issue was managed by requiring a comparison of CFD outputs of multiple personnel who have used the same code. This identifies user error not code error but nevertheless this source of error is important. He further encouraged the adoption of a "capable user" i.e. one who is sensible enough to determine appropriate settings of model inputs and review the outputs – this is a key quality control factor.
There was a discussion on "uncertainty estimates" and whether these should be part of the SUSANA MEP. Alex Venetsanos advised that this should not be in the SUSANA documentation; the intention is that it is a CFD model evaluation protocol, not an uncertainty evaluation protocol.

3.2 Discussion: Best Practice in Numerical Modelling

During Martina Scheuerer's presentation, she explained the process of measuring grid independence of a solution using Richardson refinement. It was noted however that this approach cannot be used with adaptive mesh refinement – a formal analysis of grid independence requires the whole grid to be refined.

Vladimir Molkov pointed out that certain models of turbulence are "grid independent" in the sense that they rescale certain model parameters to account for the local grid size. Therefore the question is what value is a grid independence study. BO replied that formal accuracy analysis (which is more focussed on verification that equations are solved accurately rather than validating the use of certain models) the "model" should not change between grid refinements – care needs to be taken in these circumstances. An example would be Large Eddy Simulations, where a model of turbulence is used to represent sub-grid scale eddies.

This generated a more wide ranging discussion on the incorrect use of certain models which are grid dependent. Examples given included wall functions which are often used with inappropriate near wall Y+ grid sizes. With Large Eddy Simulation, grid refinement not only changes the numerical implementation (i.e. more accurately resolved spatial gradients) but also changes the physics being modelled (grid refinement increases the spectrum of turbulence length scales being resolved directly).

3.3 Discussion: Verification and Validation

BO advised that verification test cases should be included in the SUSANA database.

A discussion was had on the Method of Manufactured Solutions, which is a way of producing numerical solutions to complex problems not amenable to analytical solutions. As MMS is able to identify coding errors, it was generally agreed that MMS was the responsibility of code developers rather than practitioners. Steve Graham reflected that the Method of Manufactured Solutions looked very time consuming and even vendors would "run in the opposite direction". The Susana consortium needs to reflect this concern in its outputs.

SG also pointed out that you have to reflect on the input data that is missing i.e. to be aware of material or boundary or initial condition parameters that are estimated rather than known with certainty.

After the presentation on the database by Alexi Kotchourko, there was a discussion on how to structure the validation database (e.g. categories the experiments). Good categorisation is vital to allow 3rd parties to find what they need.
It was noted that data on experimental setup is often limited and sometimes edited out of journal papers. As example, boundary conditions are very important but are often not communicated properly.
BO noted that in the US, there was an attempt to build a well-structured and populated validation database (AIAA?) but that this was very difficult and ultimately not successful.
While a validation database could be organised by physics, BO advised strongly against organising a verification database by this structure. Instead the database should have a set of data files/cases arranged by: analytical solution, numerical solution etc.

The discussion turned to the difference between V&V and calibration. Jonathan Puttock advised that if a validation database is available, and it is used by a practitioner for model calibration purposes then it cannot used by the same person as a validation database. In other words, we need to be clear about the difference between model calibration stages and solution validation.

3.4 Discussion: Industrial and Commercial Perspective

This session focussed on what industrial organisations, involved in CFD simulations on safety critical applications, routinely do to ensure quality standard on their results.

After his presentation Harald Dimmelmeier from Areva noted that what the nuclear regulator wants to see depends on jurisdiction. In Europe, CFD studies are more commonly used as performance based proof of safety, however in the US, the regulator looks for lumped parameter (system response type) models of complete systems. The system response models, being simpler, can be run with a very broad range of inputs and so can provide statistical / non-deterministic analysis of complete systems. The latter models do not attempt to represent physics directly, but seek to represent how the “system response parameters” vary over a wide range of inputs.

There was a discussion on how “approval” for use of codes (CFD codes) might work. Simon Coldrick and BO agreed that it is a mistake to approve **codes** for certain applications.
Steve Graham said it is possible to develop a Model Evaluation Protocol for a complete tool (such as the LNG protocol that Simon Coldrick presented on Day 1) but that is not possible when “model” refers to a “physics component” such as a model of turbulence, combustion etc.

4. Organization of Expert Workshop

The organization of the workshop was mainly done and driven by KIT, NCSRD and EE.

NCSRD took up the responsibility to collect several useable and appropriate hotels in the surrounding of Athens, based on a list of specifications, e.g. availability of meeting rooms and appropriate technical infrastructures within the meeting rooms, availability of enough guest rooms, lunch- and coffee-services as well as evening dinners, general service and support, accessibility of location by local public transport and last but not least, to find a location to concentrate in relaxed atmosphere on the work shop content and additionally to foster bilateral communication as well as group discussion apart from the time schedule of workshop. All information needs to get exchanged with coordinator, thus NCSRD processed in short communication (daily exchange of achieved status) with the coordinator. The major tasks of NCSRD concerning the arrangements and organisation of the Athens work shop can get highlighted as follows:

- Pre-collection of appropriate locations
- Pre-discussion with locations according to the specifications and conditions
- On-site check of locations
- Comparison of proposals (costs and conditions)
- Mentor between coordinator and location in all administrative issues

EE took up the responsibility to arrange the attendees to the workshop in general based on a list of potential experts suggested by the consortium. EE launched the communication with potential experts, communicated the scope of workshop to the potential experts, exchange of workshop topics and aligned suitable date for the workshop. Because of the tasks, EE drafted the first topics to the workshop agenda (aligned with experts meaning and SUSANA aims), pronounced pre-invitations and drafted first list of “potential attendees”. Because of these sensible tasks, EE stood in short communication (daily exchange of achieved status) with the coordinator. The major tasks of EE concerning the arrangements and organisation of the Athens workshop can get highlighted as follows:

- Launching of communication with potential experts
- Alignment of work shop topics with the experts
- Alignment of potential dates of the work shop

KIT held the overall responsibility of the work shop in general concerns.

5. Financials to the Executed Expert Workshop

eliminated

6. Appendix 1 Invitation List

Surname	First Name	Institution /company	Expertise area? (to help ensure sufficient coverage)
Astier-Perret	Robin	Toyota	Candidate for user group - industrial / applications based
Bartzis	John G.	Department of Mechanical Engineering, University of Western Macedonia, Kozani, Greece	COST action ES1006 (Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments), Substitute National representative at the management committee.
Bauwens	Regis	FM Global	Deflagration experiments and modelling, hydrogen combustion, hydrogen safety
Benard	Pierre	Hydrogen Research Institute, UQTR	New energy applications, hydrogen storage and safety, particularly nanoporous hydrogen storage materials and CFD modelling of hydrogen releases and dispersion. Canadian representative in IEA HIA Task 19 “Hydrogen Safety”
Cleaver	Phil	DNV/GL	Model development and evaluation. Industry / applications based
Di Benedetto	Almerinda	Institute of Combustion, CNR	Hydrogen combustion theory, experimental research, and modelling, particularly - hydrogen deflagration modelling.
di Sarli	Valeria	Institute of Combustion, CNR	Hydrogen combustion theory, experimental research, and modelling, particularly - hydrogen deflagration modelling.
Dorofeev	Sergei	FM Global	Fire, deflagration and detonation modelling, CFD, hydrogen combustion, hydrogen safety
Graham	Steve	NNL	Steve has experience of modelling of hydrogen and has been involved in developing guidelines for Sellafield. He has also taken part in CFD quality and best practice initiatives in the UK and Europe
Lea	Chris	Lea CFD associates	Model application and evaluation, worked on the LNG model evaluation protocol
Iudicello	Francesca	Xaar	Best practice/ NAFEMS
Skibin	Alexander	Gidropress	Heat and mass transfer, CFD, nuclear reactor cooling, hydrogen distribution
Trucano	Timothy	Sandia National Labs	CFD, Verification and validation. Used to work with Oberkampf so pretty much best in field.
Vyazmina	Elena	Air Liquide	CFD, candidate for user group
Wen	Jennifer	University of Warwick	CFD: releases, fires, detonations
Matsuo	Prof. Akiko	Keyo University	CFD, candidate for user group
Studer	Etienne	CEA	
Tripathi	Sharad	Fluidyn	CFD provider
Prankhul	Middha	gexcon	CFD provider
Scheuerer	Martina	GRS	Nuclear safety
Oberkampf	William		expert in verification processes.
Truchot	Benjamin		Head of the Unit Dispersion, Fire, Experiment and Modelling, Direction of Accidental Risks
Seitz	Thomas		Fluid Dynamics and CFD Analyses (PEPR3-G), ENGINEERING & PROJECTS
Dimmelmeier	Harald		Section Manager "Severe Accidents"PEPA-G Radiological, Severe Accident and Building Analyses

7. Appendix 2 Agenda to the Workshop

PROGRAMME: INTERNATIONAL WORKSHOP, MODEL EVALUATION PROTOCOL FOR CFD USE IN HYDROGEN AND FUEL CELL SAFETY APPLICATIONS.

Vouliagmeni Suites, Athens, Greece, 17-18th September 2014

Support to Safety Analysis of Hydrogen and Fuel Cell Technologies:

A European FP7 Project Funded by:

Tuesday, 16th September: Welcome dinner in evening

Wed, 17th September

Session 1: Introduction

09:00-9:30	**SUSANA FP7 Project Introduction** Olaf Jedicke, (SUSANA Coordinator), Karlsruhe Institute of Technology
09:30-10:00	**Model Evaluation Protocol Structure (MEP) in the SUSANA Project** Daniele Baraldi, Joint Research Centre

Session 2: Model Evaluation Protocols

10:00-10:30	**Guidelines by MEG (Model Evaluation Group) – best practices for Model Evaluation.** Benjamin Truchot, INERIS
10:30-11:00	**Overview of MEGGE report for gas explosions** Daniele Baraldi, Joint Research Centre
11:00-11:15	*Morning refreshment Break*
11:15-11:45	**SMEDIS /LNG protocol for dispersion** Simon Coldrick, Health and Safety Laboratory UK
11:45-12:15	**CFD protocols in nuclear industry**

	Steve Graham National Nuclear laboratory UK
12:15-12:45	Roundtable discussion - "Model evaluation protocol"
12.45 -2.00	***Lunch day 1***

Session 3 - Best Practices in Numerical Modelling

14:00-14:30	**Requirements of Physical and Mathematical models for H2 safety applications: Releases/ignitions/fires**. Vladimir Molkov, University of Ulster
14:30-14:50	**Requirements of Physical and Mathematical models for H2 safety applications: detonations** Alexei Kotchourko, Institute for Nuclear and Energy Technologies, KIT
14:50-15:20	**Hydrogen combustion modelling/ deflagration** Vanessa DiSarli, Istituto di Ricerche sulla Combustione, CNR
15:20-15:35	*Afternoon refreshment break*
15:35-16:05	**Best practice in engineering simulations** Francesca Ludicello, Xaar Ltd.
16:05-16:35	**Modelling approaches to hydrogen safety issues** Jennifer Wen, University of Warwick
16:35-17:05	**Best practice guidelines for verification and validation of CFD in nuclear reactor safety applications** Martina Scheuerer, GRS (Gesellschaft für Anlagen- und Reaktorsicherheit)
17:05-17:35	Roundtable discussion - “Best practices in numerical simulations”

Wed, 17th September

Evening Meal in Hotel

Thursday, 18th September

Session 4: Validation and Verification techniques, methodology and databases

09:00-09:30	**Verification and validation: adopted definitions, approach to verification** Shane Slater, Element Energy
09:30-10:30	**The SUSANA model validation database & benchmarking** Alexi Kotchourko, Institute for Nuclear and Energy Technologies, KIT
10:30-11:00	*Morning Refreshment Break*
11:00-11:30	**Best Practice in verification of computational simulations** William Oberkampf (Consultant, previously with Sandia National Labs)
11:30-12:30	Roundtable discussion - "Verification and Validation applied to Fuel Cell and H2 safety"
12.30-14.00	**Lunch Day 2**

Session 5: Industrial and Commercial Perspective

14.00-14.30	**CFD simulation to support safe H2 deployment** Elena Vyazmina, Air Liquide
14.30-15.00	**Best practices for use of FLACS applied to hydrogen and fuel cell safety problems** Prankul Middha, Gexcon
15.00-15.30	**Challenges for CFD in practical hydrogen and fuel cell safety applications** Harald Dimmelmeier, Areva
15.30-16.00	**Explosion modelling in Shell** Jonathan Puttock, Shell
16:00-17:00	Roundtable discussion - "I&C perspectives on practical deployment of Model Evaluation Protocol"
17:00-17:15	**Closing remarks** Olaf Jedicke, (SUSANA Coordinator) KIT
17:15	**Finish day 2**

Thursday, 18th September

Evening Meal in Hotel.