Clean Hydrogen Partnership

CFD for Hydrogen Safety

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Detonation, blast waves, effect of containments

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What is CFD for Safety

What do we expect from CFD

- Provide information on what is dangerous
- Provide detailed information of the ongoing processes during facility operation
- Provide information on the possible ways to avoid unwanted processes / consequences
    - Countermeasures
    - Change in the design / operational conditions
    - Optimization of the facility operation
- Provide information enriching/replacing experimental data

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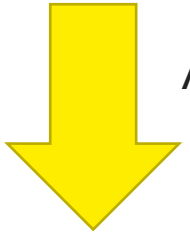
Main request to the CFD:

All obtained information must be trustworthy in the frames dictated by the task



Accepted strategy

Verification & Validation

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Reliability of CFD

SUSANA approach (tasks) to improve reliability of CFD simulations

Traditional approach to test the models and codes

- To review the state-of-the-art in CFD physical and numerical modelling
- To update and enhance verification and validation procedures for CFD models and codes
- To develop a CFD model evaluation protocol for assessment of the capability of the CFD models
- To create the infrastructure for implementation of the CFD model evaluation protocol:
  - Database of problems regarding verification of codes and models against analytical solutions
  - Model evaluation database of experiments for validation of simulations
- To compile the best practices guide in numerical simulations

SUSANA EC Project: Final report

CFD current status

- Hardware – progress is visible, however not as fast as desirable (last 30 years gave ~100 times improvement); required still much more
- Software – numerical methods does not give high level performance acceleration (meanwhile improved stability, accuracy, some of them physical effects)
- Physical models
  - Base knowledge did not create new theories or noticeably improved those which exist over decades or centuries
  - The direct numerical simulations are still very rare and more academic character rather than applied
  - The progress is focused in phenomenological models often with under-resolved or un-resolved phenomena
- Operator (‘User’) – highly educated person who understands ALL details and circumstances of his/her actions. Such person has to be knowledgeable in both mathematical and physical aspects of the software used. The idea to create software which can be used by the person who has read the manual is erroneous initially.

The codes become very complex including numerous models for numerous peculiarities of the simulated processes: see operator

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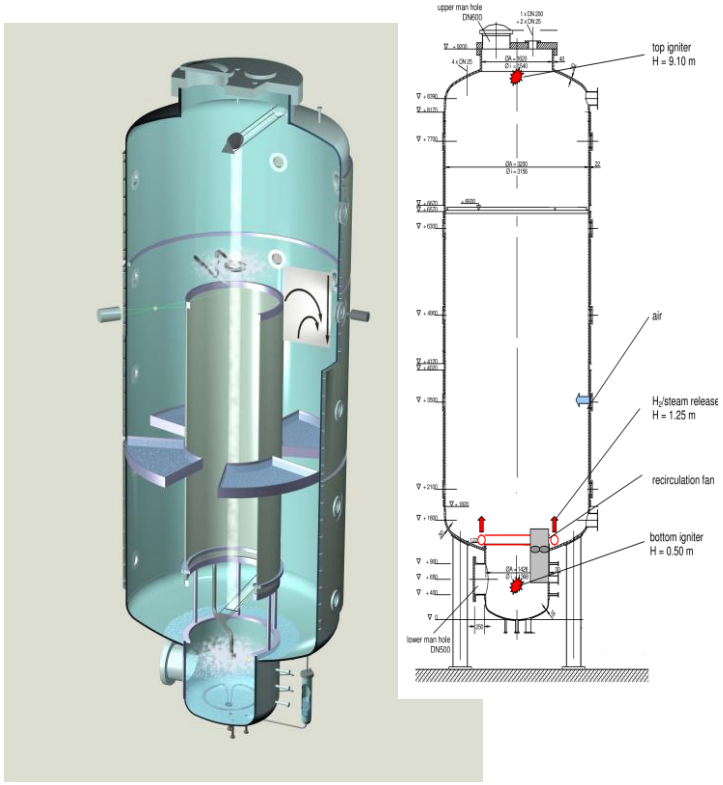
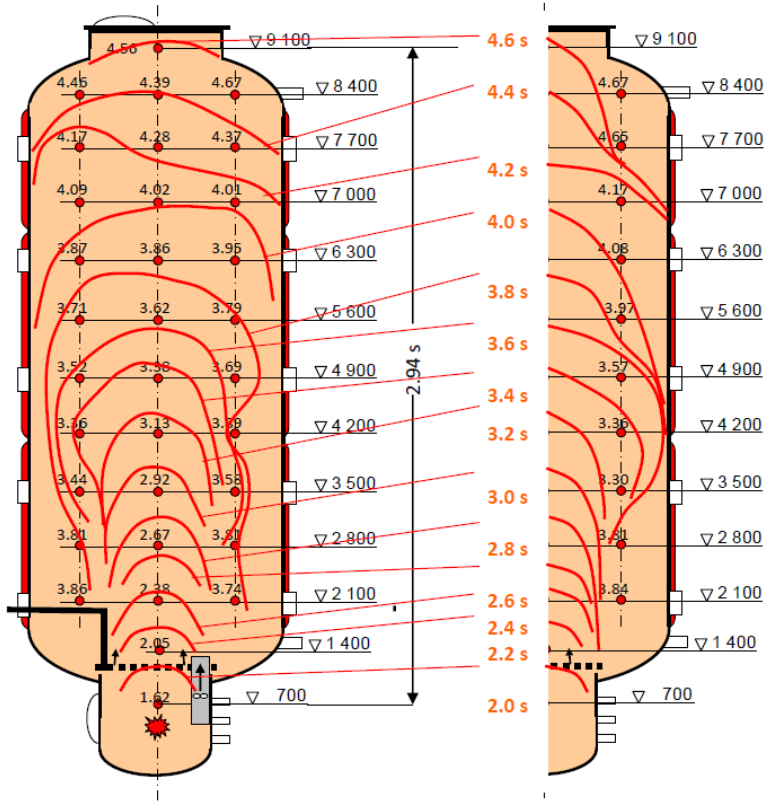
Example of validation





Source: ISP 49

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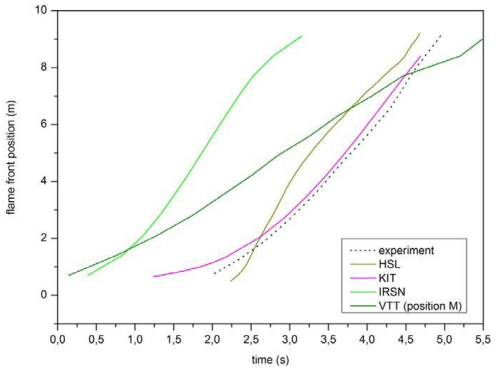
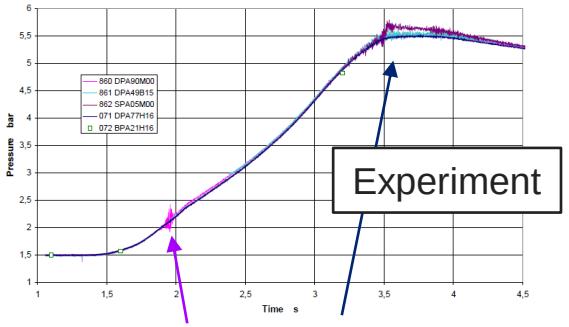
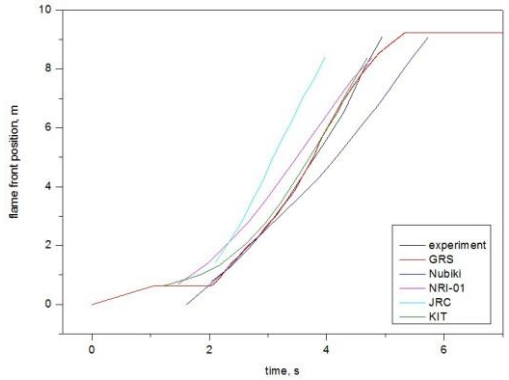
Example of validation



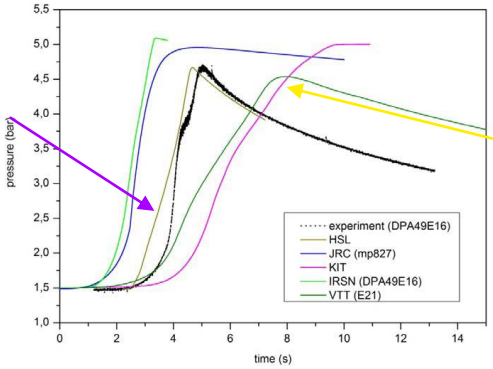


Experiment

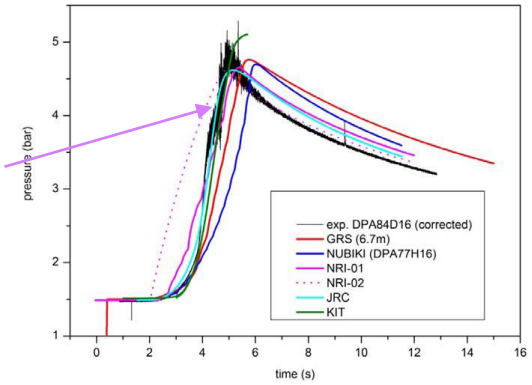
Strong acoustic effects



Does this code CFX-12 accounts for the flame instabilities?



Acoustic-parametric instability model switched on/off



Blind Simulations

Post-Blind Simulations

Are these codes valid ?
User effect or code is wrong?

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The SUSANA best practice guide lines

- The whole range of hydrogen safety relative phenomena such as: release and dispersion, ignition and jet fires, deflagration and detonation.
- It includes aspects of CFD user education and training.
- All issues of CFD simulations are discussed:
  - physical models (release, turbulence and combustion models),
  - problem setup (domain and mesh design and boundary and initial conditions),
  - numerical options (solver type, spatial and temporal discretization schemes, convergence criteria)
  - analysis of the simulation results (validation, sensitivity and interpretation of the results).

Extension of the traditional approach to simply test the models and codes

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Commercial code usage

Validation of a commercial code?

- If a scientist or a group of scientist has performed a set of very successful simulations using e.g. commercial code, does it mean the code is validated?
- If anybody else will make any simulation using the same code, this simulation results are trustworthy ?
- Typical message from a user of a commercial code

Hello Everyone,

I got some warnings and errors during the Simulation. I am doing LES simulations from ….
The warnings are as followed:
….

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Summary

How to prove trustworthy of the CFD simulation

- Verification: Yes
- Validation as an exercise to reproduce known experiment: Useful, but proves very little concerning the code quality and reliability of the results for any other simulations
- Validation as blind simulation of experiment: Useful, but proves very little concerning the code quality and reliability of the results for any other simulations
- Formulation of guide lines: Useful for education, but for applied safety calculation (which, e.g., should be considered by authorities) ?

The current paradigm for verifying the reliability of simulations needs to be revised

- Convincing prove that decisive phenomena are taken into account and are described adequately by the code model
- Single simulation / The simulation with experiment not widely discussed and accepted by community can not be considered as validation
- The role of simulation operator is clearly underestimated

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