University of
South-Eastern Norway

Faculty of Technology, Natural Sciences, and Maritime Sciences

Department of Process, Energy, and Environmental Technology

Campus Porsgrunn

Open-Source Tools for Advanced Modeling of Hydrogen Explosions and Safety Insights

***HySchool* Days 2025**

Porsgrunn, April 2th , 2025

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School.no

12+3 min

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Process Safety, Combustion and Explosion Research Group

Main Supervisor: Professor **Knut Vågsæther**, *USN*
Co-Supervisor: Associate Professor **Mathias Henriksen**, *USN*

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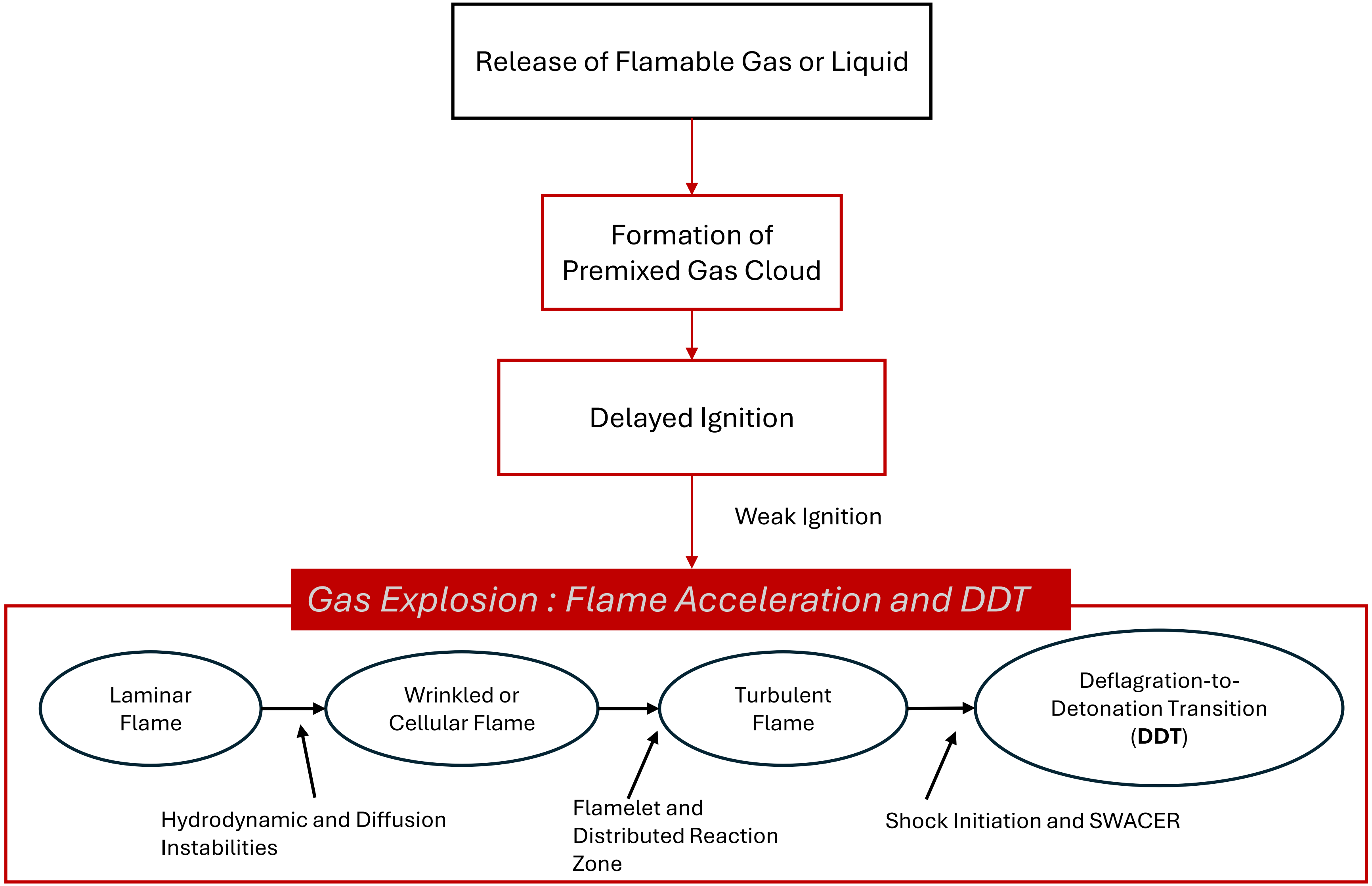
INTRODUCTION

Event Tree Analysis of Potential Consequences from Loss of Containment in Hydrogen Systems



Bjerketvedt, D. et al., 1997. Gas explosion handbook. J. Hazard. Mater. 52, 1–150.
Flame Acceleration and DDT in Nuclear Safety, OECD NEA Report NEA/CSNI/R(2000)7, August 2000.

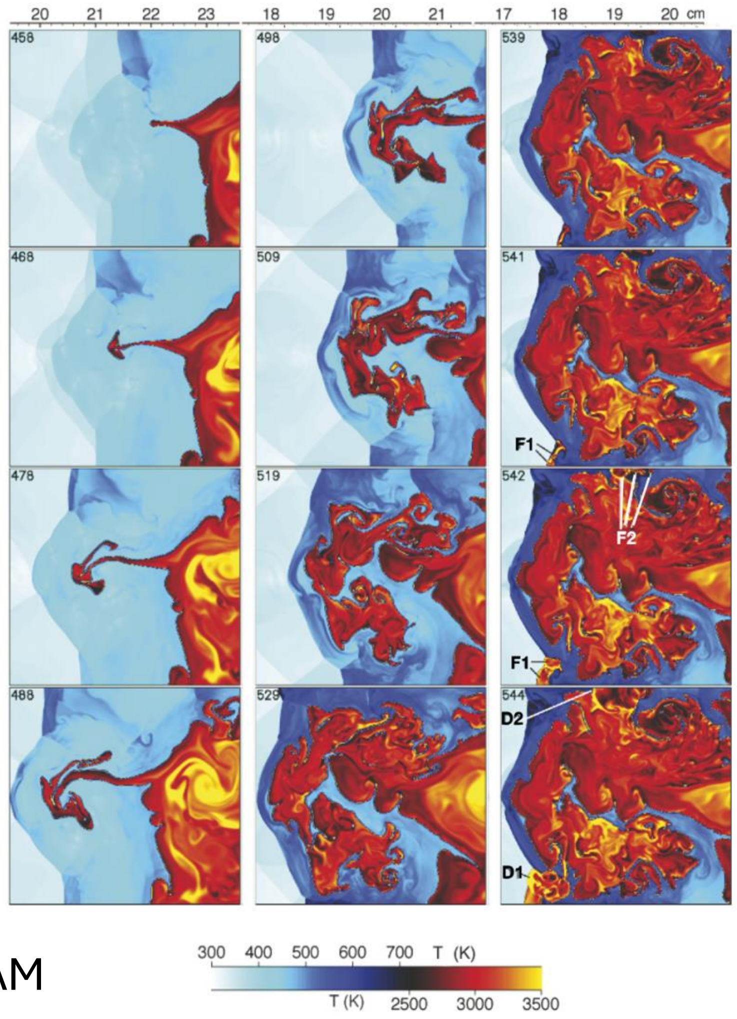
Deflagration-to-Detonation Transition

Oran, E. S., & Gamezo, V. N. (2007). *Origins of the deflagration-to-detonation transition in gas-phase combustion*. **Combustion and Flame**, 148(1–2), 4–47.

- Detonation research began in the late 19th centuary

reactants

- **Chapman–Jouguet (CJ) theory**
- **Zel'dovich–von Neumann–Döring (ZND) model**
- **Qualitative understanding of transition to detonation**
  - "Explosion within an explosion"



Numerical DDT

- Extremely high spatial and temporal resolution
  - 20 computational cells per half-reaction length
- ***Safety analyses***: macroscopic effects such as **flame speeds** and **pressure loads** on structures
- *Vågsæther K. et al. (2007)* introduced the methodology for modeling DDT on course meshes

K Vaagsaether, V Knudsen, and D Bjerketvedt. "Simulation of Flame Acceleration and DDT in H2-air Mixture with a Flux Limiter Centered Method". International Journal of Hydrogen Energy 32.13 (Sept. 2007), pp. 2186–2191.

- *Ettner F. et al. (2014)* implemented the modelling approach in OpenFOAM

Florian Ettner, Klaus G. Vollmer, and Thomas Sattelmayer. "Numerical Simulation of the Deflagrationto-Detonation Transition in Inhomogeneous Mixtures". In: Journal of Combustion 2014 (2014), pp. 1–15.

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Problem statement

Main objective

Develop a predictive model for deflagration-to-detonation transition (DDT) to improve consequence analysis in hydrogen safety applications.

Secondary Objectives

- Develop a CFD solver in **OpenFOAM** to simulate flame acceleration (FA) and DDT in a single framework
- Accurately predict DDT in **homogeneous** and **inhomogeneous** gas mixtures using **coarse meshes**
- Ensure **scalability** and **applicability** to full-scale hydrogen safety scenarios

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Methodology

Numerical Modeling

- **Computational Fluid Dynamic (CFD) software** OpenFOAM
  - Compressible ***Navier-Stokes Equations***

Criteria	Pressure-based Solvers (SIMPLE/PISO/PIMPLE)	Density-based Solvers (Riemann solvers)
Flow Regime	Incompressible to mildly compressible flows	Compressible flows, shocks, supersonic/hypersonic conditions
Equation Coupling	Weak coupling of pressure-velocity equations	Fully coupled solving of conservation equations
Numerical Stability	Implicit(semi) Solvers → Stable for larger time-steps	Explicit solvers → CFL limited → smaller time-steps
Computational Cost	Lower computational cost per iteration	Higher computational cost per iteration
Shock Handling	Inadequate	Handles shocks and discontinuities robustly
OpenFOAM 9 default solvers	Combustion: XiFoam, reactingFoam, …	Combustion: no default Non-combustion: rhoCentralFoam

Libraries developed by ***blastFoam****

**An Open-Source CFD Solver for Compressible Multi-Fluid Flows with Application to Blast and Explosions*. Retrieved from https://www.blastfoam.org/

Combustion Model

- Base Solver: The standard OpenFOAM ***XiFoam*** solver
  - Weller's Flame Wrinkling Model
  - Flamelet Regime

$$\frac{\partial(\rho b)}{\partial t} + \nabla\cdot(\rho\mathbf{u}b) - \nabla\cdot\left(\frac{\mu_t}{Sc_t}\nabla b\right) = \rho_u S_u \Xi|\nabla b|$$

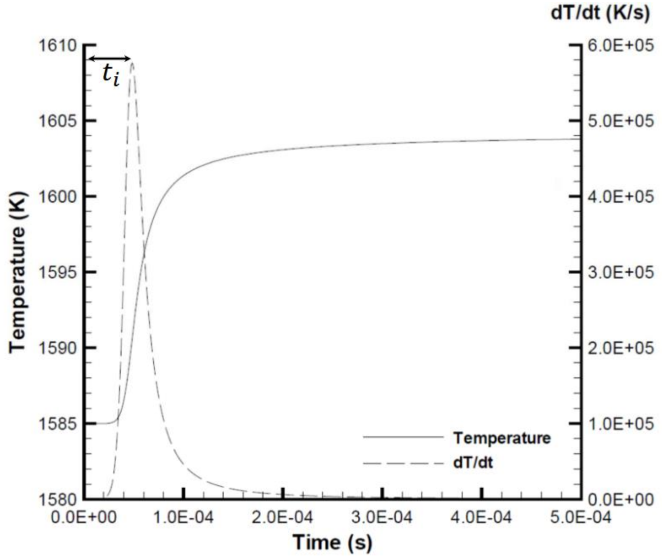
- Implementation of ***auto-ignition model***
  - Cantera and SDToolBox
  - Induction Time
    - Constant Volume Explosion

Cantera
Chemical Kinetics • Thermodynamics • Transport Processes

$$t_{\text{ind}} = t_{\text{ind}}(p, T_u, \phi), \quad \tau = \frac{t}{t_{\text{ind}}}$$

$$\frac{\partial(\rho\tau)}{\partial t} + \nabla\cdot(\rho\mathbf{u}\tau) - \nabla\cdot\left(\frac{\mu_t}{Sc_t}\nabla\tau\right) = \frac{\rho}{t_{\text{ind}}}$$

Model	t_i (μs)	Δ_i (mm)
ZND (thermicity peak)	50.4	15.4
CV (dT/dt_{max})	49.2	13.3
CP (dT/dt_{max})	45.2	14.5



- Implementation of ***detonation source term***

- Final model:

$$\boxed{\frac{\partial(\rho b)}{\partial t} + \nabla\cdot(\rho\mathbf{u}b) - \nabla\cdot\left(\frac{\mu_t}{Sc_t}\nabla b\right) = \begin{cases}\rho_u S_u \Xi|\nabla b|, & \tau < 0.99,\\ \rho\frac{1-b}{\Delta t}, & \tau \geq 0.99.\end{cases}}$$

S. Browne et al. SDToolbox - Numerical Tools for Shock and Detonation Wave Modeling, Explosion Dynamics Laboratory. Explosion Dynamics Laboratory, 2021.

Density-base solver

mech2Foam

Auto-generates a fuel-specific thermophysical properties file (Py3)

Adaptive Mesh Refinement (AMR)

OpenFOAM 9

MMXFoam

M**ulti-**M**ode-e**X**plosion-**Foam

DEFLAGRATION

AUTO-IGNITION

Python 3 using Cantera and SD Toolbox libraries script auto-generates t_{ign} look-up table file

DETONATION

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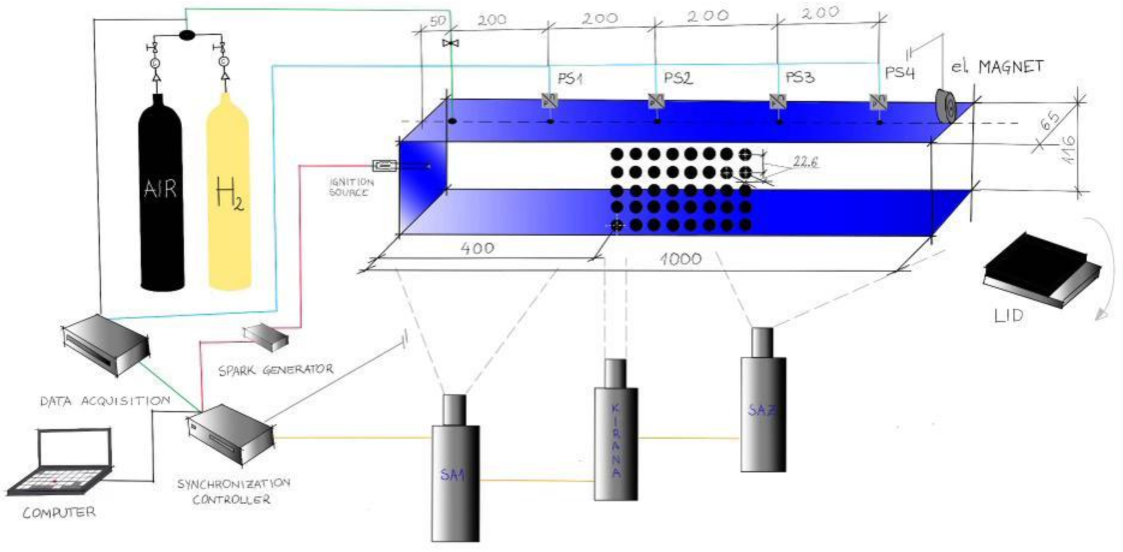
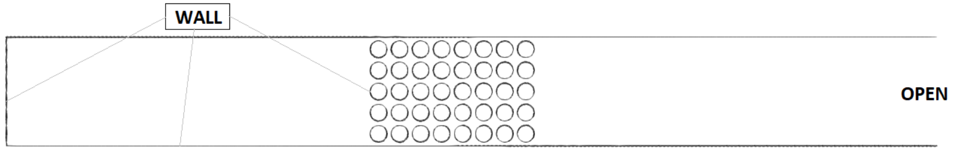
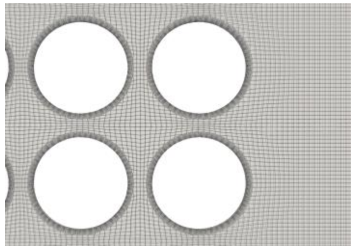
Validation Case and Results

Experimental and Numerical Setup



Experimental Apparatus:
- 1-meter rectangular open-ended explosion chamber
- 40 (18x650 mm) cylindrical obstacles → BR = 0.77
- Gas Supply System (premixed H2-air)
- Spark Ignition System and Porous Lid System
- 4 Pressure Transducers (Kistler 7001 and 603B)
- High Speed Cameras:
  - Photron SA-1 (Flame Luminosity): 8000 fps
  - Kirana (Schlieren setup): 500 000 fps
  - Photron SA-Z (Flame Luminosity): 120 000 fps
- Synchronus Triggering System and Data Acquisition

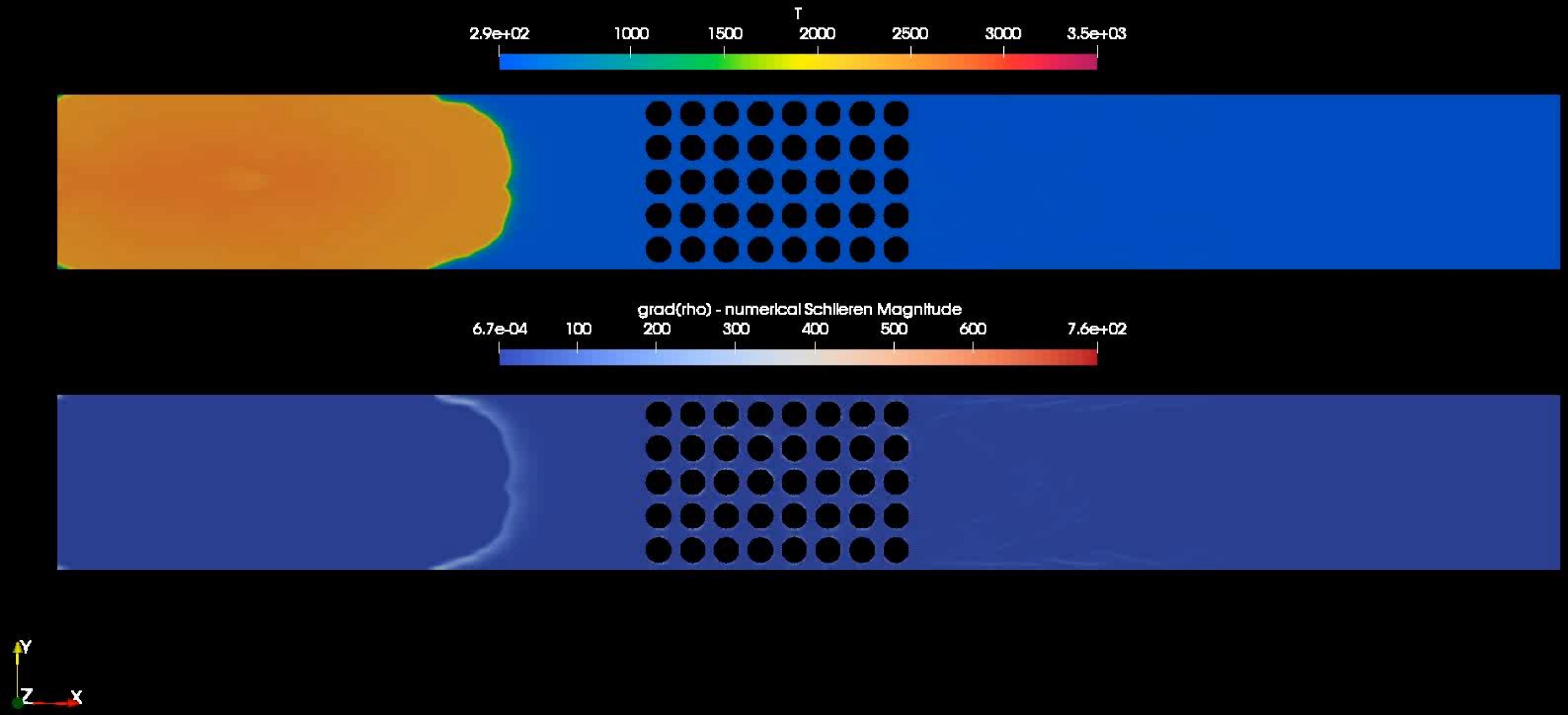




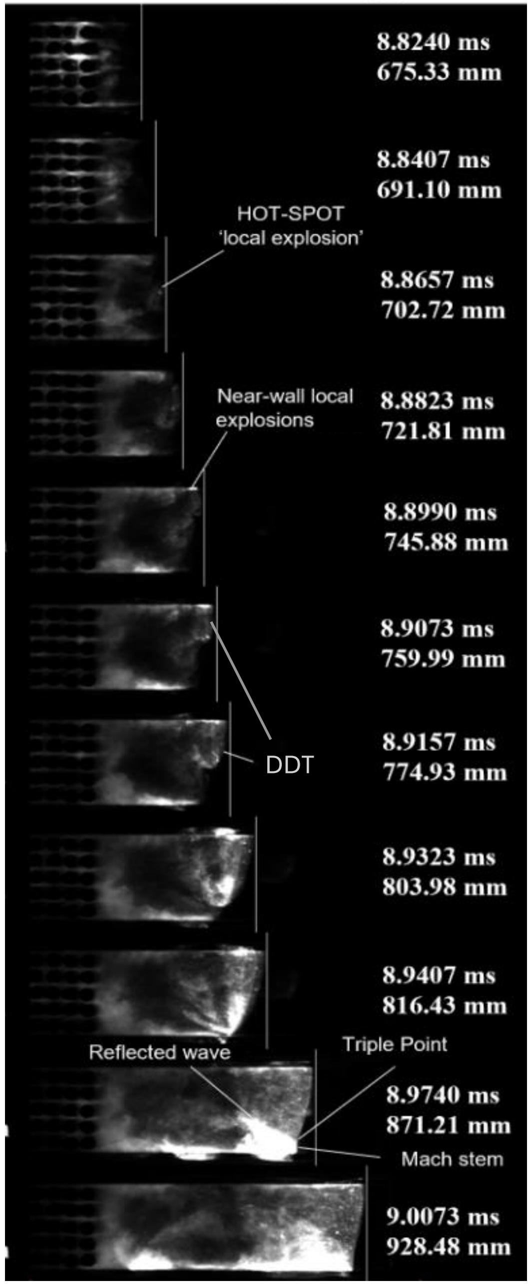
Numerical Domain and BC:
- 2D domain (1000x116 mm)
- Static and dynamic mesh
- Boundary conditions:
  - WALL: non-slip adiabatic wall
  - OPEN: total pressure

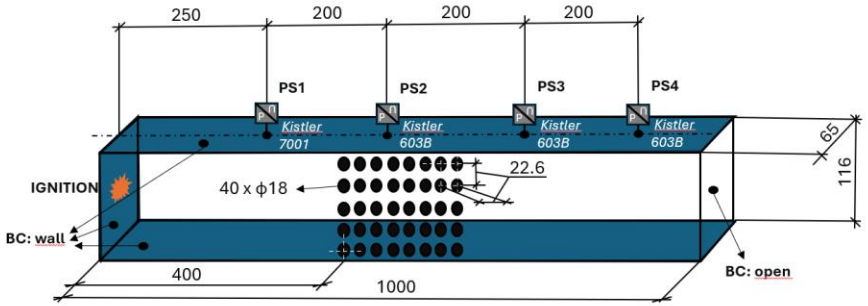
Computational Fluid Dynamic Solver:
- OpenFOAM 9: ***MMXFOAM***
- Thermopysical and Transport properties:
  - Gas Composition: Homogeneous **ϕ = 1.1** H2-air generated with ***mech2Foam***
- Turbulence model: **k-omega SST**
- Compressible solver: **HLLC** (shock capturing)
- Combustion model:
  - **Deflagration** + **Detonation** source term

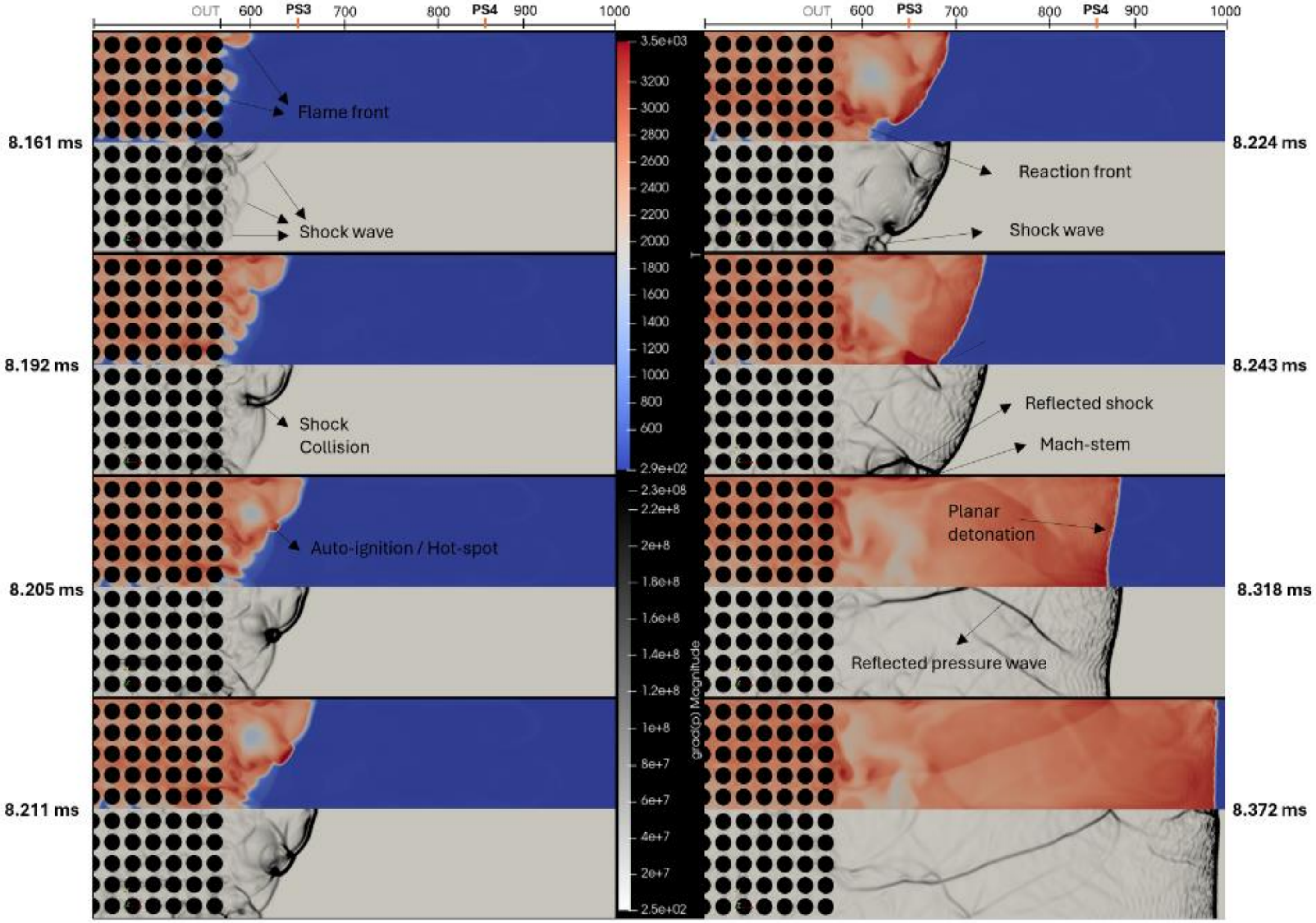
Auto-ignition ⌛


T
2.9e+02
1000
1500
2000
2500
3000
3.5e+03
grad(rho) - numerical Schlieren Magnitude
6.7e-04
100
200
300
400
500
600
7.6e+02
Y
Z
X

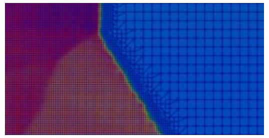
Photron SA-Z (120 00 fps): **T00062**



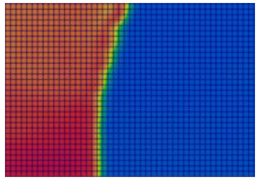




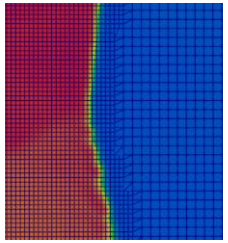
CASE 1



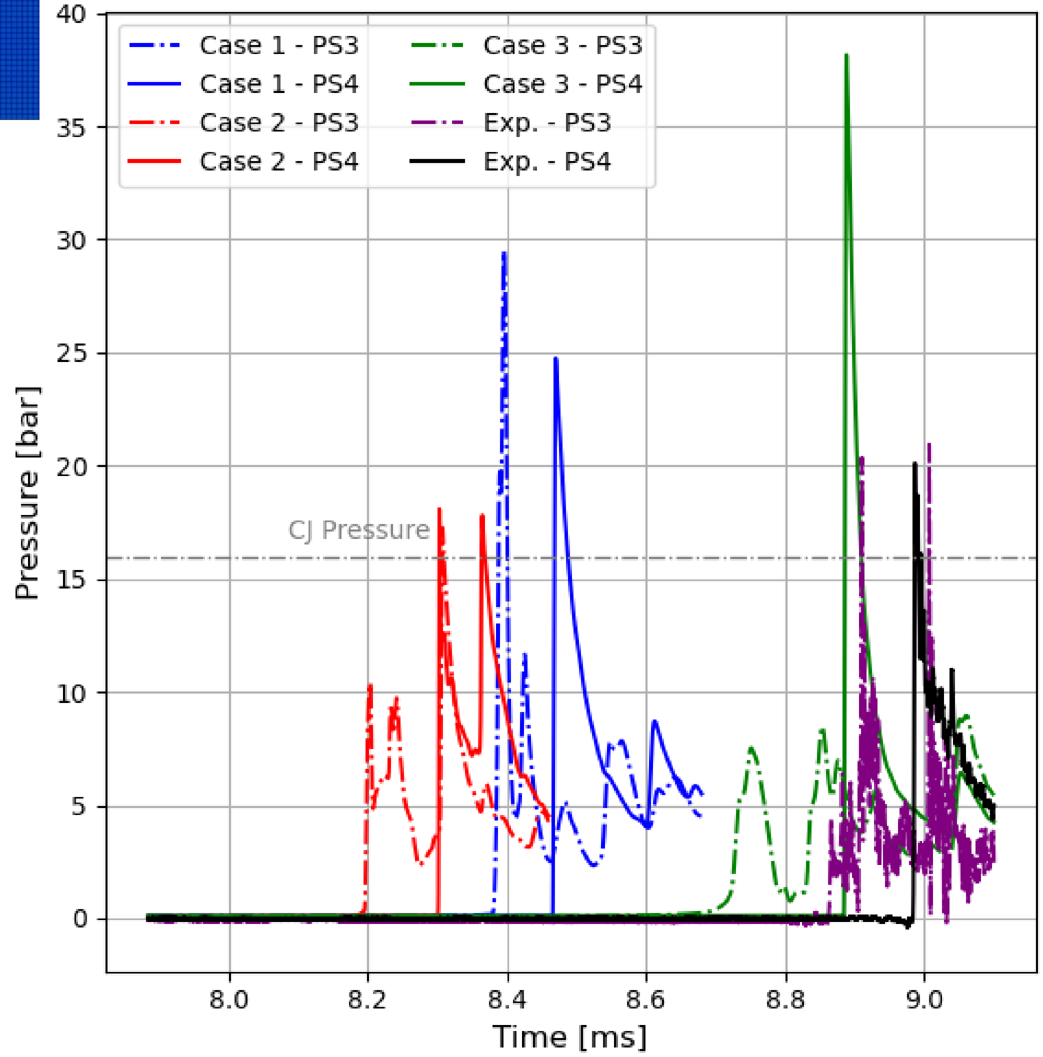
CASE 2

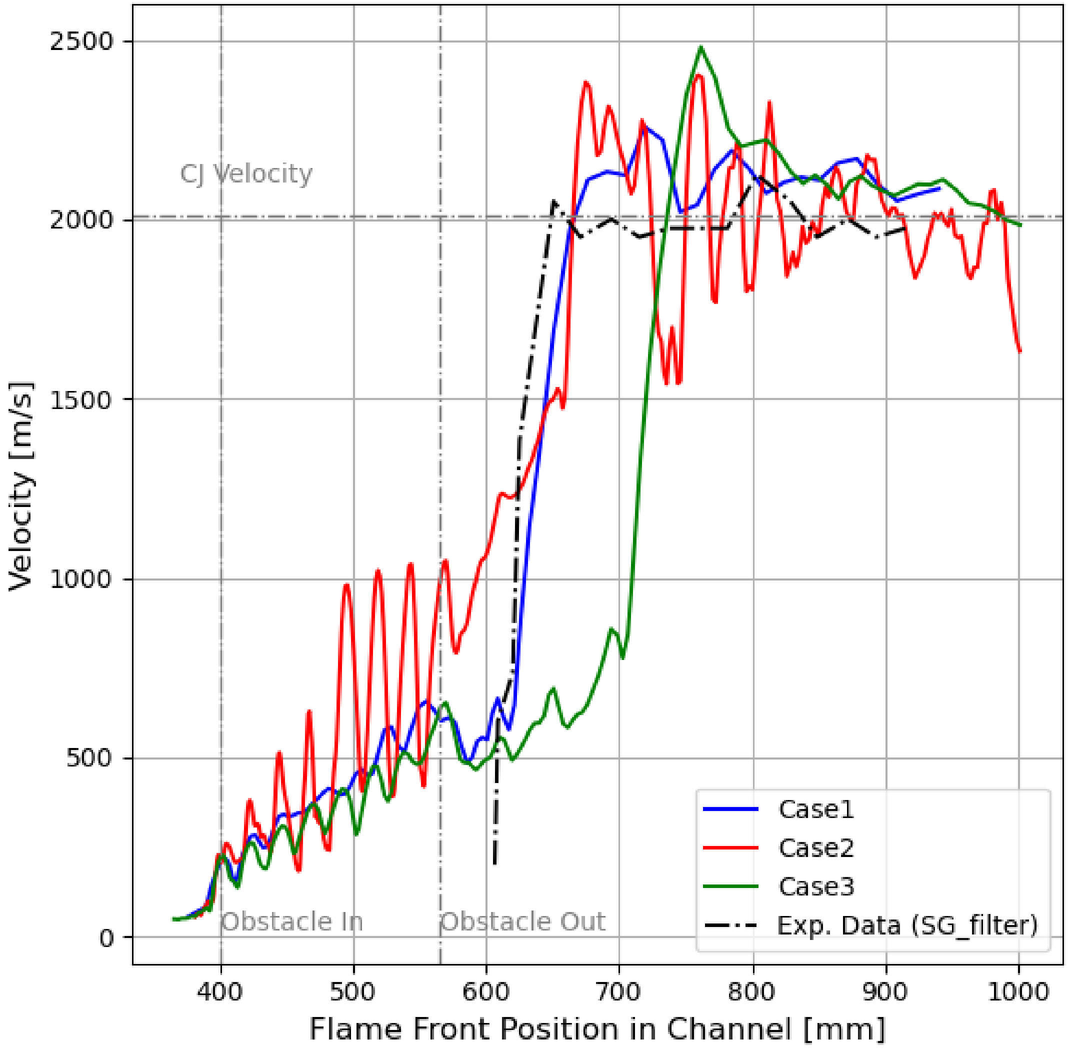


CASE 3



Case	Mesh	AMR	Base/Min. Mesh (mm)	Run Time (h)	DDT	$p_{3,max}$ (bar)	$p_{4,max}$ (bar)
1	26 152	Yes	2 / 0.5	21	Yes	29.5	24.7
2	116400	No	1 / 1	40	Yes	17.3	18.1
3	26 152	Yes	2 / 1	5	Yes	9.0	38.1
4	26 152	No	2 / 2	0.75	No	6.4	6.6





FUTURE DEVELOPMENT

Density-base solver

Pressure-base solver
Ma<0.3

OpenFOAM 9

Adaptive Mesh Refinement (AMR)

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M**ulti-**M**ode-e**X**plosion-**Foam

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Conclusion

Conclusion

- Hydrogen Technologies – Low Carbon Technologies
- Risk Assessment of Hydrogen Technologies
- Consequence Analysis – Gas Explosions
- Research Goals:
  - Develop a CFD solver in **OpenFOAM** to simulate flame acceleration (FA) and DDT in a single framework
    - Solver developed for safety studies and engineering purposes
  - Accurately predict DDT in **homogeneous** and **inhomogeneous** gas mixtures using **coarse meshes**
  - Ensure **scalability** and **applicability** to full-scale hydrogen safety scenarios

Acknowledgements:

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THANK YOU!

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