Modelling in FLACS
Activities and prospects

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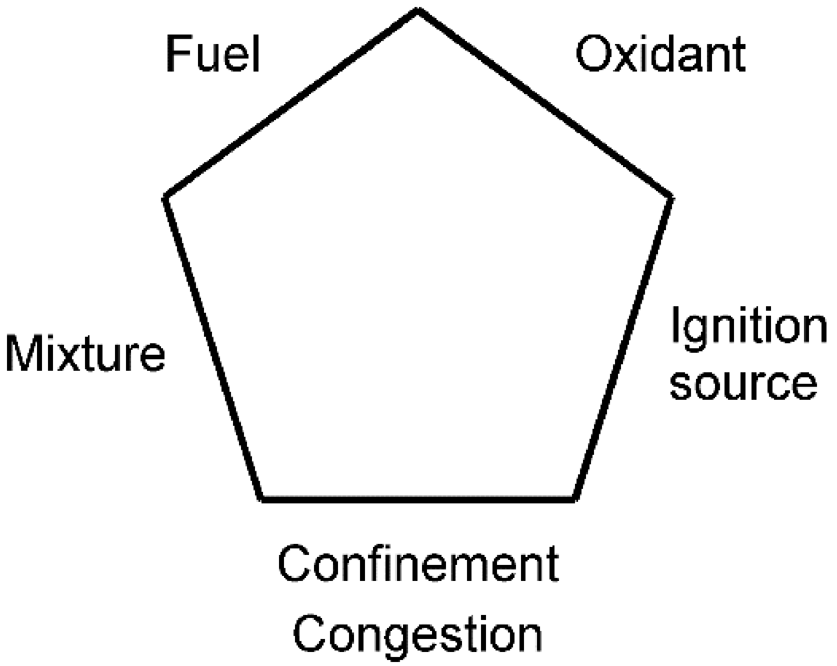
FLACS

Outline

- Introduction
- Activities
- Prospects
- Summary
- Acknowledgements

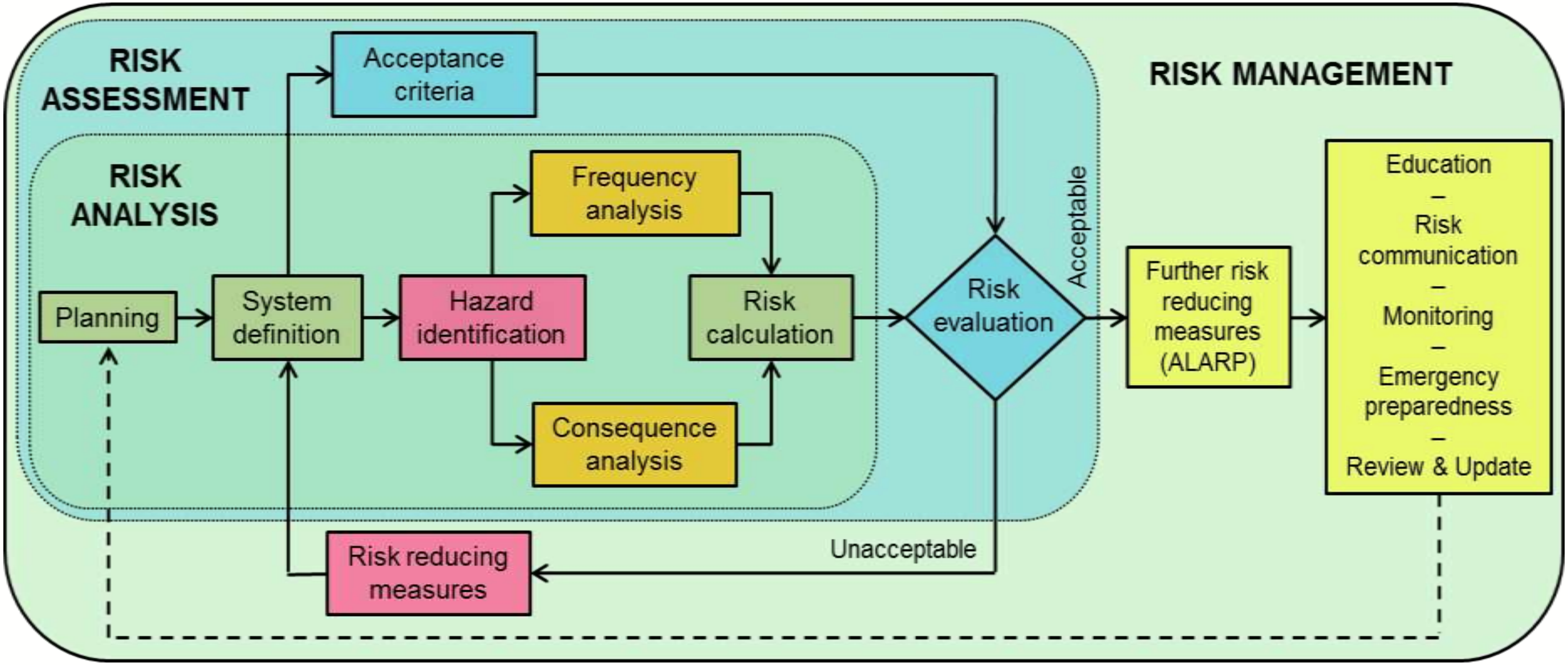


Background

- Gexcon develops the computational fluid dynamics (CFD) code **FLACS**
- FLACS includes the porosity / distributed porosity (PDR) solver **Flacs** for simulating flow phenomena in complex geometries
- FLACS is primarily an engineering tool used for **consequence analysis** and **design of risk-reducing measured** in the process industry

Risk management

General flow diagram for risk analysis, risk assessment and risk management:

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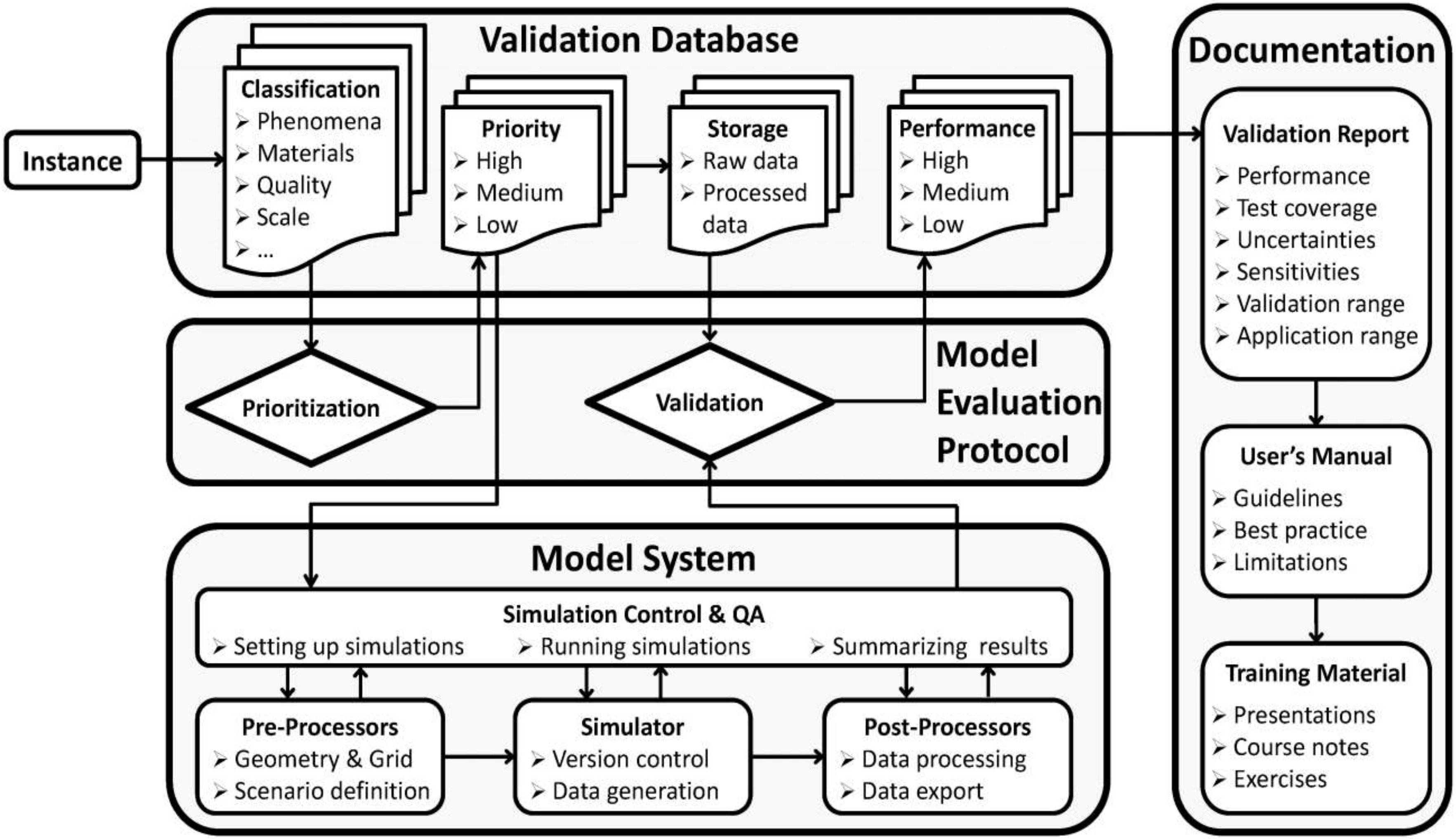
ACTIVITIES

Gexcon R&D

- GexCon R&D develops the CDF/PDR solver Flacs
- Currently 13.2 developers: 7 PhDs + 4 colleagues currently pursuing PhDs

Integrated validation framework



JIP MEASURE

Modelling **E**scalating **A**ccident **S**cenarios and the **U**se of **R**isk-reducing technology for **E**xplosion safety

Fundamental aspects of fuel-air explosions

Premixed combustion

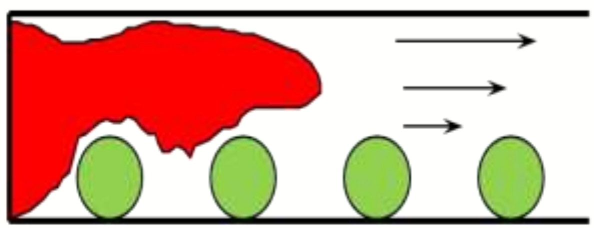
→ Expansion ⟺ Pressure build-up

Ignition

$$S_T \propto u'^{A} \, \ell^{B} \, S_L^{\,C} \, \nu^{D}$$

DDT?

Enhanced rate of combustion



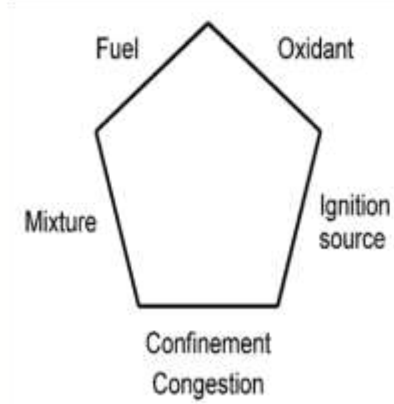
Turbulent reacting flow

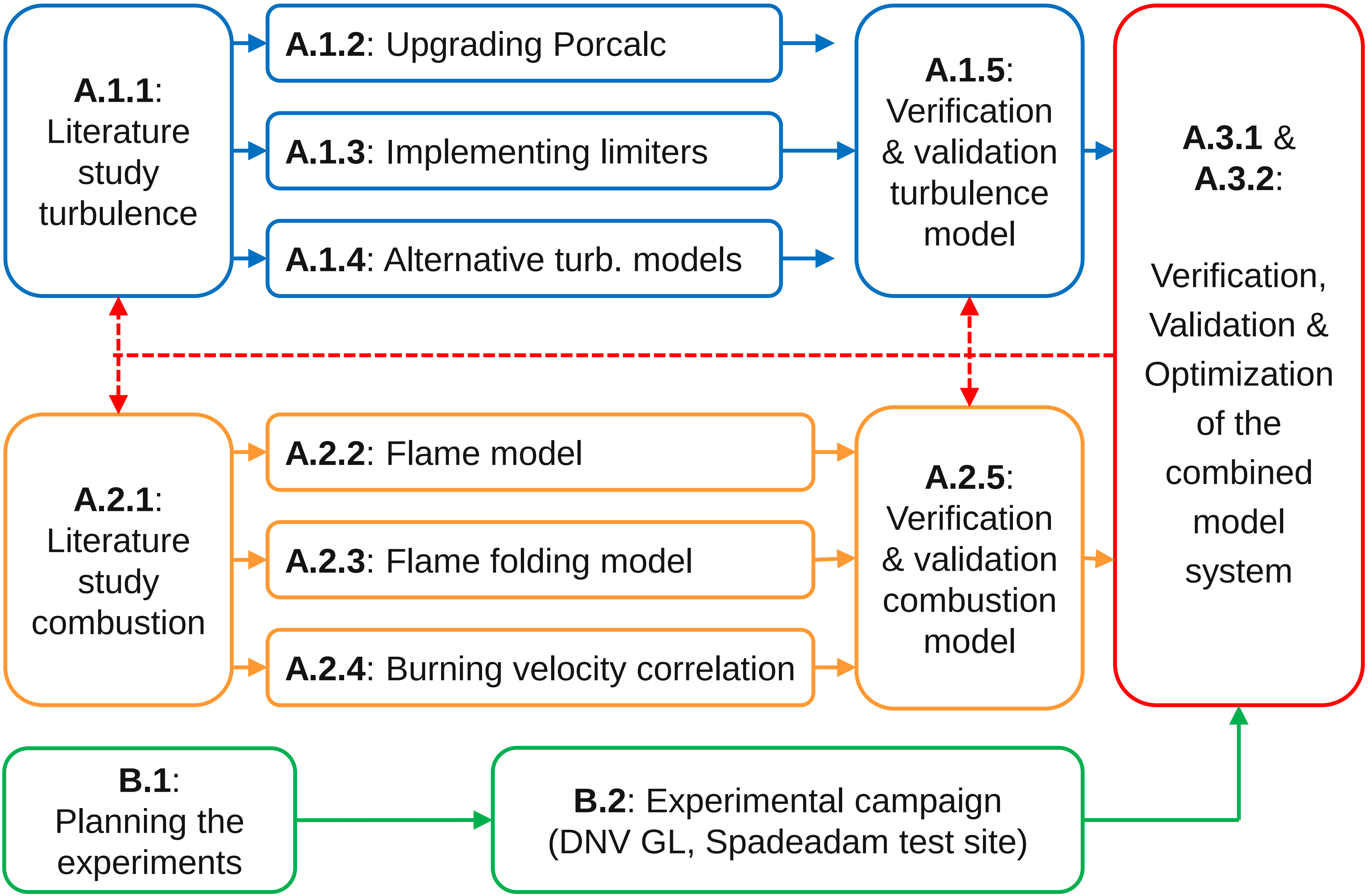
$$\ell = ?$$

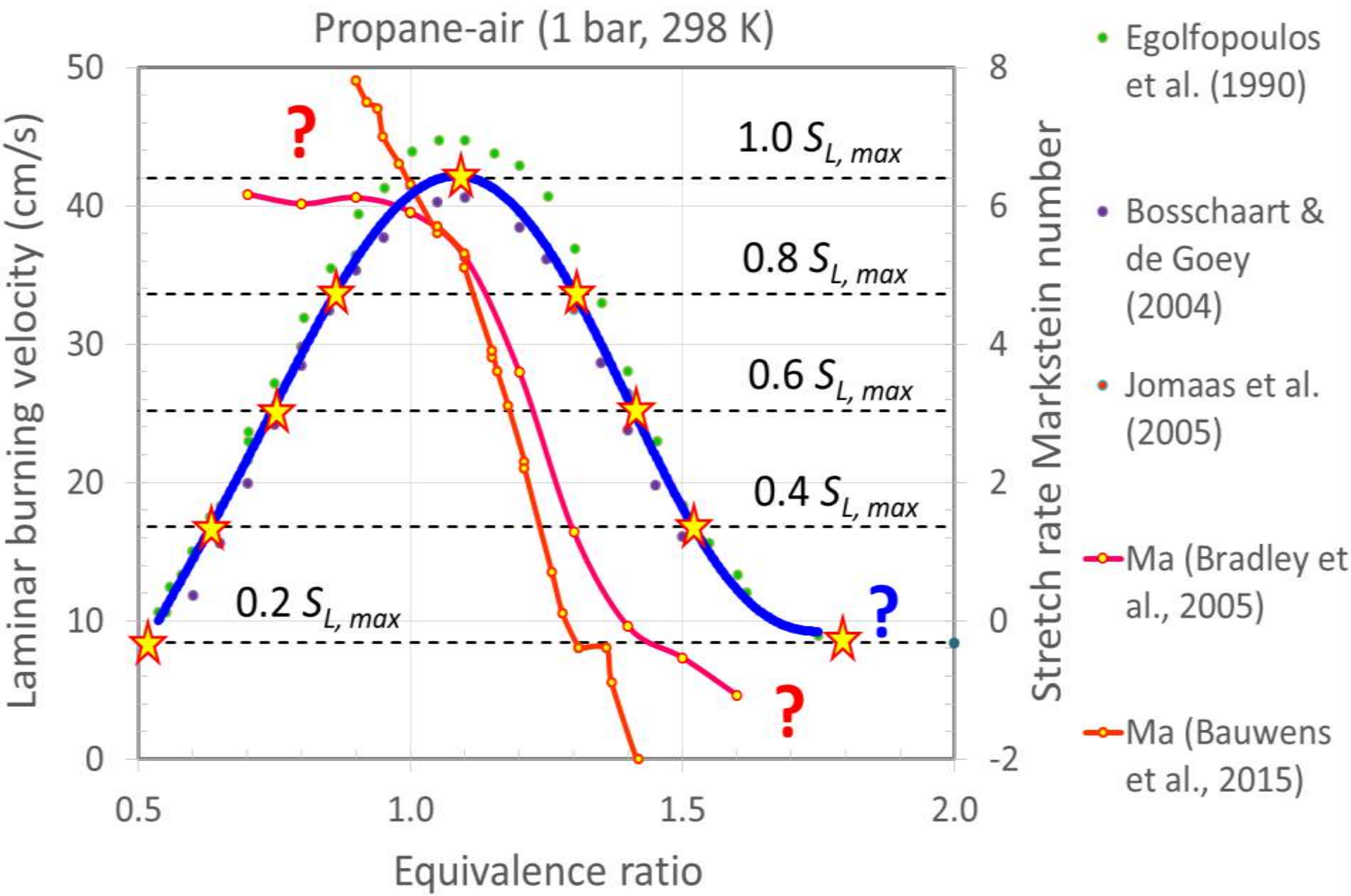
$$P_k = G_s + G_w + G_b + G_0$$

Interaction with obstacles

→ Turbulence generation

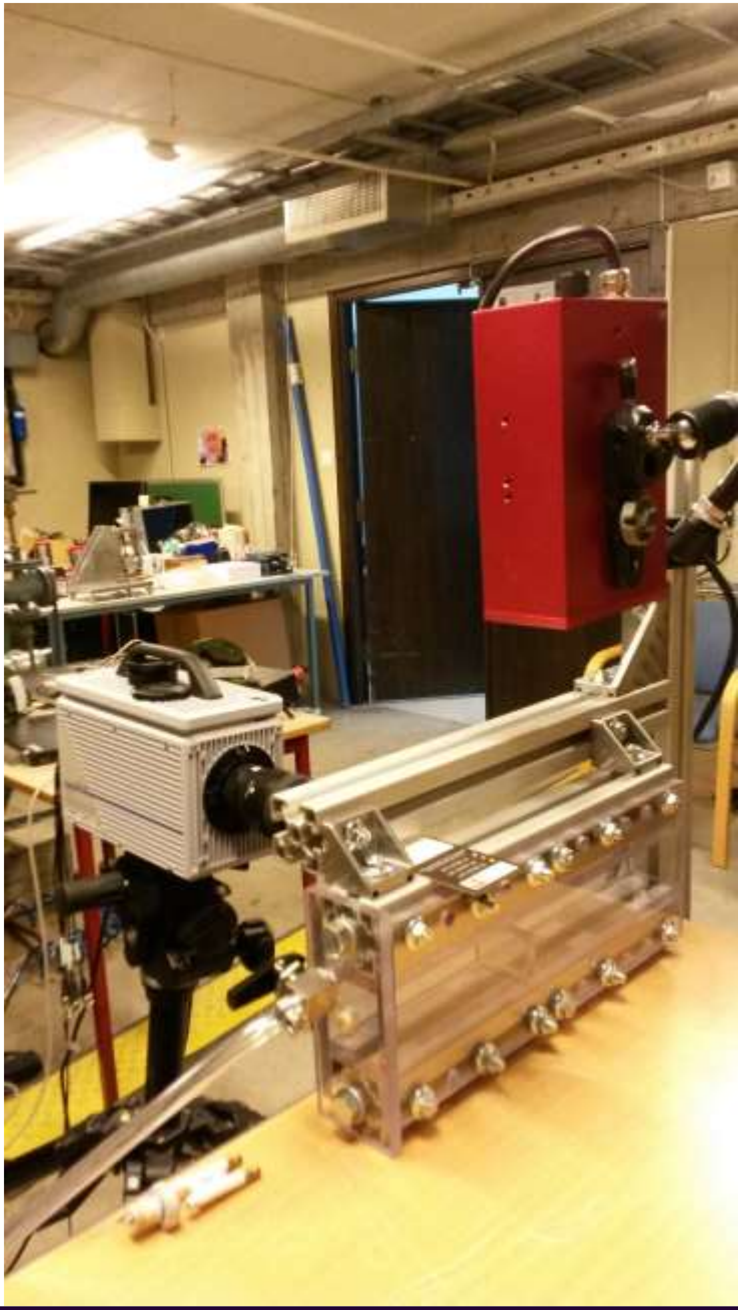



A.1.1: Literature study turbulence
A.1.2: Upgrading Porcalc
A.1.3: Implementing limiters
A.1.4: Alternative turb. models
A.1.5: Verification & validation turbulence model
A.3.1 & A.3.2:
Verification, Validation & Optimization of the combined model system
A.2.1: Literature study combustion
A.2.2: Flame model
A.2.3: Flame folding model
A.2.4: Burning velocity correlation
A.2.5: Verification & validation combustion model
B.1: Planning the experiments
B.2: Experimental campaign (DNV GL, Spadeadam test site)


Propane-air (1 bar, 298 K)
Laminar burning velocity (cm/s)
Stretch rate Markstein number
Equivalence ratio
1.0 $S_{L, max}$
0.8 $S_{L, max}$
0.6 $S_{L, max}$
0.4 $S_{L, max}$
0.2 $S_{L, max}$
?
?
?
0
10
20
30
40
50
-2
0
2
4
6
8
0.5
1.0
1.5
2.0
Egolfopoulos et al. (1990)
Bosschaart & de Goey (2004)
Jomaas et al. (2005)
Ma (Bradley et al., 2005)
Ma (Bauwens et al., 2015)

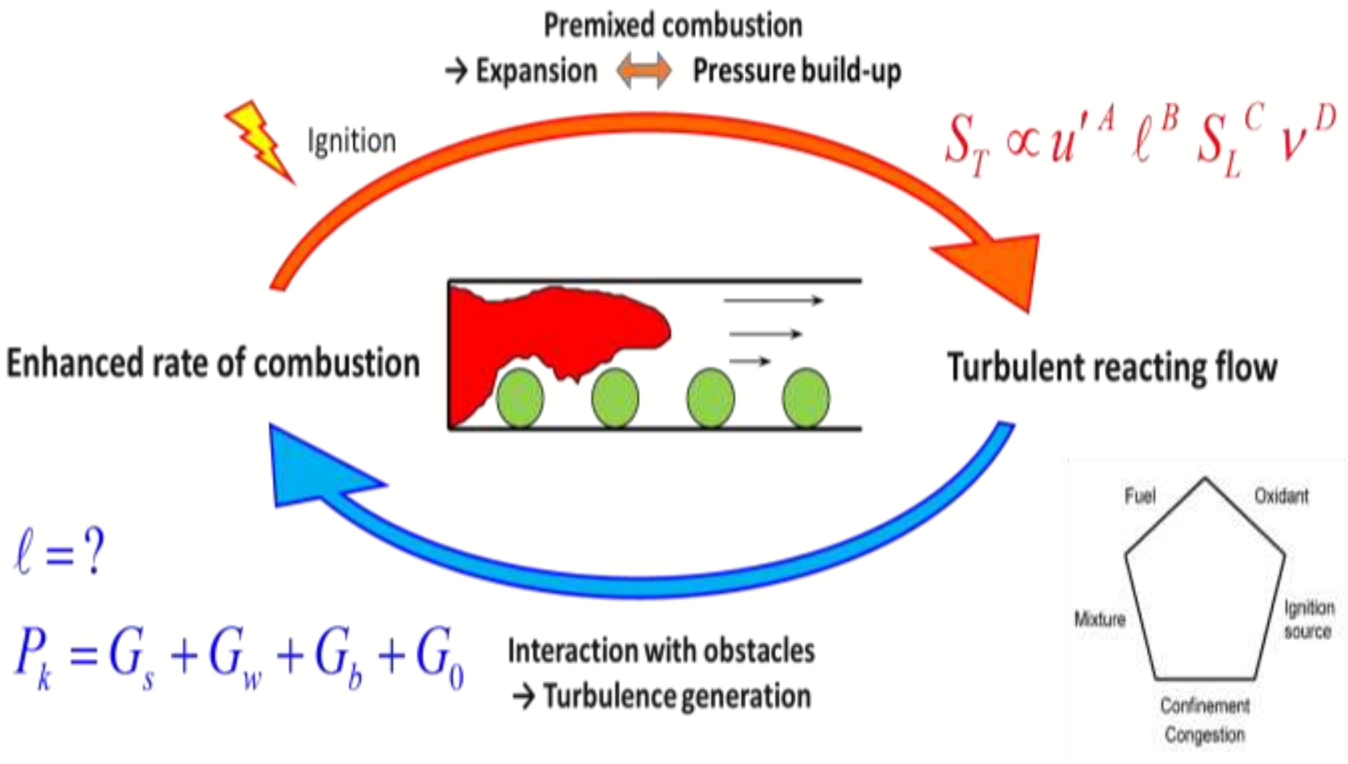
Experiments at HiT

- Part of Hy3DRM project
- The goal is to characterize flow and turbulence in wakes downstream of bluff bodies during explosions
  - High-speed camera + laser sheet
  - Particle image velocimetry (PIV)
- Limited data available: CMI, Imperial College, Loughborough, etc.
- Important for validating subgrid models in CFD tools



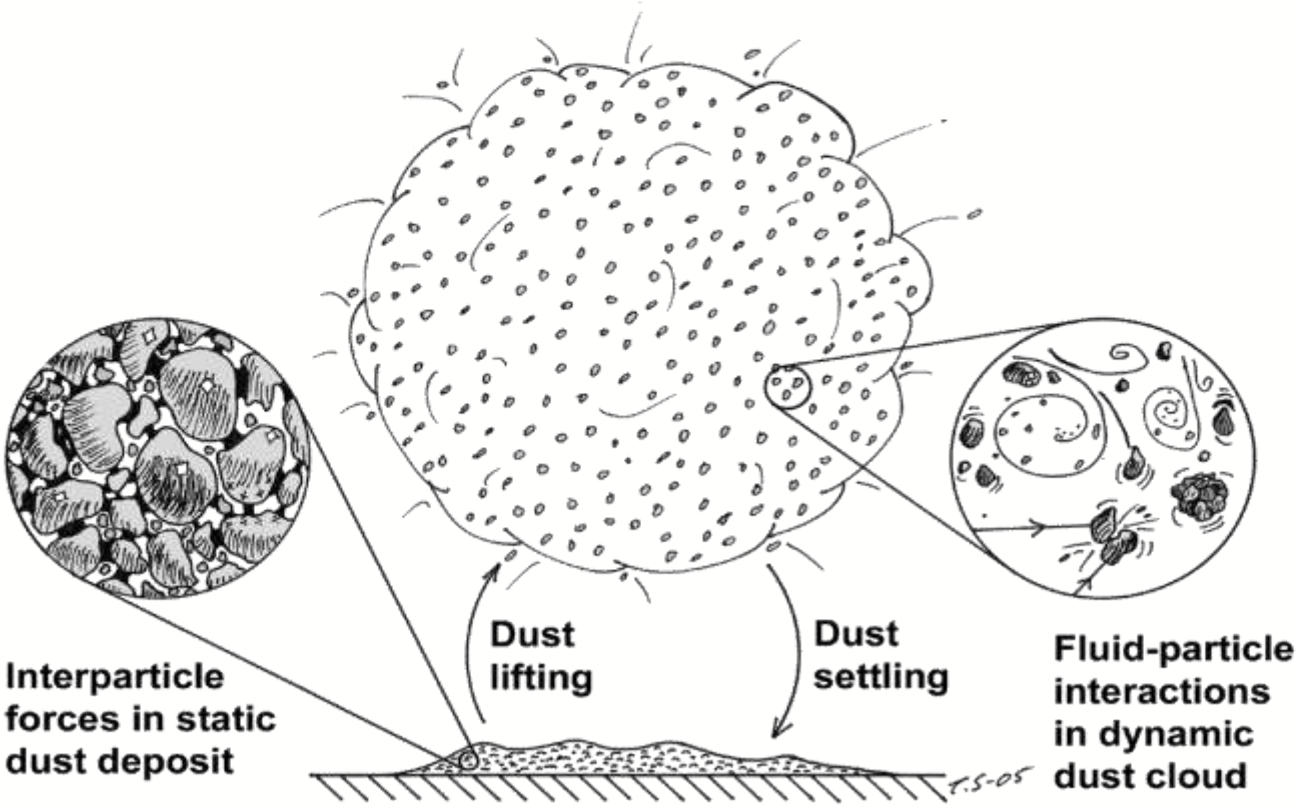
Parameter optimization

- Industry PhD project
- Established cooperation with optimization group at University of Bergen

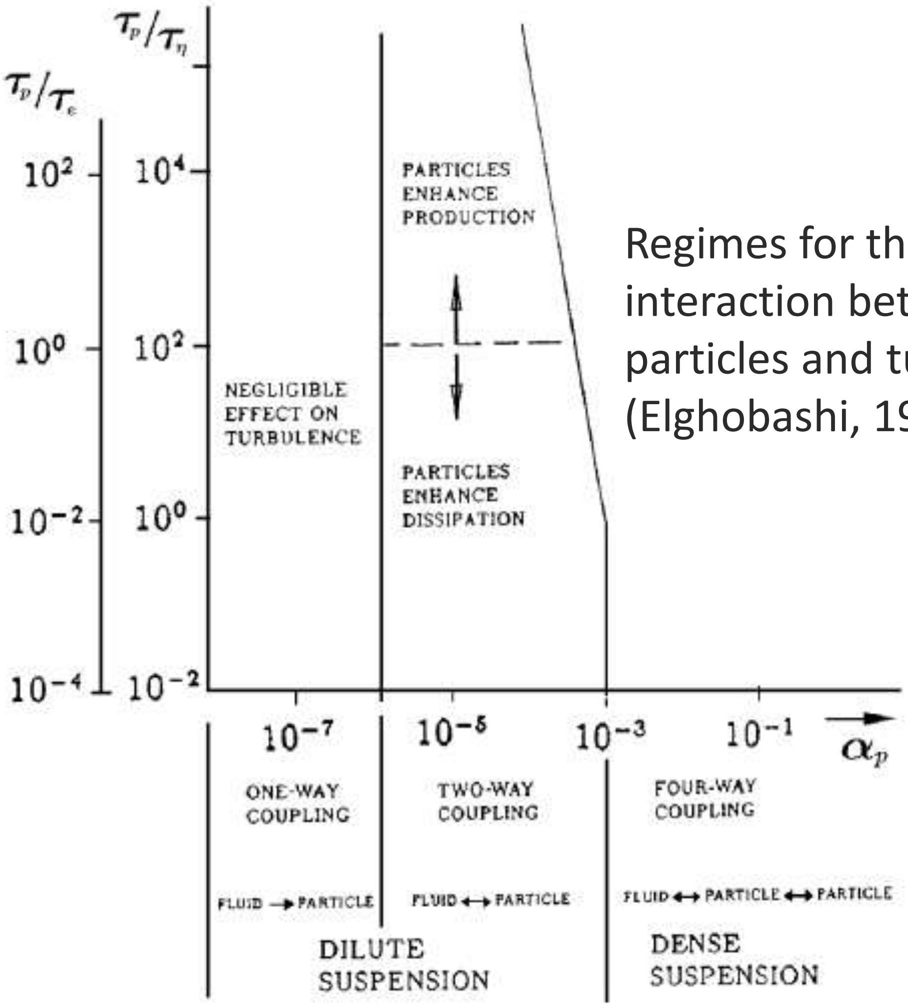


Dust explosion modelling

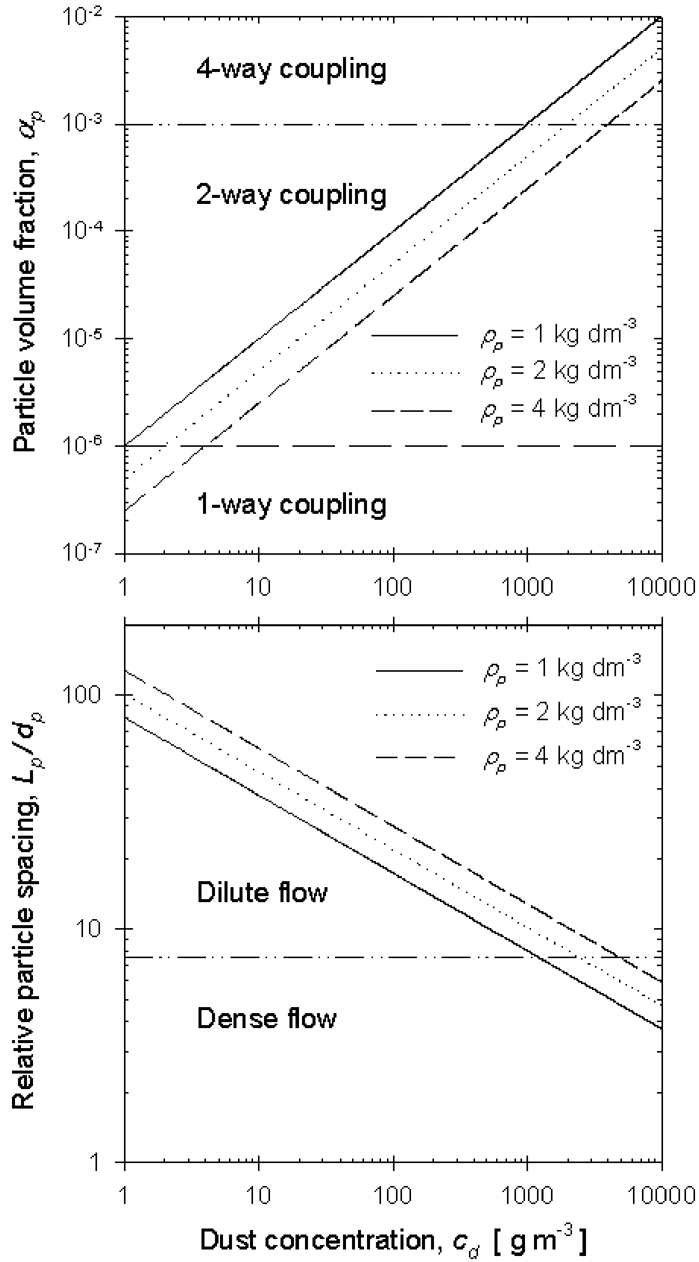
- Industry PhD project continuing the work from the DESC project
- Established cooperation with FSA in Germany and University of Greenwich (Stefan Zigan and Lahiru Lulbadda Waduge)



Particle-laden flow



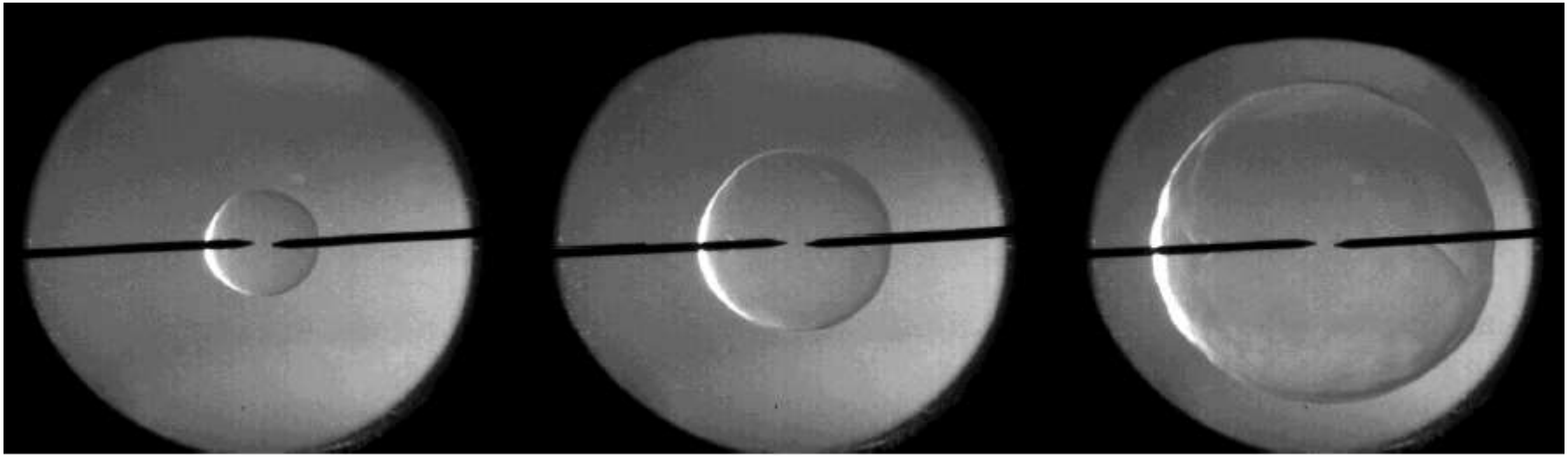
Regimes for the interaction between particles and turbulence (Elghobashi, 1994)



Mist explosion modelling

- Industry PhD project continuing the work from previous work on transformer explosions etc.
- Established cooperation with Cardiff University (Prof. Philip J. Bowen)

- Flame propagation in ethanol mist:



Hydrogen safety

Compressor in ISO container

Inside the container

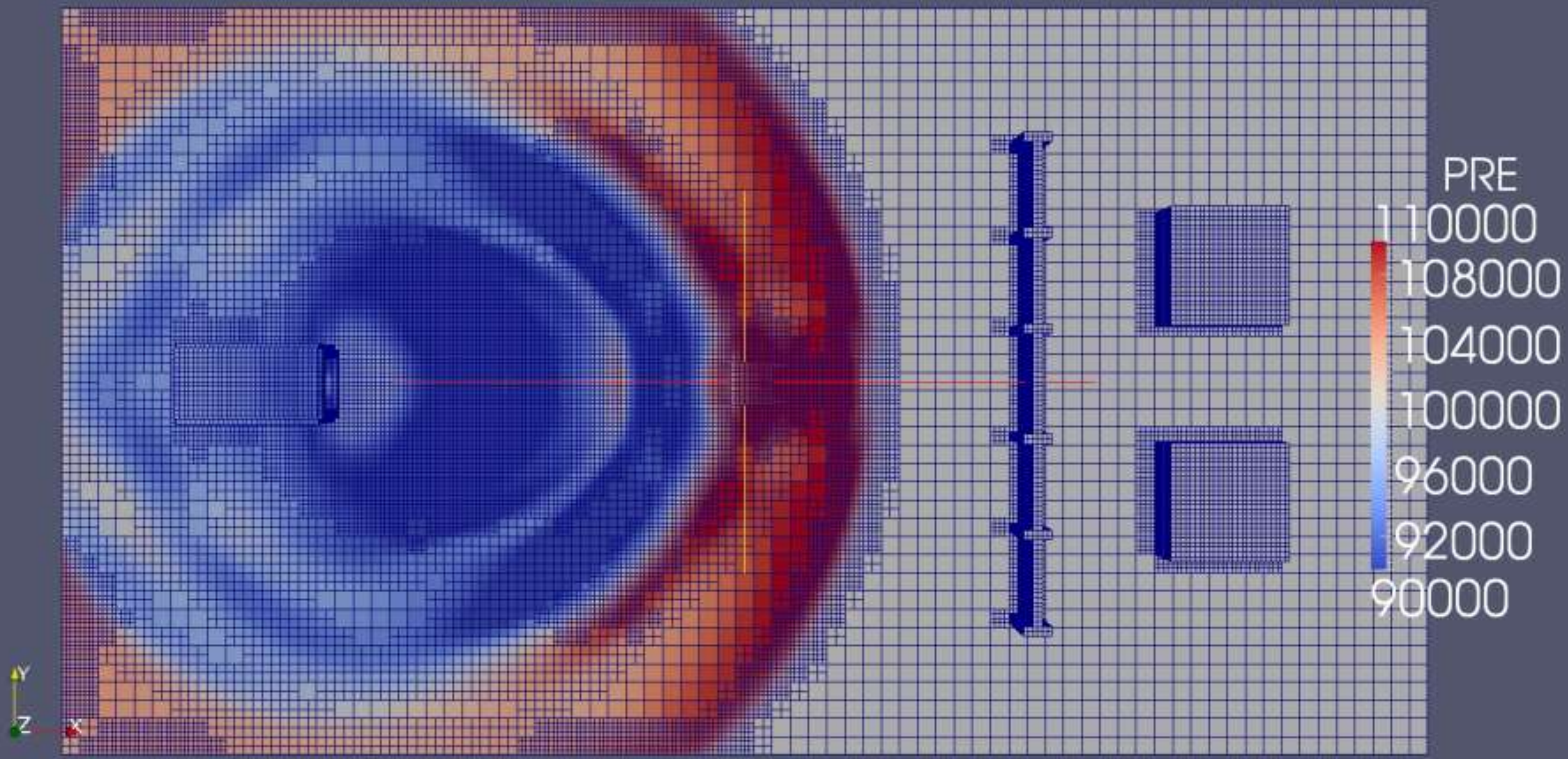
HySEA

www.hysea.eu

HySEA

- Improving **Hy**drogen **S**afety for **E**nergy **A**pplications through pre-normative research on vented deflagrations
- **Call**: H2020-JTI-FCH-2014-1-FCH-04.3-2014 – “Pre-normative research on vented deflagrations in containers and enclosures for hydrogen energy applications”
- **Consortium**: Gexcon (Coordinator), University of Warwick, University of Pisa, Fike Europe, Impetus Afea and University of Science and Technology of China (USTC)
- **Start-up date**: 1 September 2015 (three-year duration)
- Further & updated information: **www.hysea.eu**

Flacs 3: Initiated work on AMR solver

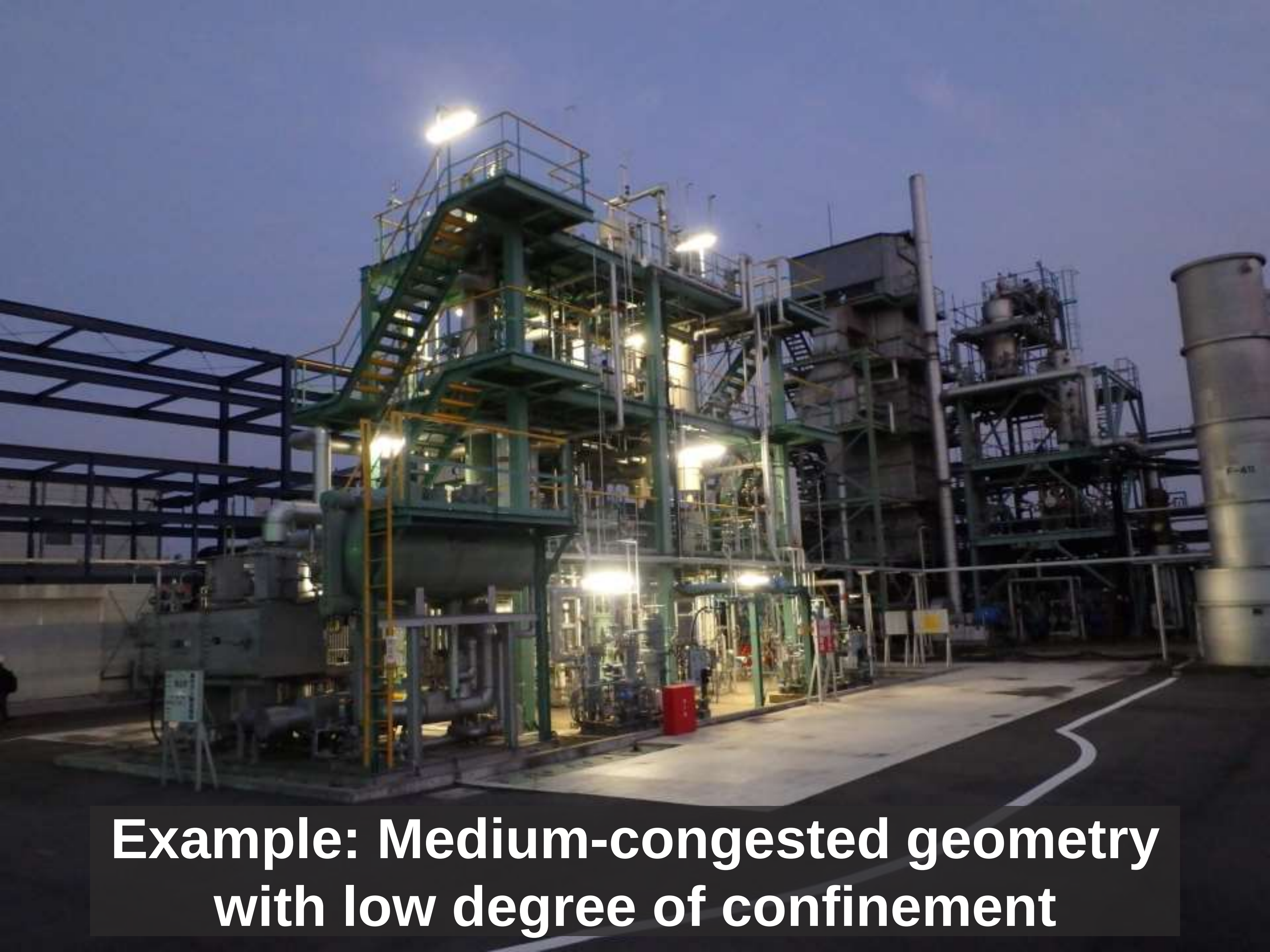


Apollo Blast simulator (courtesy of Arno Klomfass, Fraunhofer EMI)


PROSPECTS

Beyond explosions

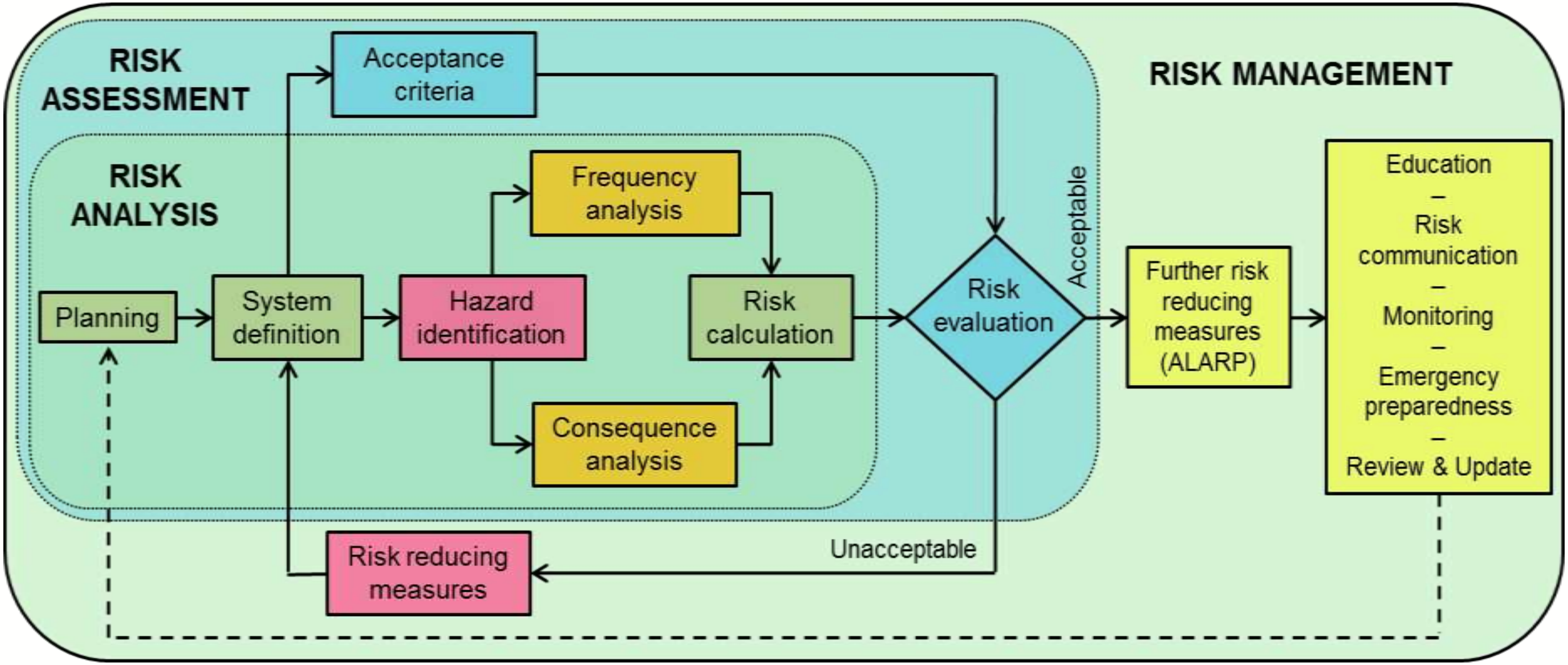
- CFD tools such as FLACS are routinely used for quantitative risk assessment (QRA).
- The modelling of complex 3D geometries in typical process facilities represents a **significant investment** for the owners and/or operators of the plants.



Example: Medium-congested geometry with low degree of confinement

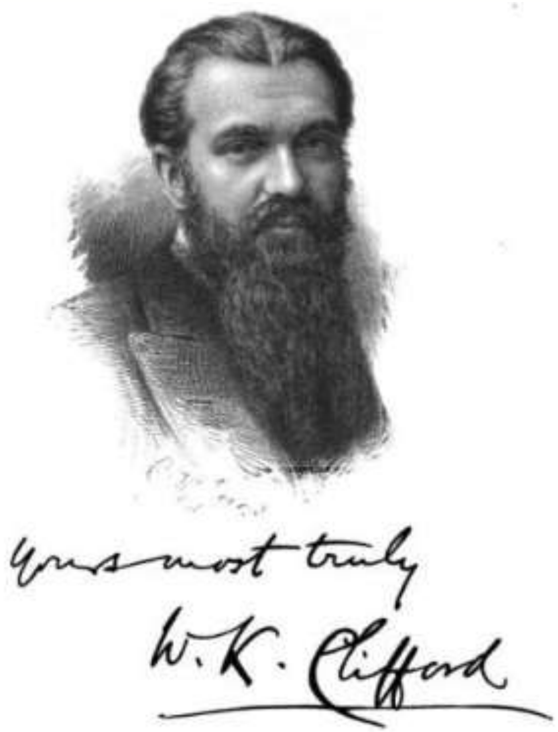
Risk management

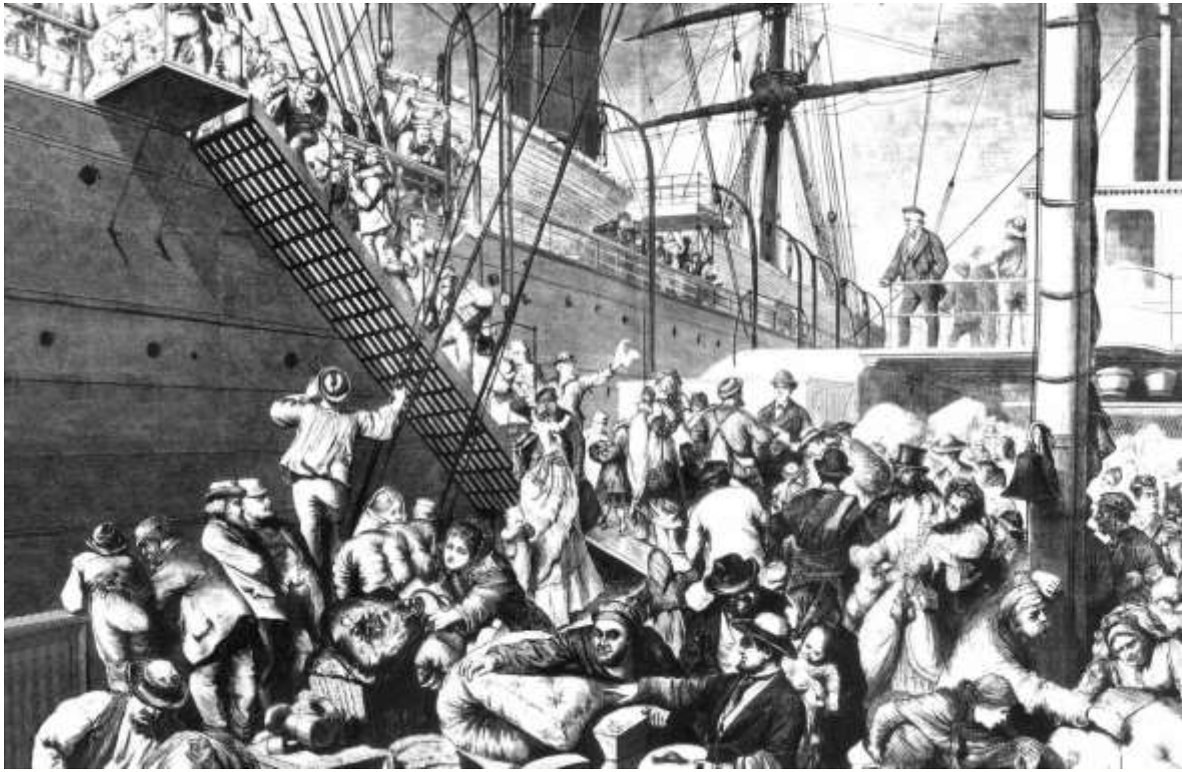
Risk management is *"the business of believing only what you have the right to believe"* DeMarco & Lister (2003): "Waltzing with Bears"

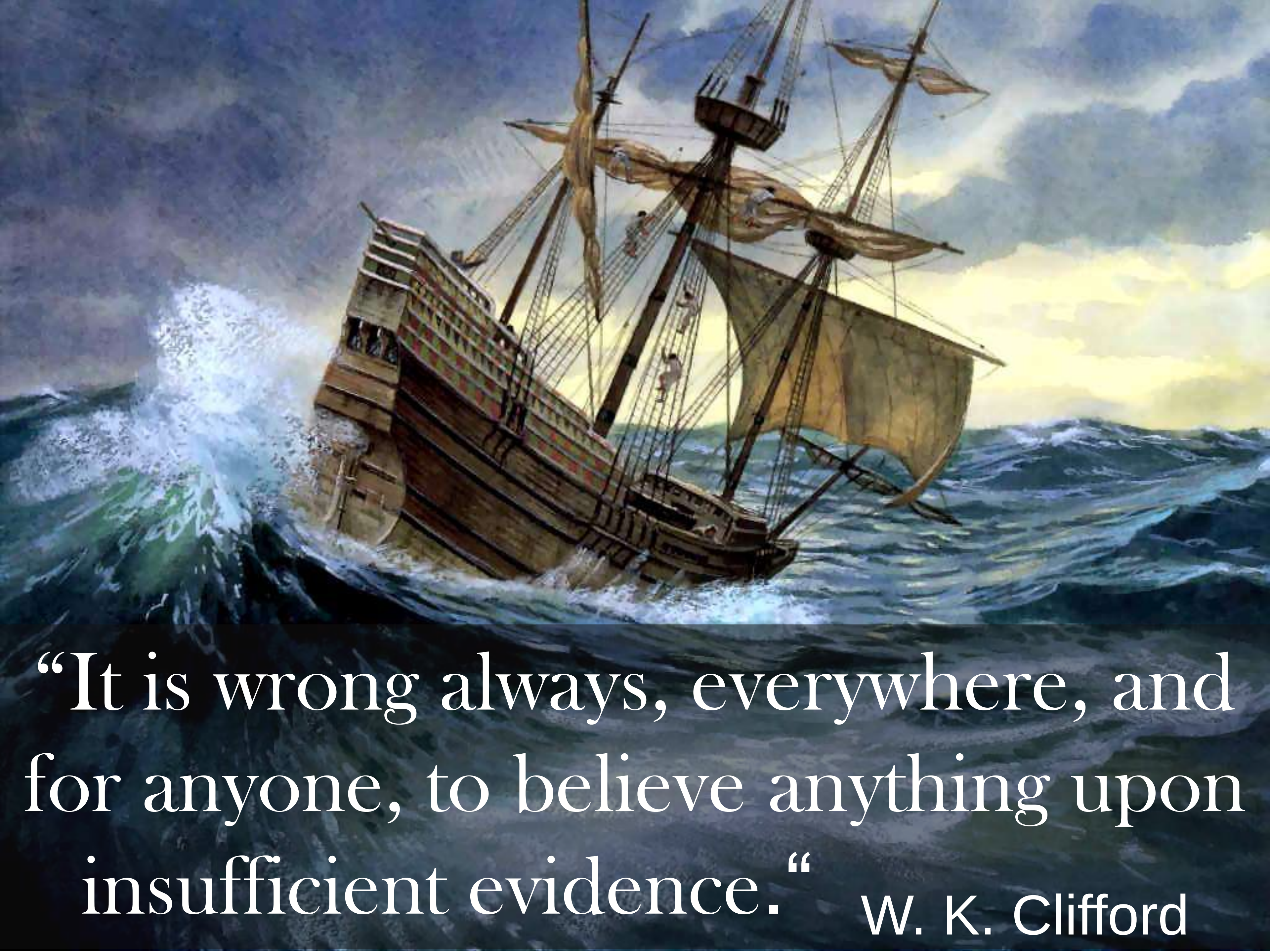


What do we have the right to believe?

- The Monthly meeting in *London's elite Metaphysical Society* at Grosvenor Hotel, London on 11 April 1876
- William Kingdon Clifford (1845-1879): «**The Ethics of Belief**»






"It is wrong always, everywhere, and for anyone, to believe anything upon insufficient evidence."
W. K. Clifford

Motivation

- The purpose of risk assessments include:
  - Systemizing knowledge and uncertainties about phenomena, processes and activities in systems,
  - Describing and discussing the results of the analysis in order to provide a basis for evaluating what is tolerable and acceptable,
  - Comparing and optimizing different design options and risk reducing measures.
- There is significant uncertainty associated with most risk assessments – however, this may be of secondary importance as long as the use of procedures and information* is consistent.

* Data, Assumptions, Knowledge, etc.

Motivation

- Numerous factors influence the level of safety an organization can achieve for a given system:
  - Safety culture
  - Potential for loss
  - Maturity of the technology
  - Risk perception / awareness
  - Safety functions and processes
  - Safety training & emergency preparedness
  - Relevant standards and legislation
  - etc.

Hierarchy of principles for risk reduction:

- Inherent safety
- Prevention
- Passive mitigation
- Active mitigation
- Procedural safety
- …

Motivation

- Statistical records from accidents and near misses demonstrate that engineered safety and administrative procedures cannot replace risk awareness, competence and a healthy safety culture:
  - Human errors account for about 80 percent of all events – only 20 percent involve equipment failure [DoE].
  - About 70 per cent of the events caused by human error can be traced to latent organizational weaknesses – only 30 percent are due to mistakes by individuals [DoE]

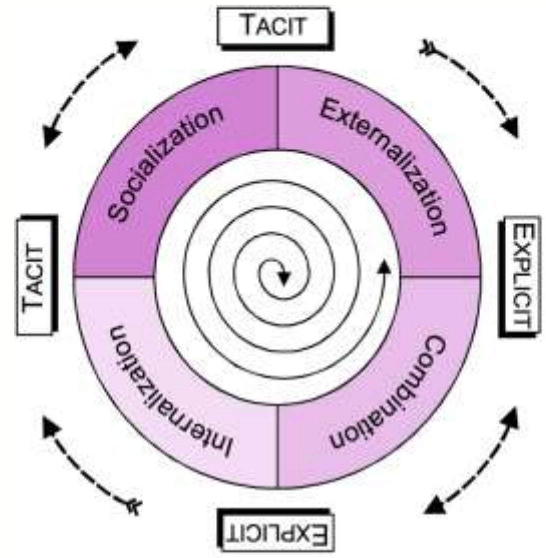
Motivation

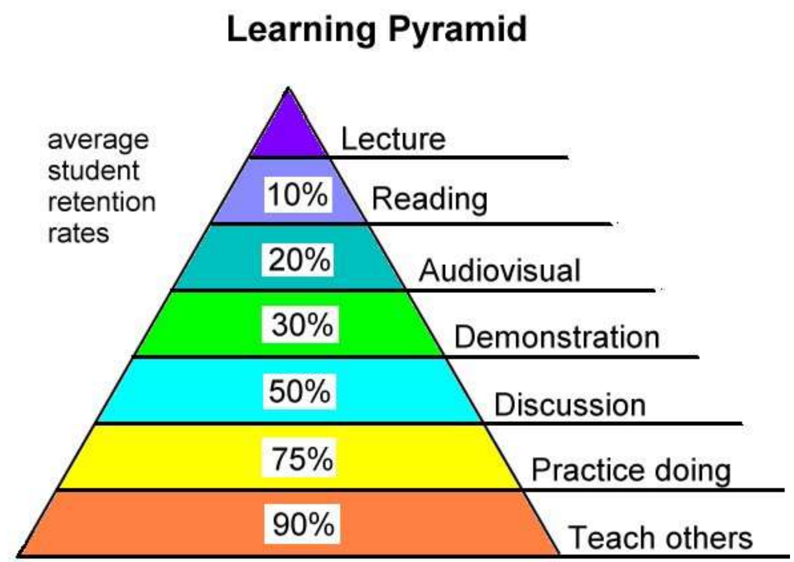
- Management of the operational risk* in industrial facilities should take into account:
  - The risk analysis/assessment
  - Previous events and near misses
  - Safety barriers / risk-reducing measures
  - Modifications and the age of the installation
  - Technological developments
  - The likelihood of natural disasters and malicious attacks
  - Safety culture, risk awareness, etc.

* **Risk management** refers to a coordinated set of activities and methods used to direct an organization and to control the risks that can affect its ability to achieve its objectives.

What if …

- We could extend the use of detailed 3D models to other aspects of risk management than ‘simple’ QRAs?
- We could create a framework for risk management that facilitates learning in organizations through discussion and practice?
- We could use virtual site-specific geometry models, continuously updated (“as is”, not “as built”) in the daily operation of process plants?
- We could define the next paradigm in risk management!





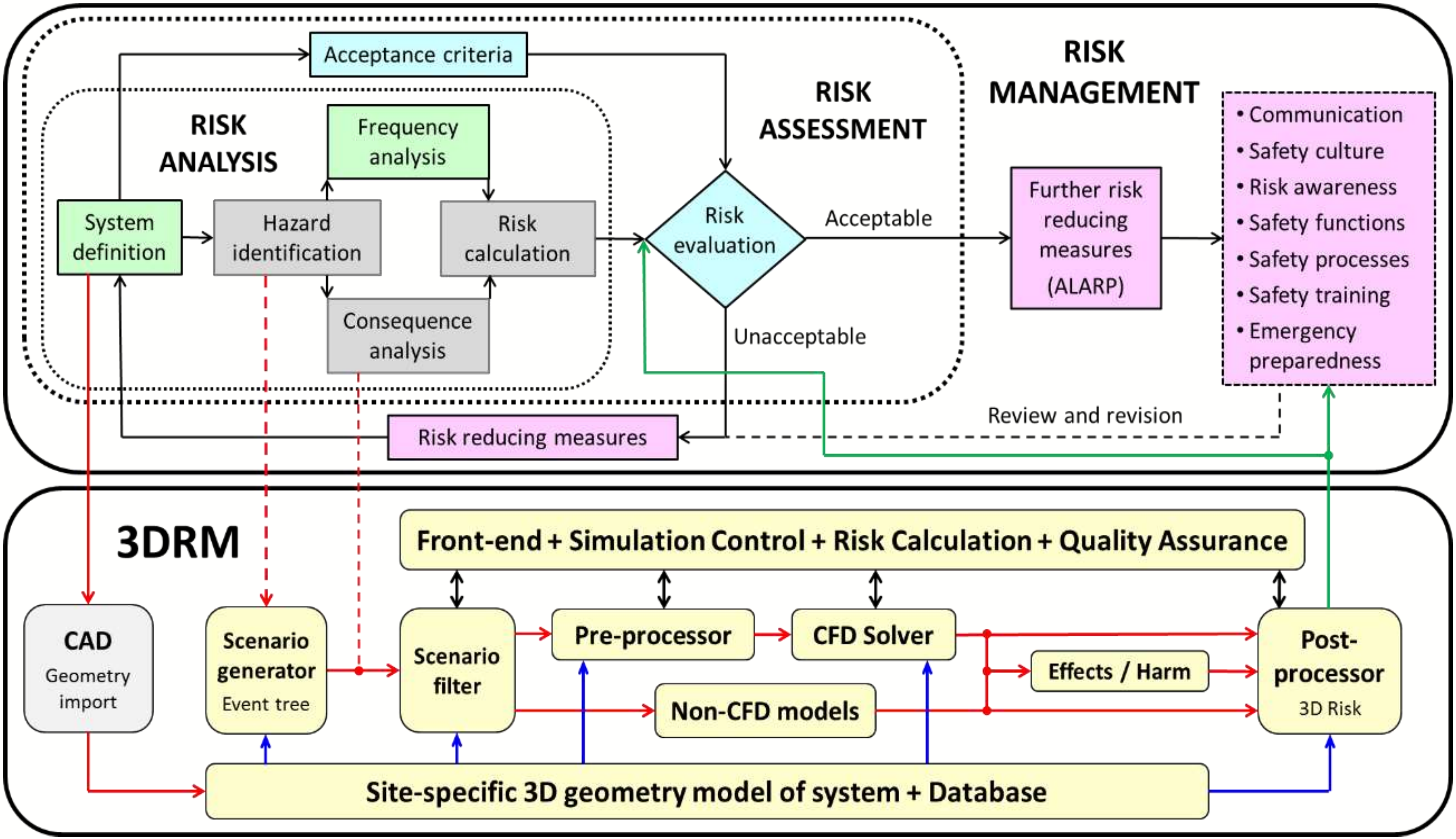
Source: National Training Laboratories, Bethel, Maine

3DRM

3D Risk Management (3DRM)

- 3DRM is an integrated risk management framework for a specific facility, characterized by interactive use of a detailed 3D geometry model, a CFD tool, and other models and libraries.
- Within the 3DRM framework, the quantitative risk assessment (QRA) becomes a (more or less) continuous processes that evolves throughout the lifetime of the facility.
- Realization of the 3DRM concept entails both development of software products and related consulting services.
- The 3DRM concept is inspired by Agile principles for software development, which put particular emphasis on people, teams, continuous integration and knowledge sharing in organizations.
- 3DRM is <u>not</u> an ‘expert system’!

Schematic representation of 3DRM



Typical workflow for QRA part

- Importing (or manually constructing) the 3D geometry model for the system.
- Identifying and registering inventory of hazardous materials in the virtual 3D model.
- Identifying and registering potential release locations in the virtual 3D model – set up links to inventory.
- Identifying and registering potential ignition sources in the virtual 3D model.
  - Two main categories: Specified location (turbines, flares, etc.) and distributed (hot work, lightning, etc.).
- Identifying and registering main safety functions in the virtual 3D model (post-processing)
- Registering personnel densities in virtual 3D model (post-processing – personnel risk).
- Registering relevant boundary conditions: terrain, wind rose, relevant codes and standards, …

Communication

- Simulating selected scenarios (automated process):
  - Wind simulations – provides the initial conditions for:
  - Release and dispersion scenarios (flammable/toxic) – provides the initial conditions for:
  - Detector optimization studies based on 3D concentration probability density functions, and
  - Simulation of jet and pool fire scenarios, and
  - Simulation of gas explosion scenarios, and
  - Simulation of escalating accident scenarios.
- Estimating the effect (harm) to structures (including structural response) and main safety functions.
- Estimating the effect (harm) on personnel caused by physical parameters (personnel risk).
- Optimizing detector layout or other prevention and mitigation measures based on harm criteria.

Can be automated

- Calculating and visualizing risk contours in the virtual 3D model.
- Analysing results, implementing risk-reducing measures, ALARP, updating calculation, …

…

Towards 3D risk management

- The 3DRM concept is not limited to QRAs, and operative use of the virtual 3D model may include aspects such as:
  - Visualization of the 3D geometry model, including metadata, in the control room, at training centres, on portable devices, etc.
  - Visualization of scenarios from QRA (training, …), incidents, etc.
  - Hazardous area classification – visualizing zones and equipment
  - Work permits – highlighting specific areas during maintenance
  - Interactive training/site visits for employees, subcontractors, etc.
  - ISO 9000 compliance – issue tracking, documentation, etc.
  - Gas detector optimization based on QRA – various optimization criteria: detecting leak, minimizing damage, etc.
  - Emergency preparedness and emergency response: GPS tracking in 3D geometry, visualizing sensors and alarms, etc.
  - Etc.

Pros and cons of 3DRM

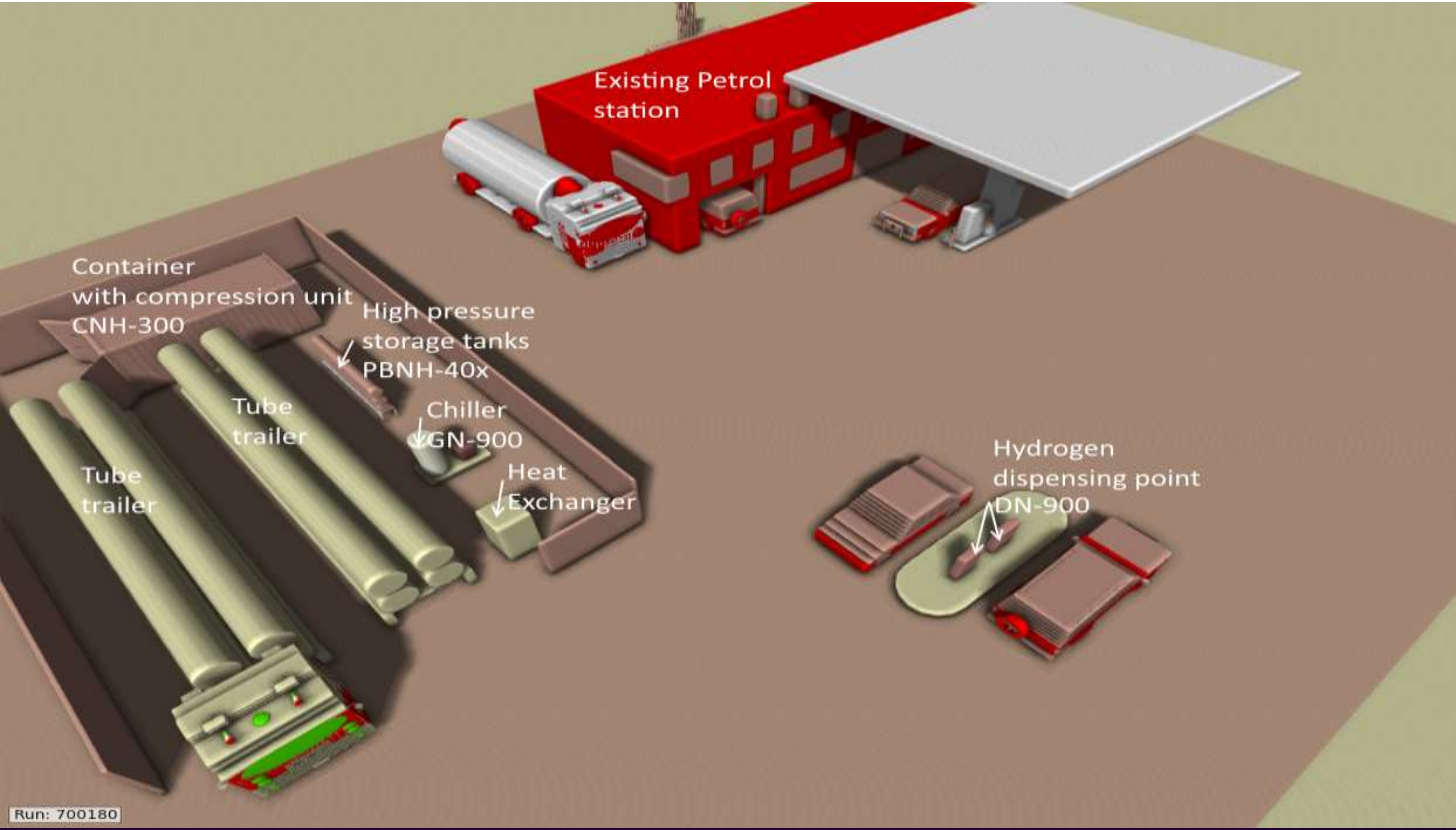
- Advantages:
  - Step-wise implementation
  - Communication with and/or between stakeholders
  - Competence building: CFD vs. Engineering models, …
- Limitations:
  - Implementation cost
  - Not an ‘expert system’ (probably an advantage …)
  - Full implementation requires dedicated end-user

Case study

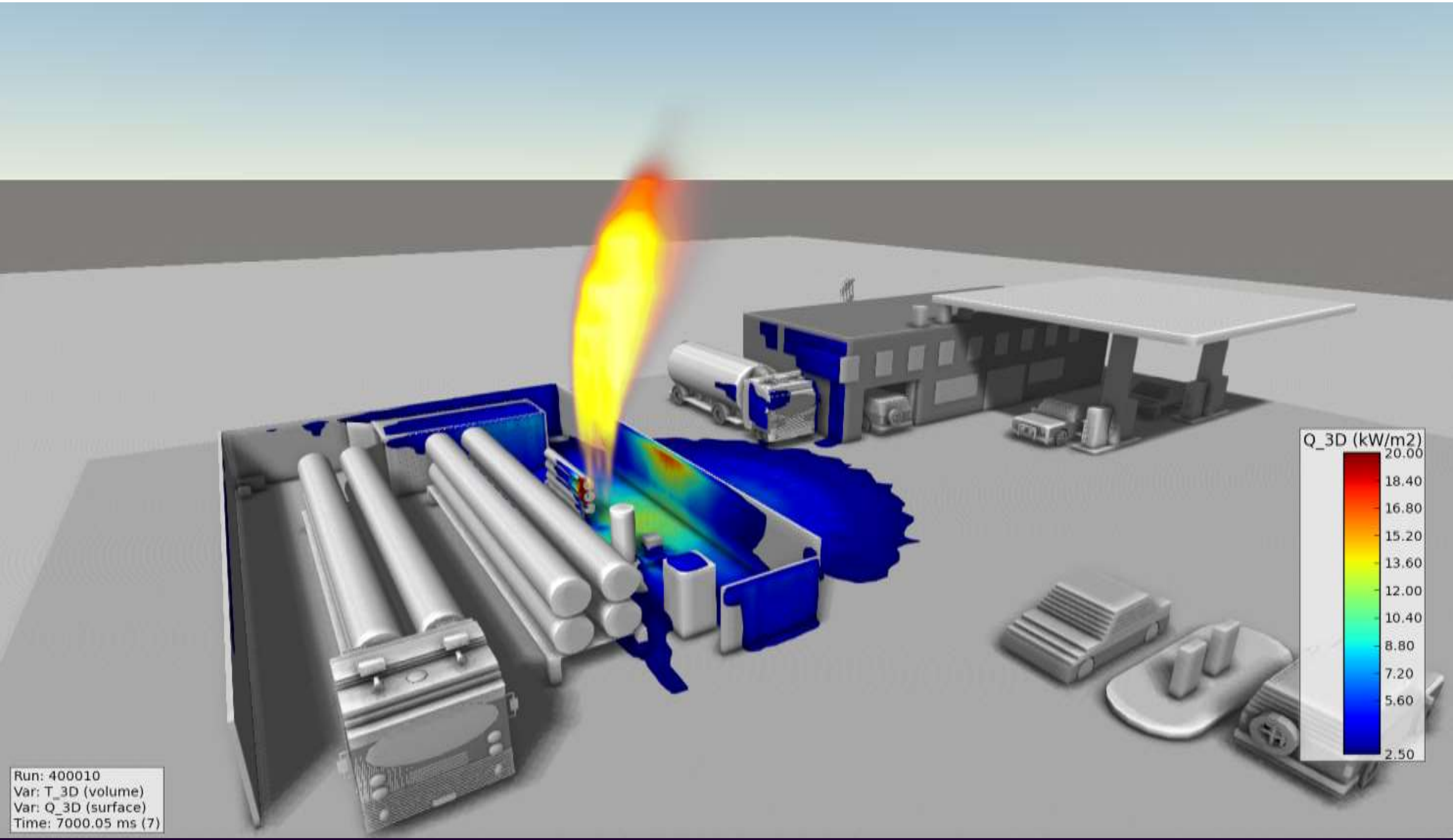
- … while we are waiting for the dedicated end-user.
- Generic filling station: 100 kg day^{-1} reference [H2FIRST]
  - Compressor in 20 ft. ISO container compresses hydrogen from tube trailer to high-pressure storage tanks.
- Simplified fault trees [HyRAM / Sandia reports] and event trees for selected accident scenarios:
  - 168 dispersion simulations
  - 168 jet fire simulations
  - 672 gas explosion simulations

FLACS simulations:
- 1008 simulations
- 2-3 days on HPC cluster

Hypothetical filling station

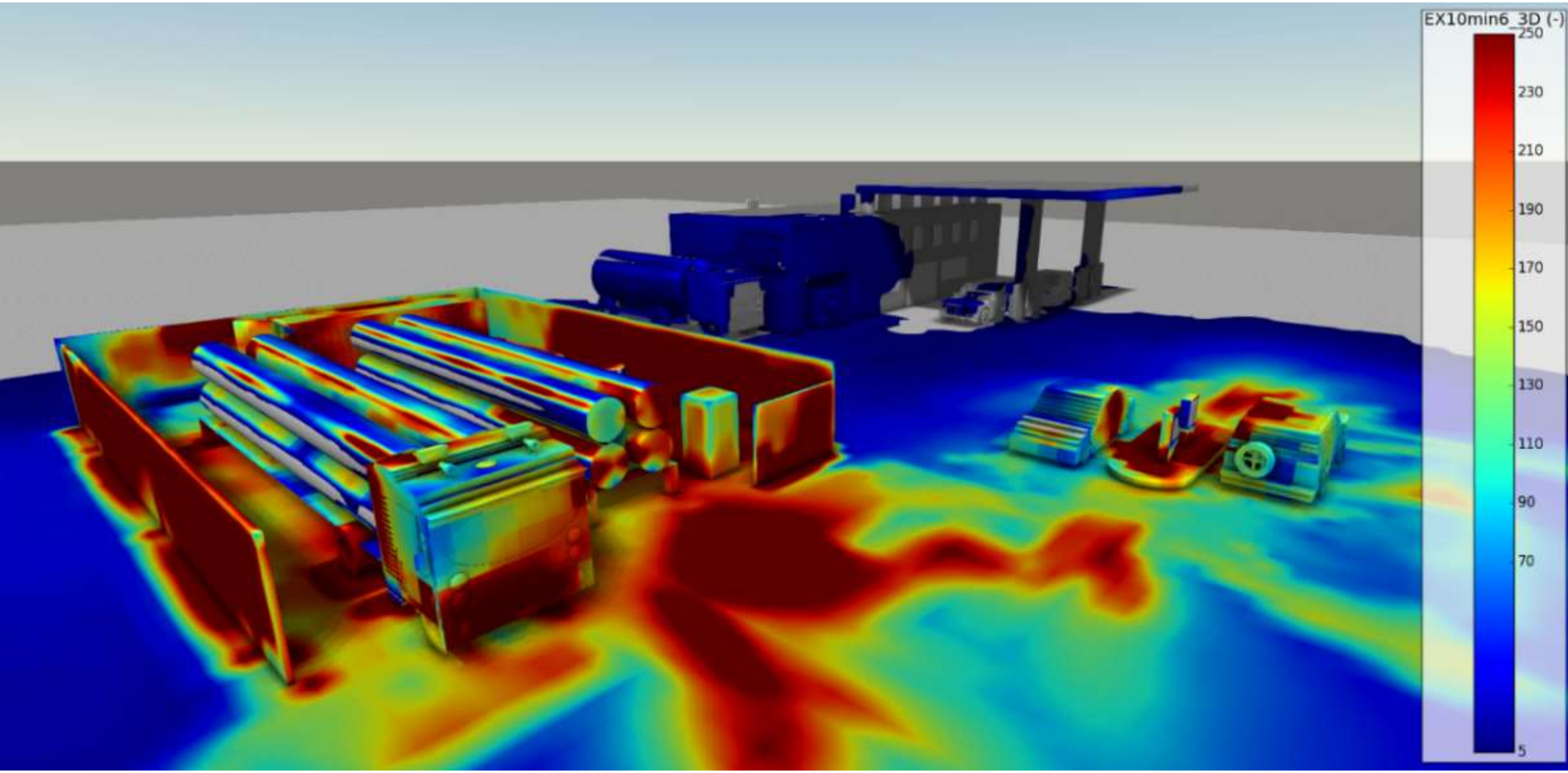


Example: Jet fire scenario

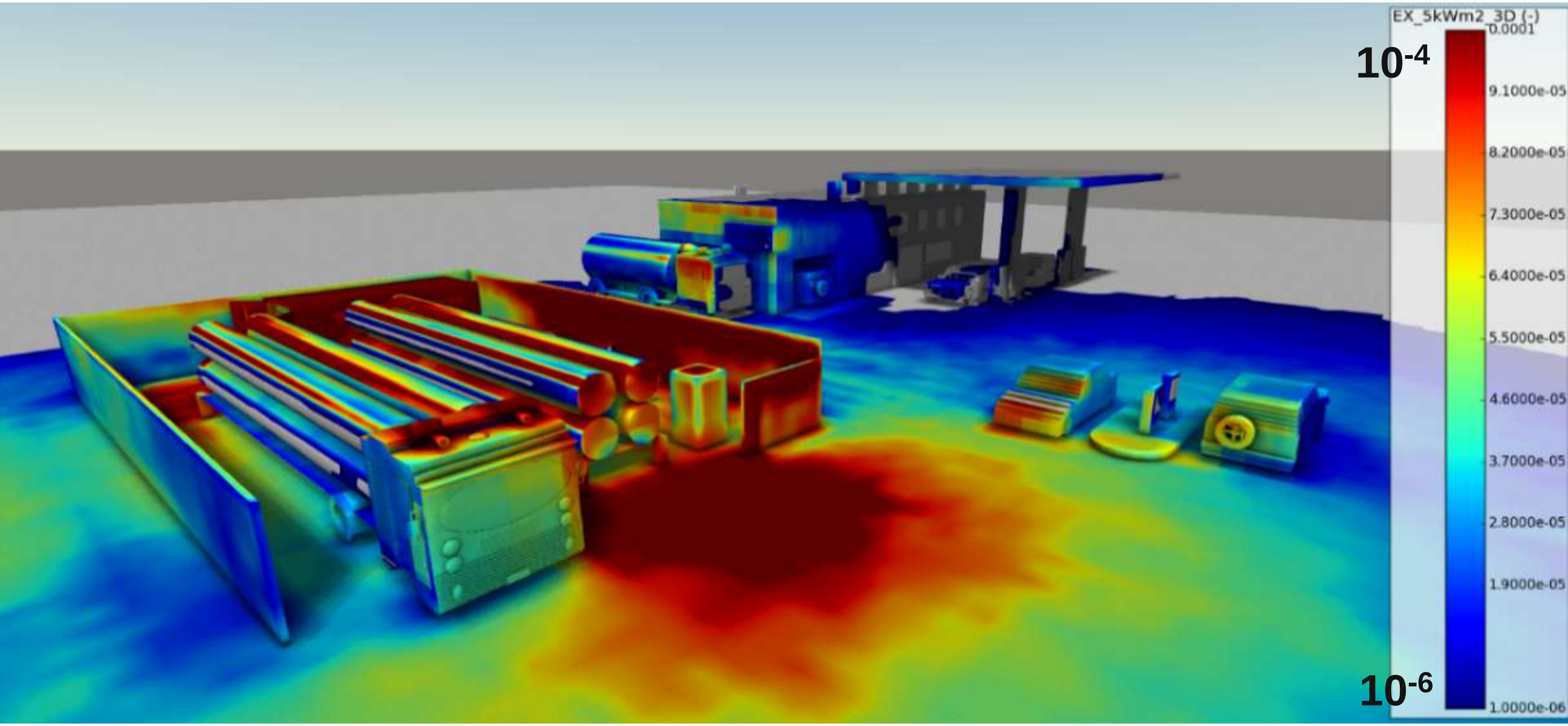


FLACS

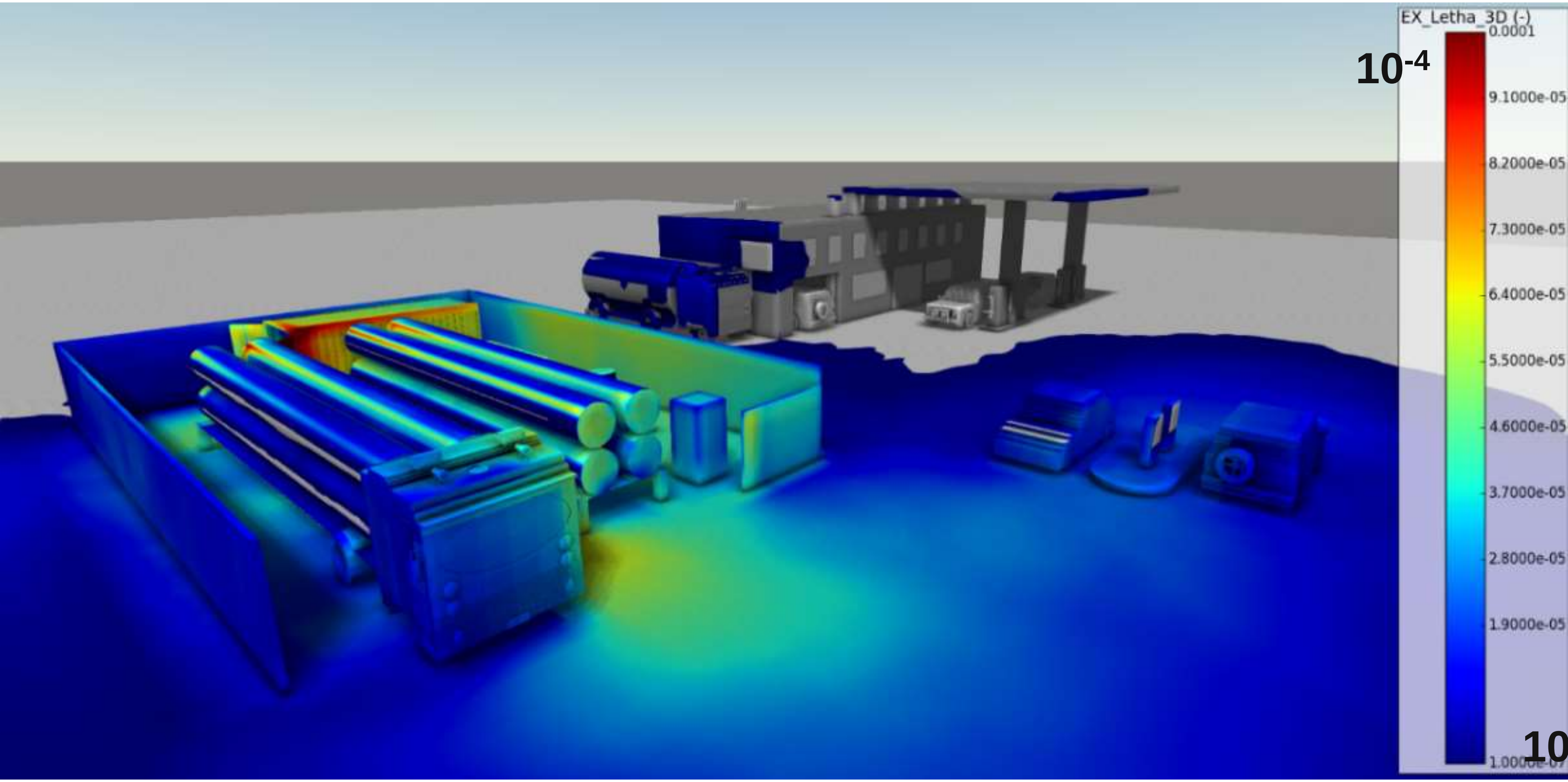
Heat radiation contours: $f > 10^{-6}$ yr^{-1}



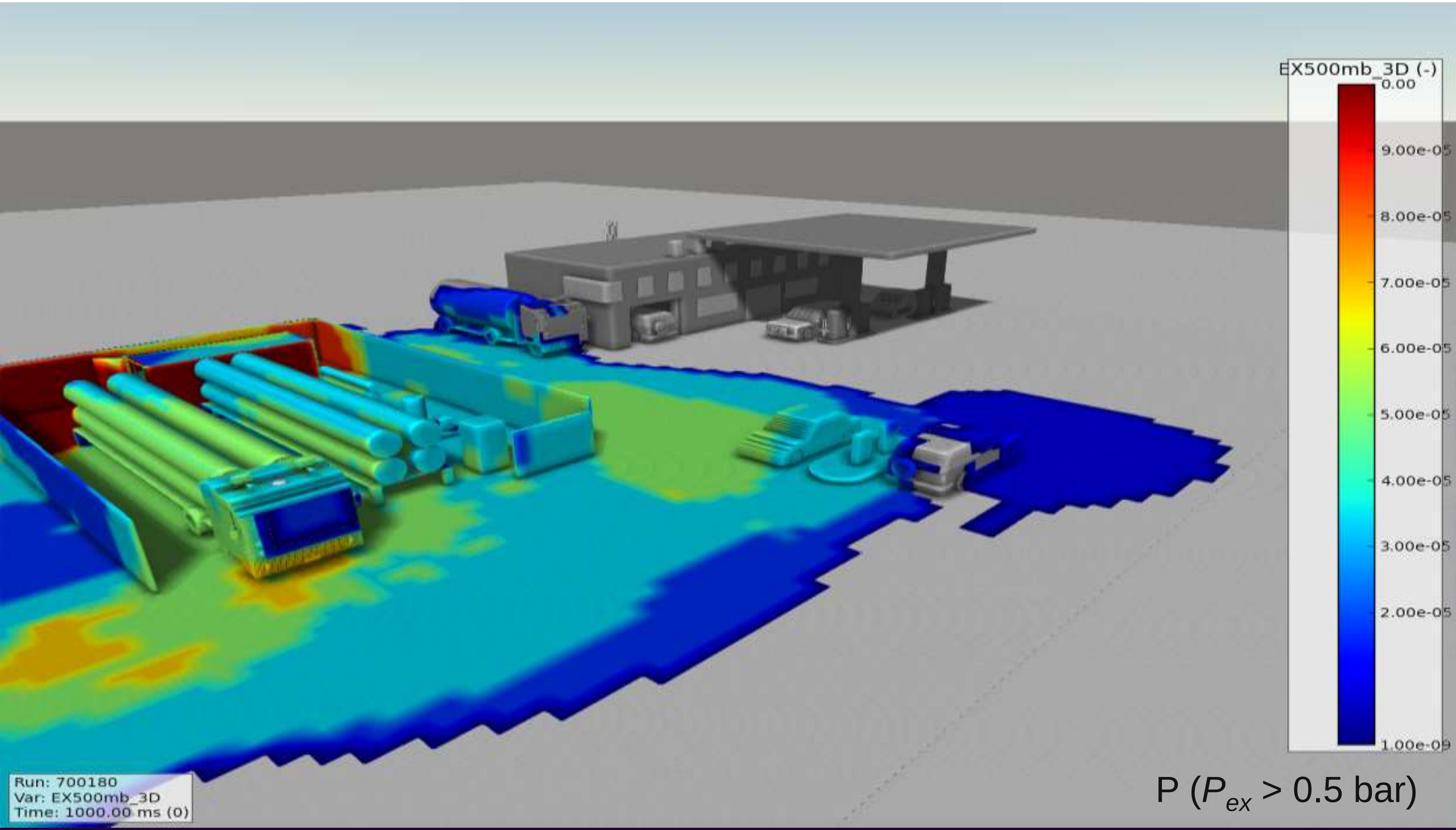
Frequency contours: Q_{rad} > 5 kW m^{-2}



Lethality frequency – jet fire

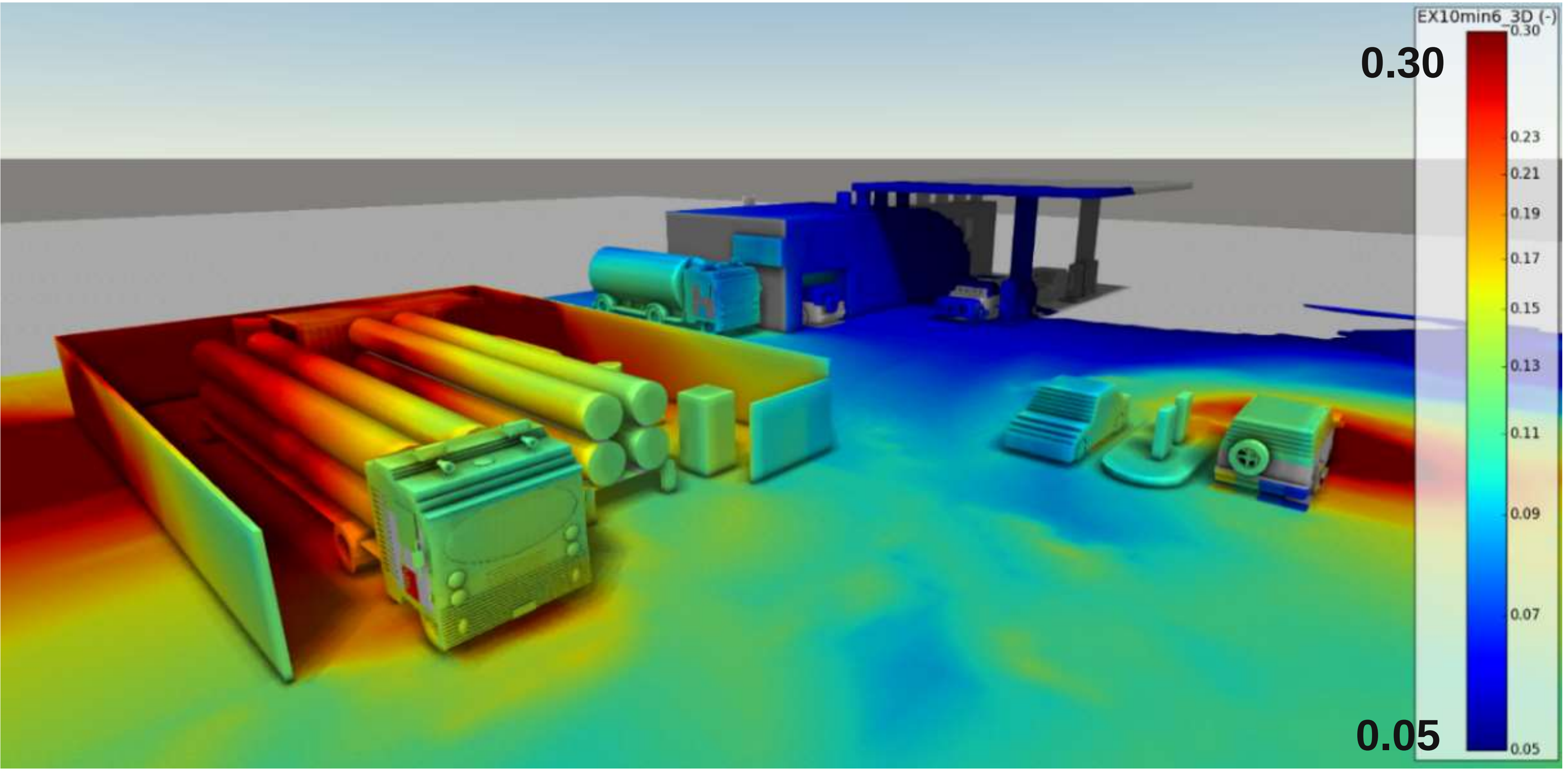


Frequency contours: P_{ex} > 0.5 bar



P (P_{ex} > 0.5 bar)

Over-pressure contours: $f > 10^{-6}\ yr^{-1}$



Summary

- Modelling of explosions occurs at various levels:
  - Detailed numerical simulations aimed at revealing fundamental physical phenomena.
  - Pragmatic CFD modelling, often based on the porosity/distributed resistance (PDR) approach, aimed at providing engineering estimates for industrial design.
  - Simpler engineering models, typically based on empirical correlations.
- There is increasing focus on model validation:
  - Providers of software products for safety applications need to document validation against relevant large-scale experiments.
  - There is an urgent need for more reliable predictions (indications) of the occurrence of deflagration-to-detonation-transition (DDT) in large-scale complex geometries.
  - Simulation of safety gap scenarios provides an interesting challenge for modellers.
- The 3DRM concept from Gexcon has several advantages:
  - It combines state-of-the-art CFD/PDR models and simpler engineering models
  - The primary focus is on risk communication in organizations and between stakeholders

Acknowledgements

- The Research Council of Norway (RCN) supports the **Hy3DRM project** under the ENERGIX program, and the PhD projects under the Industry PhD funding scheme.

- Statoil, Total, ExxonMobil, ENGIE (GDF Suez), DNV GL and BP sponsor JIP MEASURE. The experimental campaign is conducted in cooperation with Shell.

- The European Commission supports the **HySEA project** through the Fuel Cells and Hydrogen Joint Undertaking (FCH 2 JU) under the Horizon 2020 Framework Programme for Research and Innovation.

Questions?