

## Hydrogen safety: modeling of flame acceleration and detonation onset

### Motivation

Hydrogen, increasingly popular as an alternative fuel, presents unique challenges due to its high reactivity and associated ignition and explosion hazards. With the expected rise of hydrogen production and use in both public and industrial locations, understanding and predicting the consequences of gas explosion are crucial for ensuring safety. Hydrogen is stored in tanks in liquid or gaseous form under high pressure. If the pressure in the tank rises due to any technical failure, some hydrogen must be released to prevent the tank from rupturing. The sequence of events involved in accident scenarios typically include the release of fuel into congestion, flow-obstacle interactions (responsible for the generation of background turbulence that later feed into the flame dynamics), the formation and delayed ignition of a reactive cloud, the propagation and acceleration of the resulting flame front and its possible transition to detonation. Appropriate modeling of the underlying physics will ultimately enable accurate overpressure predictions and safer design of facilities. The goal of this project is to study under which conditions the released hydrogen, if ignited, can lead to a detonation and how this can be prevented. In this project, fully resolved simulations of canonical problems such as flame propagation in channels with obstacles will be performed to inform model development that may be used for industrially relevant scales and congestion types. Shell has an extensive database of large-scale explosion experiments that can be used for validation.

### Project description and research goals

The aim of this project is to set up simulations for different configurations where hydrogen flames transition into detonations. The focus lies on the influence of detailed diffusion processes, the initial distribution of hydrogen, the turbulence intensity as well as the geometry where the hydrogen burns. Additionally, the feasibility of different simulation approaches should be investigated as well as up-scaling of the observed phenomena be discussed. Figure 1 (left) shows a large-scale explosion of a hydrogen/air cloud engulfing a piece of congestion that could be typically found in process facilities. In Fig. 1 (right), simulation results of a canonical configuration (i.e. a wavy channel) where an initially slow hydrogen flame transitions into a detonation front is shown.

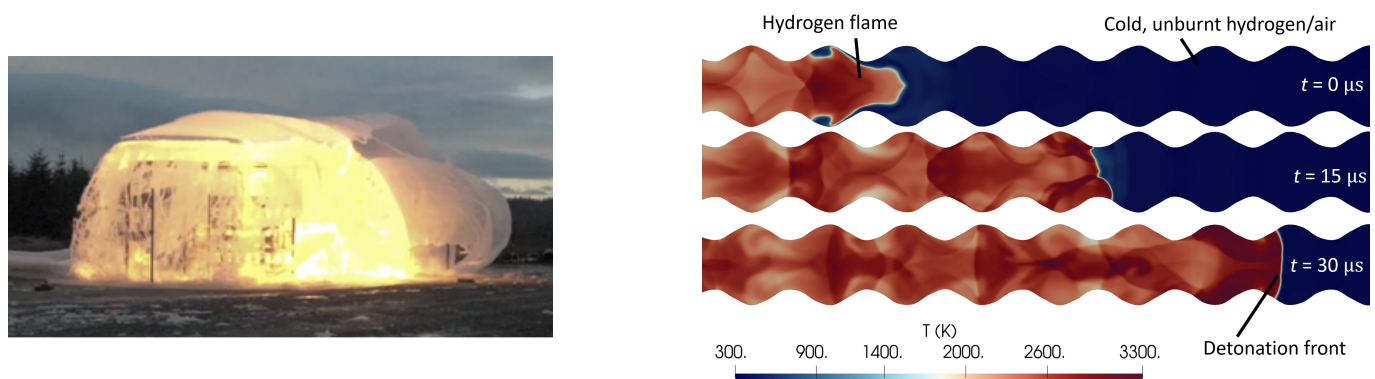


Figure 1: Left: Experiment of hydrogen detonation at Shell. Right: Simulation of a hydrogen flame that transitions into a detonation.

Simulation tools are available. Therefore, this work will focus on conducting the simulations and postprocessing the results. Due to the collaboration with Shell, students will be able to interact with explosion/combustion scientist from Shell, Netherlands. Short-term visits to the Energy Transition Campus in Amsterdam can also be arranged.

### Tasks

- Literature review to learn about deflagration-to-detonation transition and simulations with OpenFOAM;
- Perform numerical simulations of the development of detonations for hydrogen flames;
- Assess different models with regard to accuracy and simulation times, e.g. adaptive mesh refinement;
- Evaluate and analyze the simulation results;
- Write a thesis and present your results.

### Prerequisites

- Basic knowledge in fluid dynamics, programming with MATLAB, Python or similar
- Beneficial: knowledge in C/C++, experience with computational fluid dynamics (CFD), OpenFOAM

### Contact

If you are interested, feel free to contact:

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