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CFD for Hydrogen Safety

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Role of Computational Fluid Dynamics, where to apply, typical phenomena, risk evaluation, and mitigation

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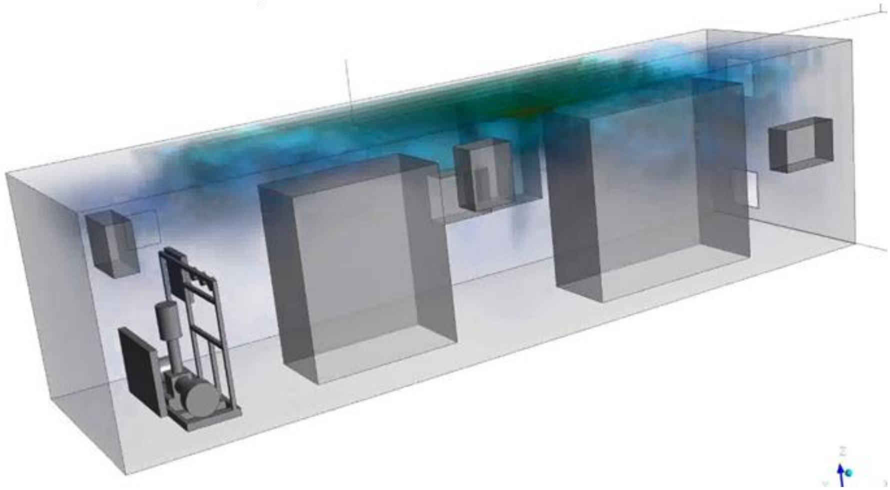
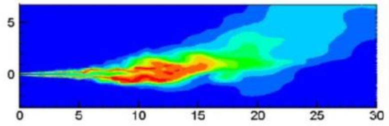
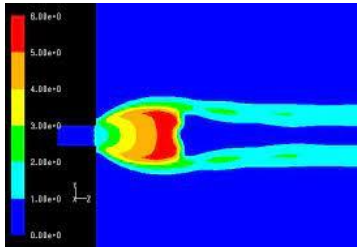
What is CFD?

- ✓ CFD consists of a set of numerical modeling tools able to simulate and predict the behavior of single-phase and multiphase fluid flows
    - CFD is a transdisciplinary field between fluid mechanics, applied mathematics, and engineering)
    - Development of CFD is closely linked to that of computers (highly intensive in terms of CPU and memory usage)
- ✓ the use of applied mathematics, physics and computational software to simulate and visualize how a gas, liquid or multi-phase mixtures flows and reacts
- ✓ based on the Navier-Stokes equations
- ✓ the state-of-the-art simulation tool for predicting space and time resolved mixing and combustion phenomena
- ✓ CFD gives an insight into flow patterns that are difficult, expensive or impossible to study using traditional (experimental) techniques
- ✓ replacing or complementing simplified engineering correlations and lumped parameter codes







What is CFD?

PRE-PROCESSING

Solid Modeler → Mesh Generator

Solver settings

SOLVER

Equations solved on mesh

- ✓ Transport equations
  - Mass
  - Momentum
  - Energy
- ✓ Equation of State
- ✓ Supporting physical models

- ✓ Physical models
  - Turbulence
  - Combustion
  - Multiphase
  - Phase change
  - Moving mesh
  - Etc …

- ✓ Material properties
- ✓ Boundary conditions
- ✓ Initial conditions

POST-PROCESSING

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Experiments vs. Simulations

EXPERIMENTS

Quantitative description of flow phenomena using ***measurements***

- ✓ for one quantity at a time
- ✓ at a limited number of points
- ✓ for a laboratory-scale model
- ✓ for a limited range of problems and operating conditions

Error sources: measurement errors, flow disturbances by the probes

SIMULATIONS

Quantitative prediction of flow phenomena using ***CFD*** software

- ✓ for all desired quantities
- ✓ with high resolution in space and time
- ✓ for the actual flow domain
- ✓ for virtually any problem and realistic operating conditions

Error sources: modelling, discretization, iteration, implementation, users

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Definition

- HARM = adverse effect, consequence, physical injury or damage to health or property
- HAZARD = potential source of HARM
- RISK = probability * severity of HARM

  = cost expectation

✓ SAFETY is the freedom from unaccepted RISK

Determined by society and individually

Technical term:
RISK = probability x damage

Source: ISO/IEC Guide 73:2002

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Where CFD is used in Risk Analysis?

Qualitative Methods → **Quantitative** Methods

HAZID, HAZOP
Preliminary analysis accounting for external factors

→ ~ 100 Scenarios

FMEA, SABINE, Fault tree,…
Detailed anaylsis of process and mitigation measures

~ 50 Scenarios

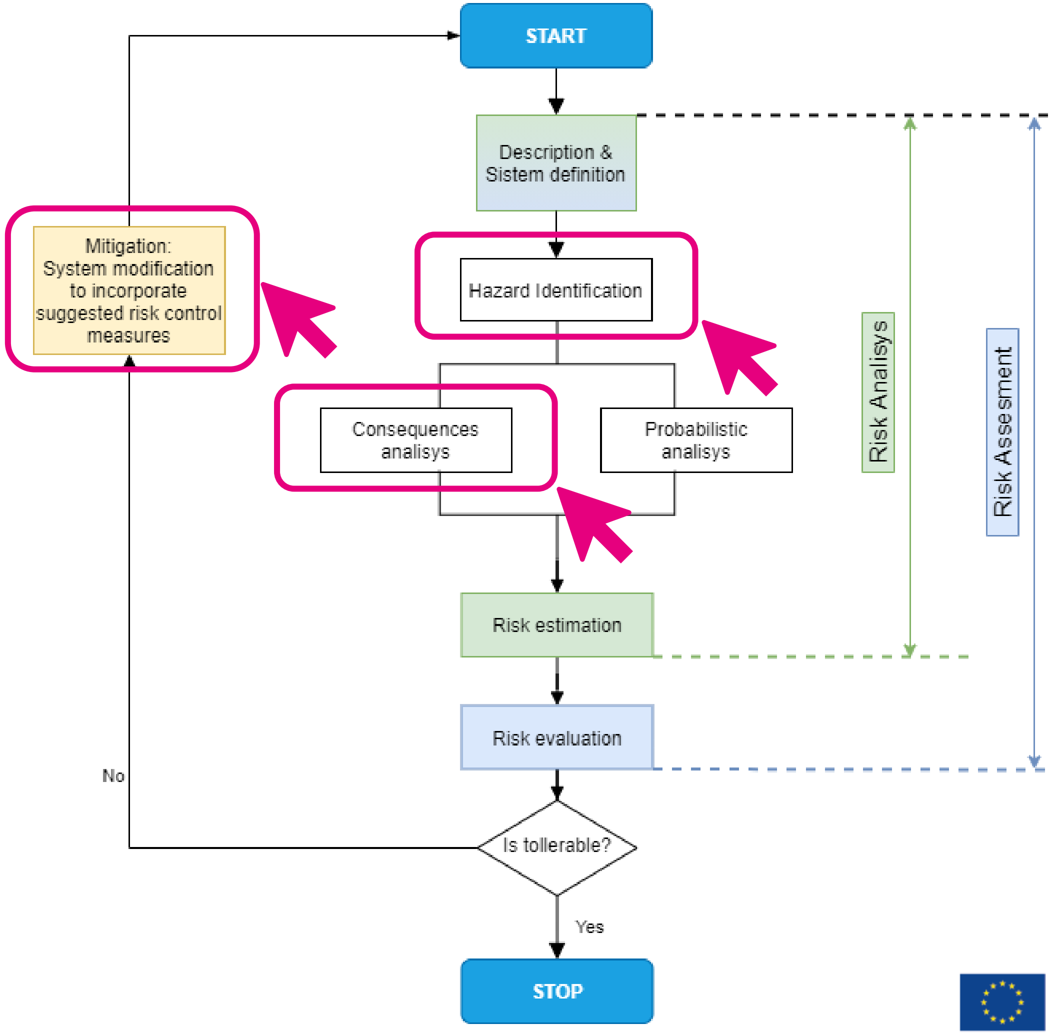
QRA
Detailed determination of probabilities and consequences with experiments and simulation, CFD,…

~ 10 Scenarios

… replacing or complementing simplified engineering correlations and lumped parameter codes

Role of CFD in QRA (Quantitative Risk Assessment)

- Supporting **Hazard Identification** (does a flammable mixture develop? does flame accelerate?)
- State-of-the-Art tool for deterministic **Consequence Analysis**
  - Determine pressure and thermal loads on structures and persons
- Supporting proper application of **Mitigation** technology and development of mitigation strategies
- Replacing or complementing simplified engineering correlations and lumped parameter codes ….



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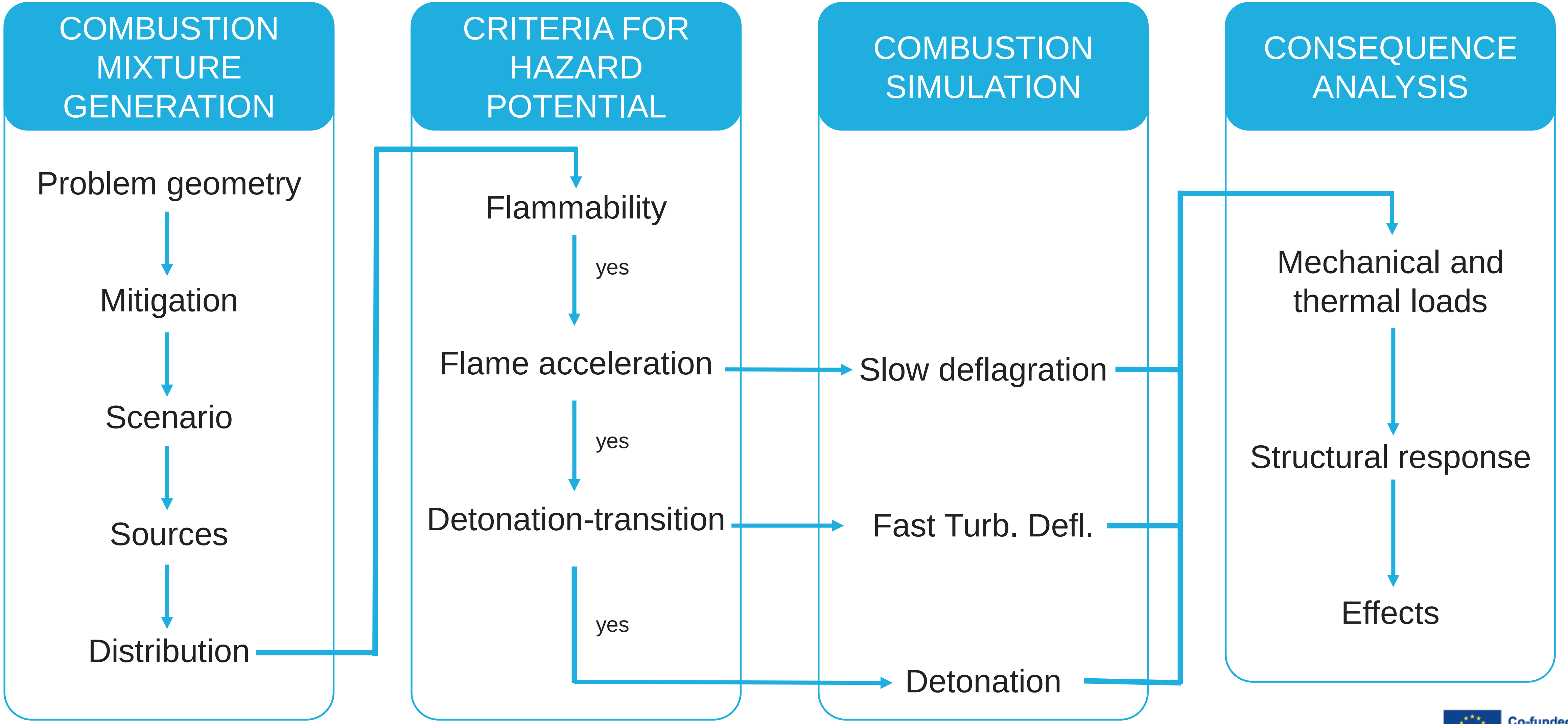
Typical Approach for Consequence Modelling



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What are problems with CFD?

CFD is

- expensive wrt computational resources, time
  (→ remedy: faster machines, new solvers)
- a complex tool requiring complex input
  without specific user guidance for hydrogen safety analysis
- seriously user dependent (→ remedy: user guidance, e.g. SUSANA)

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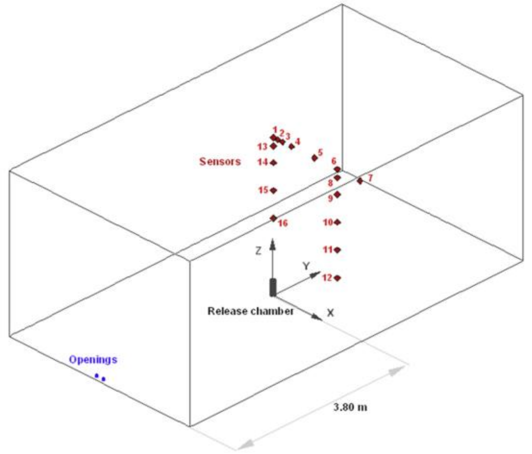
User Influence



Example: HySafe Blind Benchmark SBEPV3

Simple release experiment in empty garage-like room (1 g/s expanded for 240 s)

Participation in the benchmark was high:

- 14 different organizations with
- 10 different CFD codes and
- 8 different turbulence models

Large variation in predicted results was found in the blind phase of the benchmark, between the various modelling approaches.

Results caused heavy discussion about usefulness of CFD for hydrogen safety

(Venetsanos 2009)

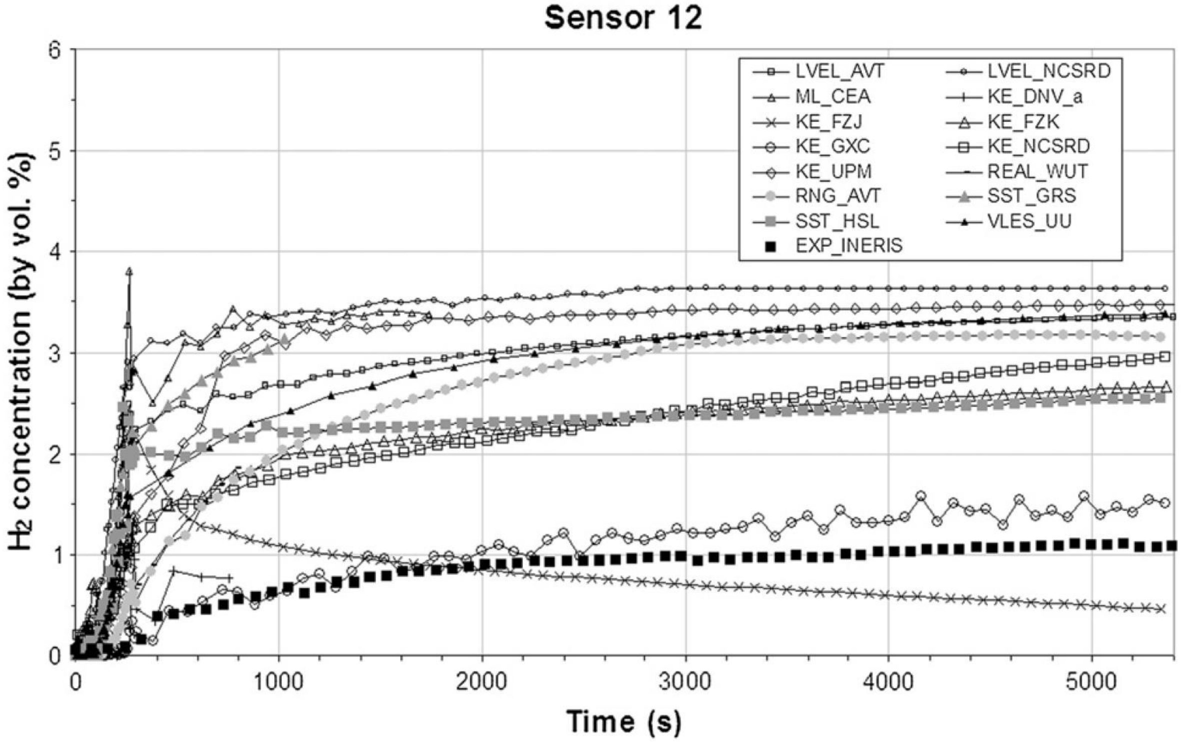


Fig. 8 – Predicted hydrogen concentration (vol. %) histories for sensor 12 (blind calculations).

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- non-linear models show strong dependence on initial and boundary values
  (→ remedy: sensitivity analysis, uncertainty quantification)
- typically a commercial product functioning as a black box with hidden implementation of critical models e.g. turbulence, combustion, etc.
  (→ trend: open source CFD)
- lacking verification and validation for relevant phenomena and scenarios
- difficult to be trusted (→ remedy: train users, authorities, etc.)

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List of available CFD models/tools

- ✓ Based on the information collected and compiled by Task Force 3 of the EHSP from CFD developers/users in the international community
- ✓ Both academic institutions, research laboratories and industry CFD users have been contacted
- ✓ To be published in the EHSP web pages as part of a document “EHSP Guidance on Hydrogen Safety Engineering” in 2023

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CLEAN HYDROGEN JOINT UNDERTAKING
(FCH 2 JU)

List of available CFD models for hydrogen safety applications

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Keep in touch/Thank you

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For further information
https://www.clean-hydrogen.europa.eu/

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