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NUMERICAL INVESTIGATIONS OF HYDROGEN RELEASE AND DISPERSION DUE TO SILANE DECOMPOSITION IN A VENTILATED CONTAINER

Rocco Rotundo

Thomas Jordan

Jianjun Xiao

Daniele Melideo

Umberto Desideri

Karlsruher Institut für Technologie

Università di Pisa

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Introduction

- Silanes (Si-H) are a group of chemical compounds consisting of a backbone of silicon and hydrogen.
- Si-H products may evolve gaseous hydrogen in the surrounding.
- Si-H emulsions are in a liquid form and are used in the tire industry nowadays.
- Typically, they are handled in IBC (Intermediate bulk containers).

Introduction

- Being emulsions, they can release gaseous hydrogen continuously.

- To preserve the mechanical integrity of the structure of IBCs and control the internal pressure, every IBC is provided of a safety relief valve on the top cap.

- IBCs are meant to be transported in containers, typically 20 ft containers.

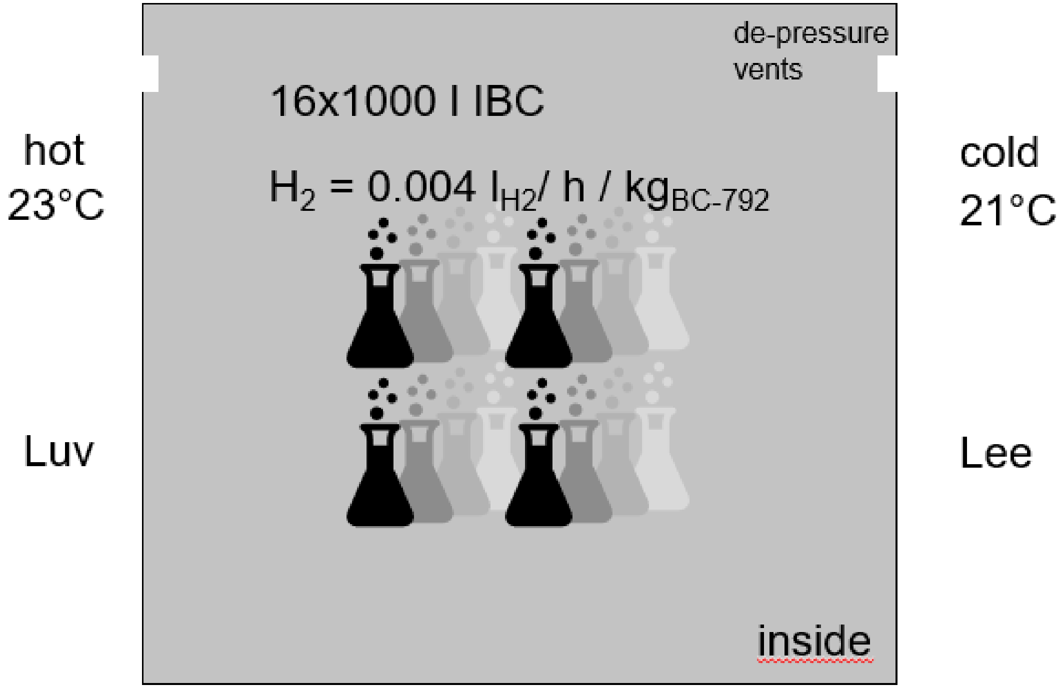
- A flammable or even explosive atmosphere might form if there is no air exchange in the container.

Introduction

- A numerical study was carried out to investigate whether standard containers are able to avoid the formation of explosive atmospheres when IBCs with Si-H are loaded in them.

- The aim is to study which are the effects of the configuration of the natural ventilation system of the containers and the influences of the external condition such as wind or sun.

- Results will provide a preliminary understanding of the release and dispersion process of gaseous hydrogen within the container for future studies.



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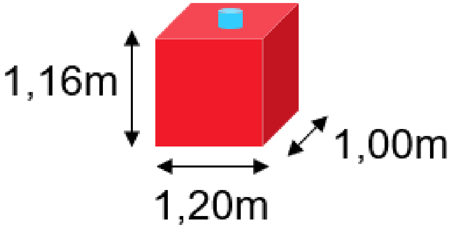
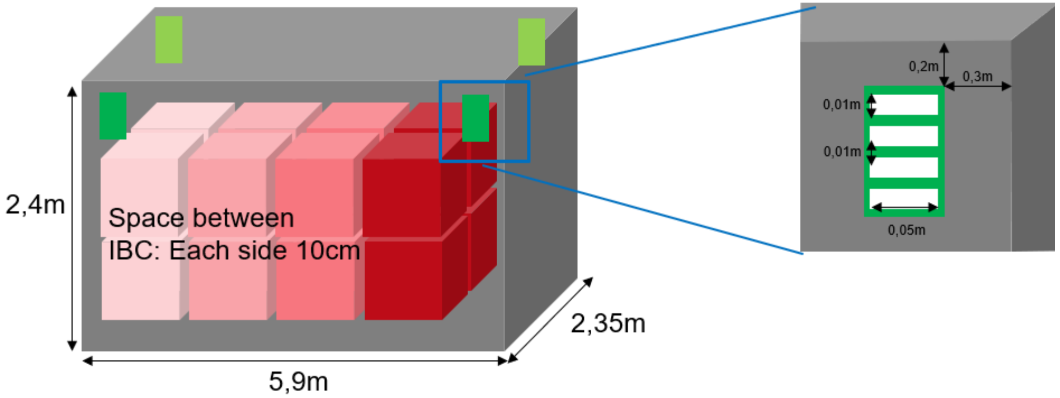
Case of study

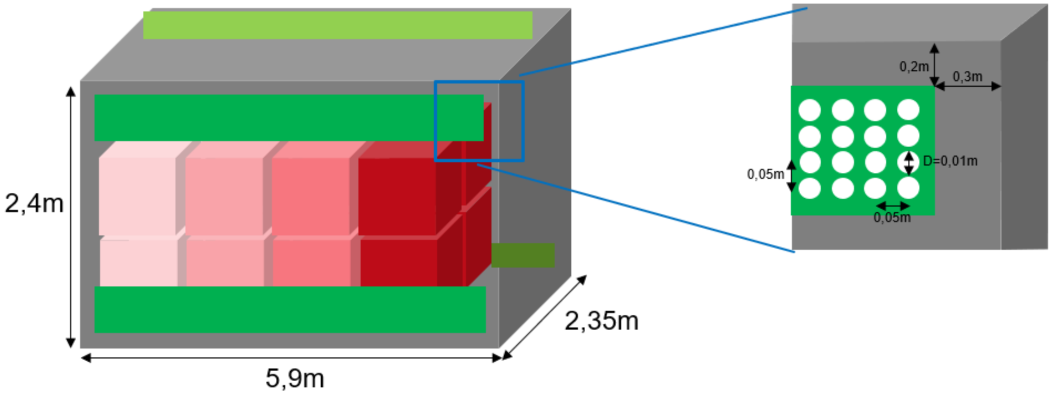


IBC

ISO Container

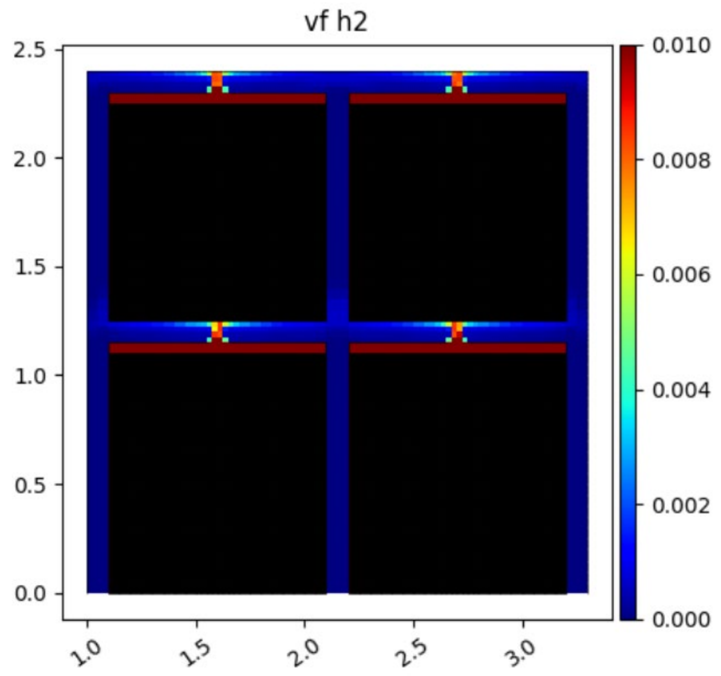
Coffee Container





Case of study

- Continuous release with every IBC ejects hydrogen continuously into the container. “Reference Case” (1)
- Pulsed release: hydrogen is released when the safety valves open. (2)
- External wind case: wind is directed straight to the vent hole with a magnitude of 1m/s. (3)
- Solar radiation case: a difference in temperature of about 2°C is assumed between the walls of the outer container. (4)
- Coffee container configuration. (5)



- Production of H_2 is for all cases equal to 0,004 $l_{H_2}/h/kg_{liquid}$

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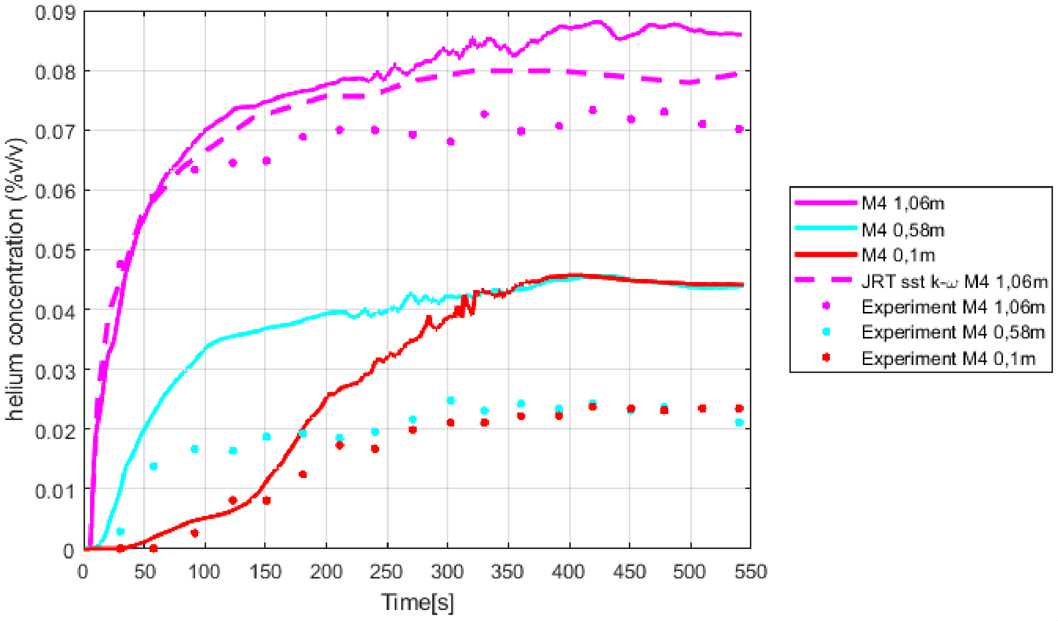
Models

- GASFLOW-MPI was used to carried out the simulations.
- Grid was evaluated reproducing an experimental study found in literature with a similar grid, where helium was released in an enclosure.
- Results are qualitatively consistent with experimental data, but not quantitatively.
- In the simulations the concentration of helium is higher than experiments, and this ensures that results are more conservative.



https://www.sciencedirect.com/science/article/pii/S0360319914033485

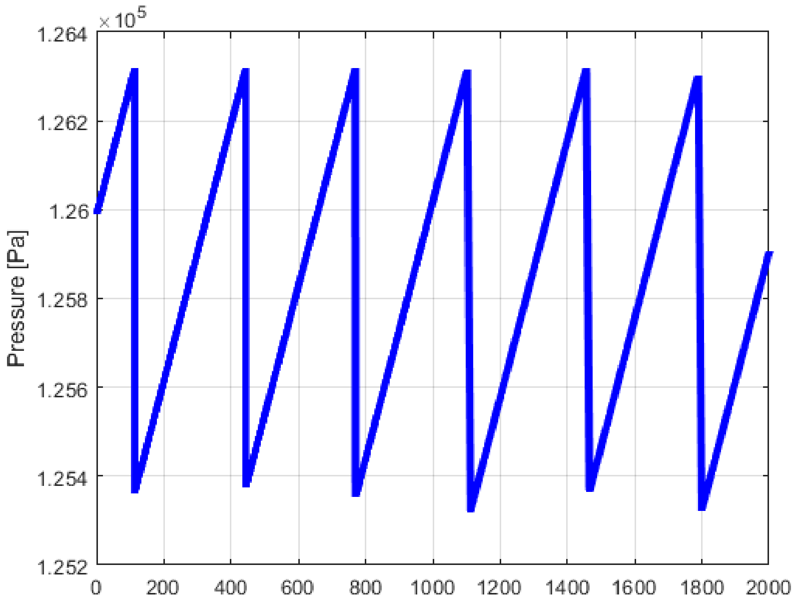
Models

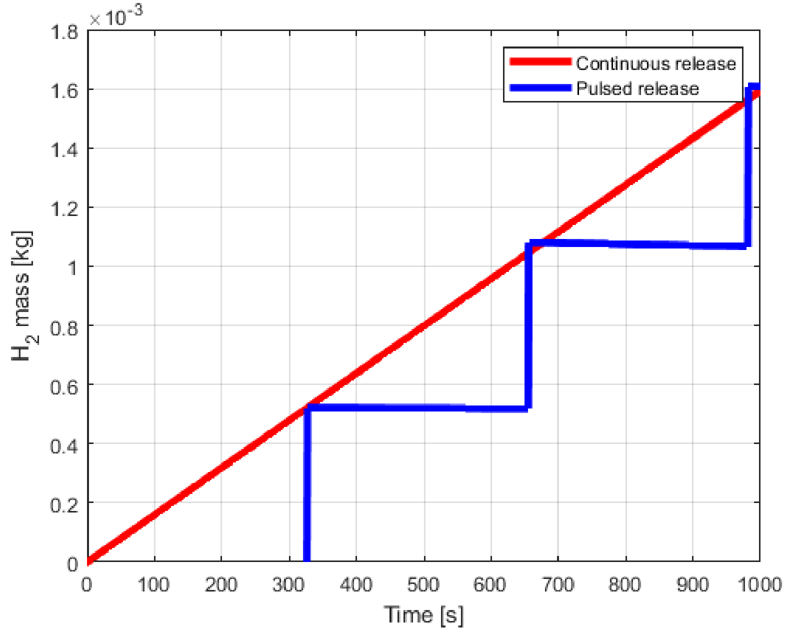
	Length [m]	Width [m]	Height [m]	Volume [m^3]	Area [m^2]
Container	5,9	2,35	2,4	33,276	13,865
IBC	1,2	1	1,016	1,22	1,2

Case	Cells on x	Cells on y	Cells on z	Total cells	Domain
1, 2, 5	79	39	34	104754	7,9x4,3x3,4 m
3, 4	99	59	54	315414	25,9x24,3x14,4m

Models

- Safety valve model was developed for this particular problem.
- The opening overpressure is 25kPa. It was assumed that the valves close when the operpressure falls to 24kPa.
- The outgoing mass flow from the valves results four orders of magnitude bigger of the continuous release mass flow.
- Openings occur every 330s.





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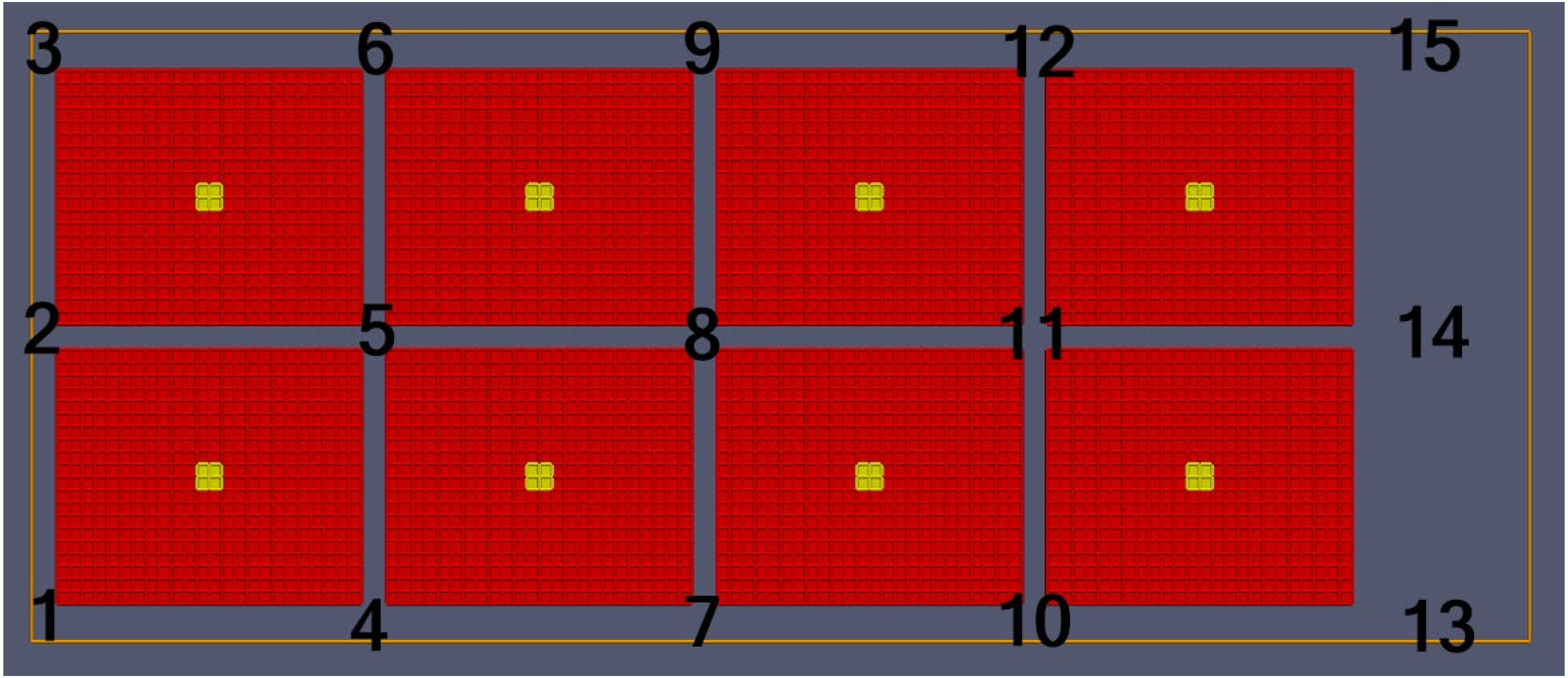
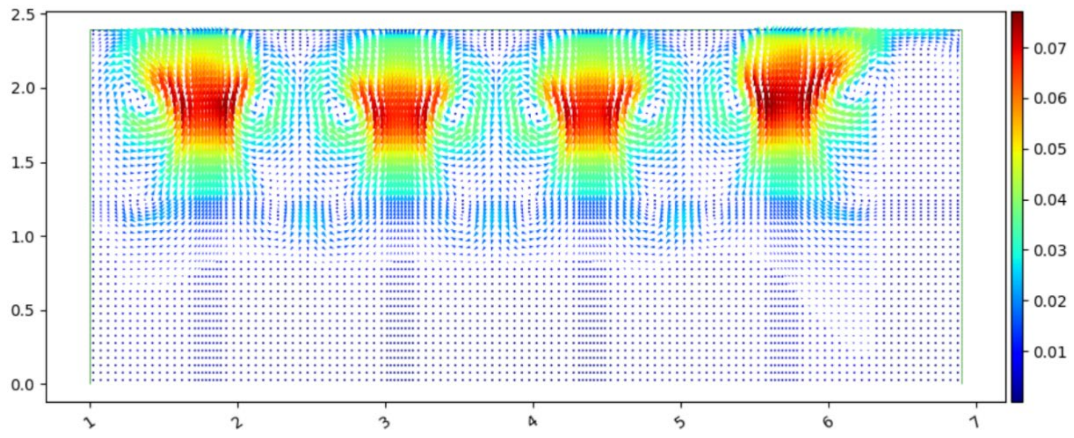
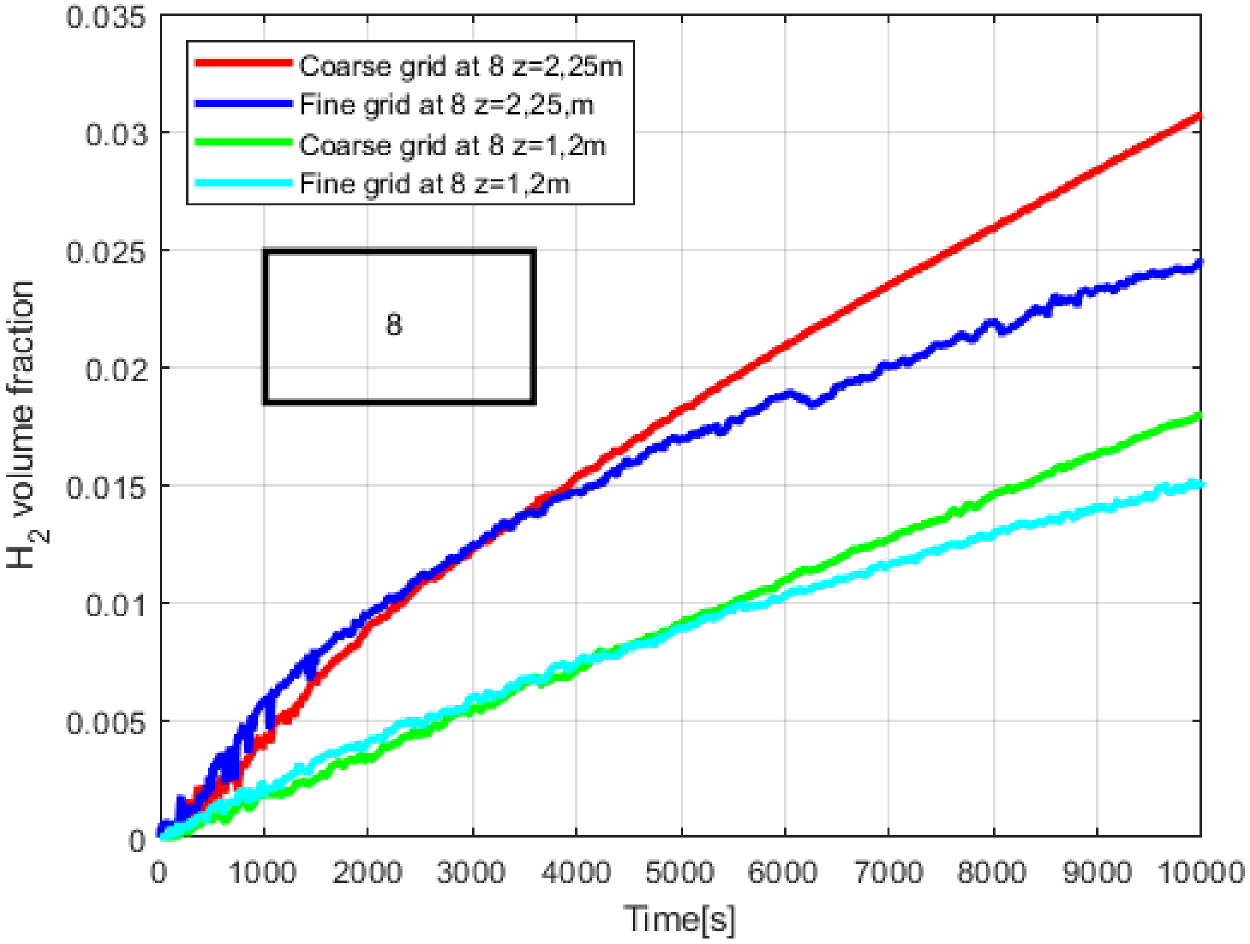
Analysis and Results



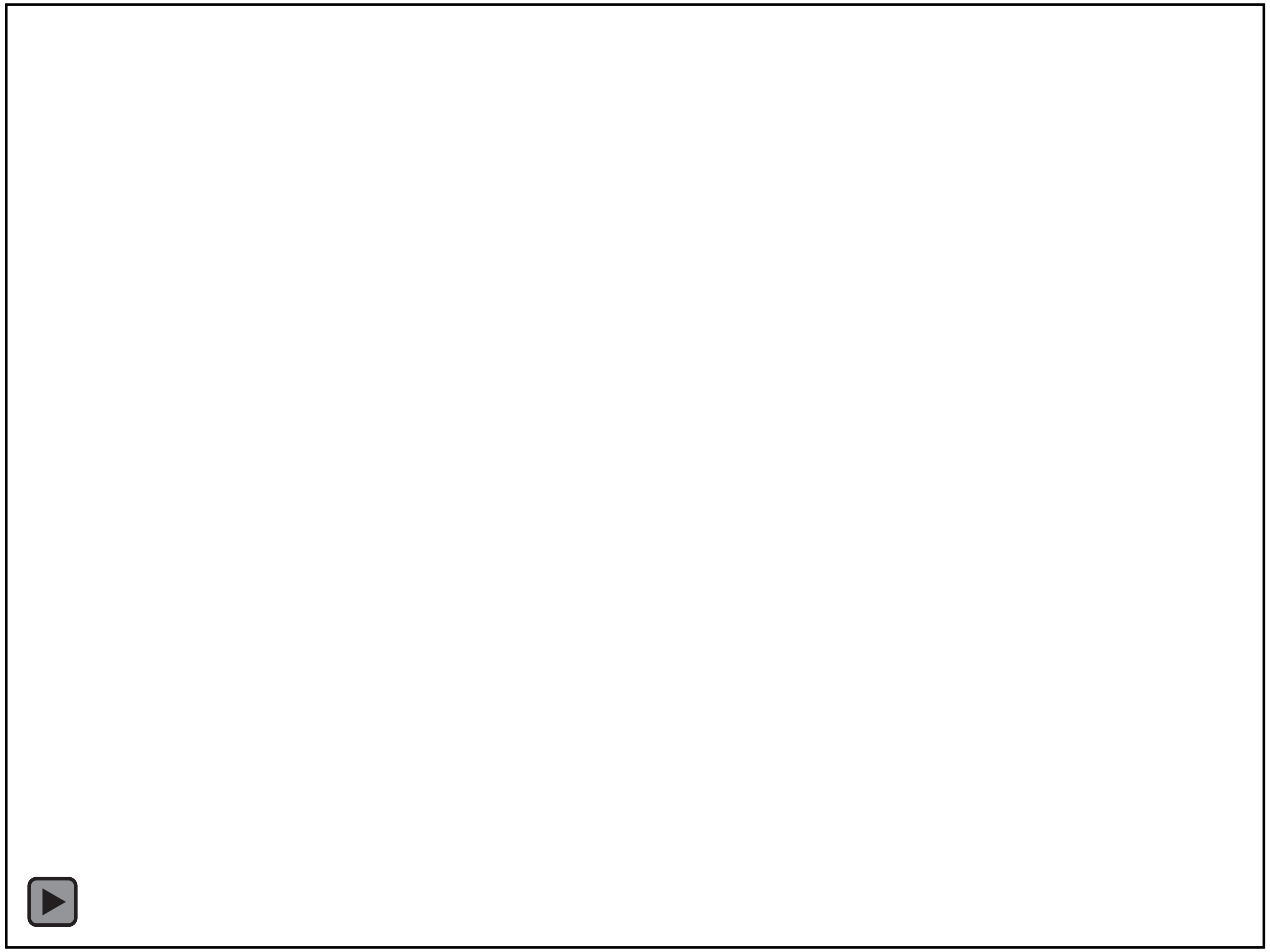
Analysis and Results

- Original mesh was doubled on each axis
- Coarse mesh provides conservative results.
- Diffusion process is stronger with a finer mesh grid.





Analysis and Results

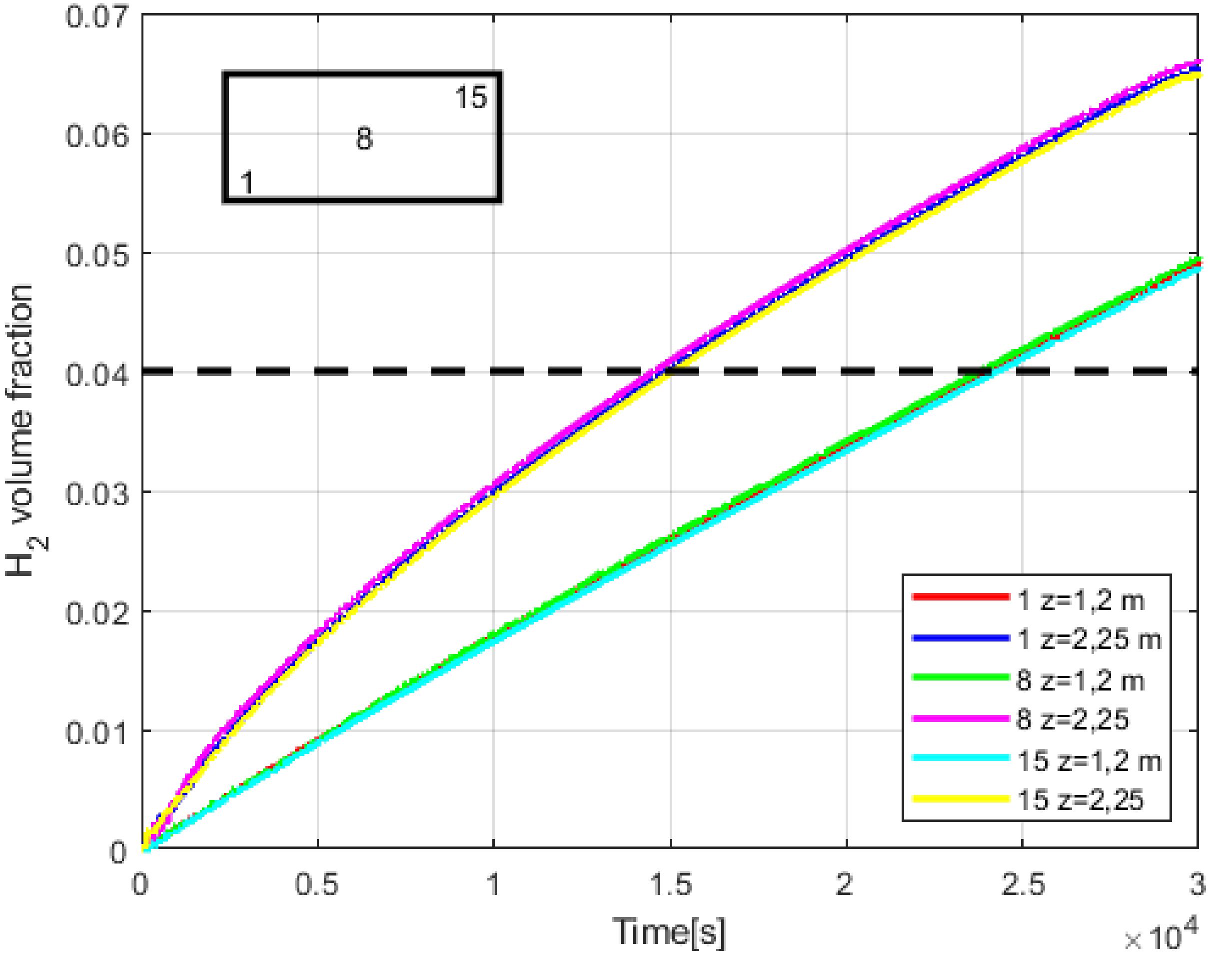


Continuous release scenario

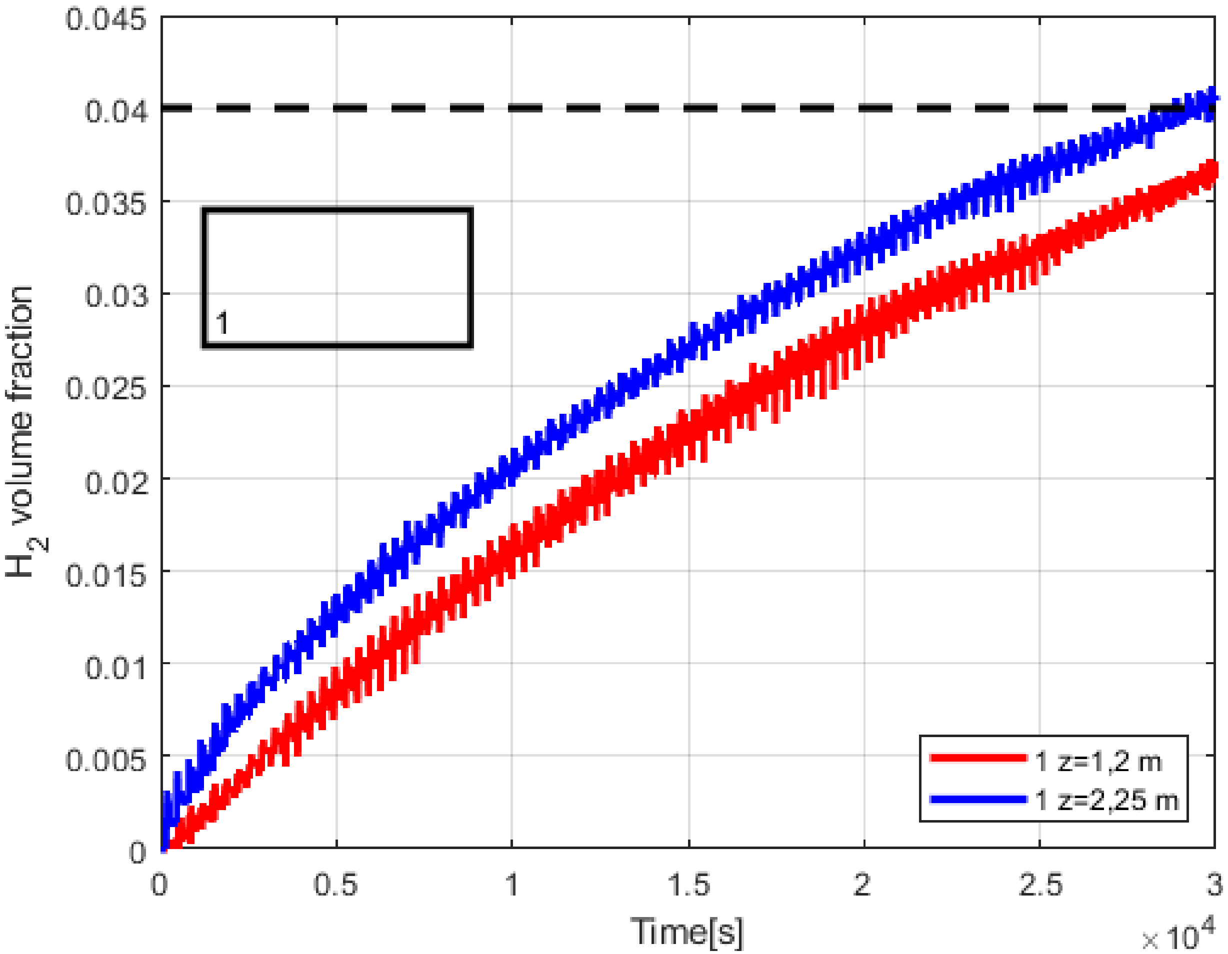
Pulsed release scenario

Analysis and Results

Continuous release scenario

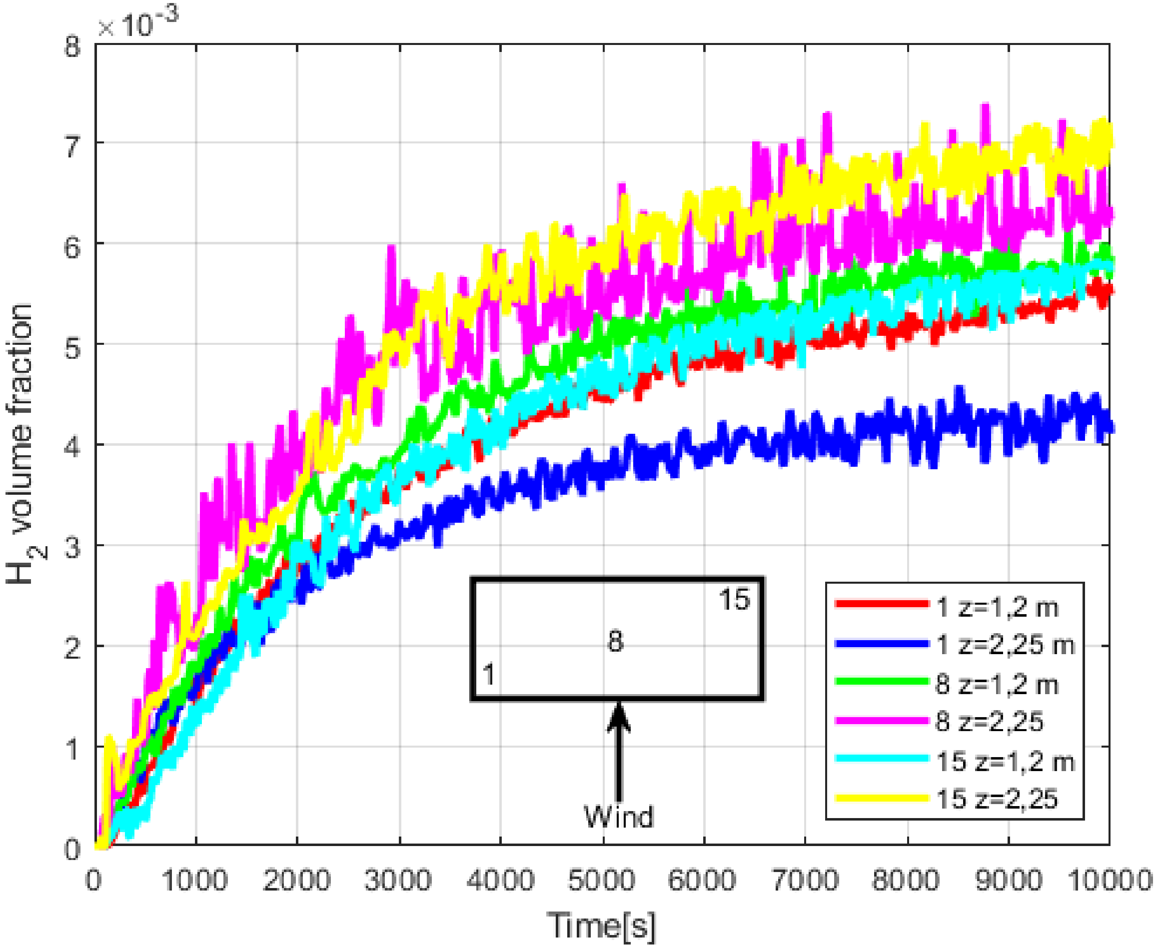


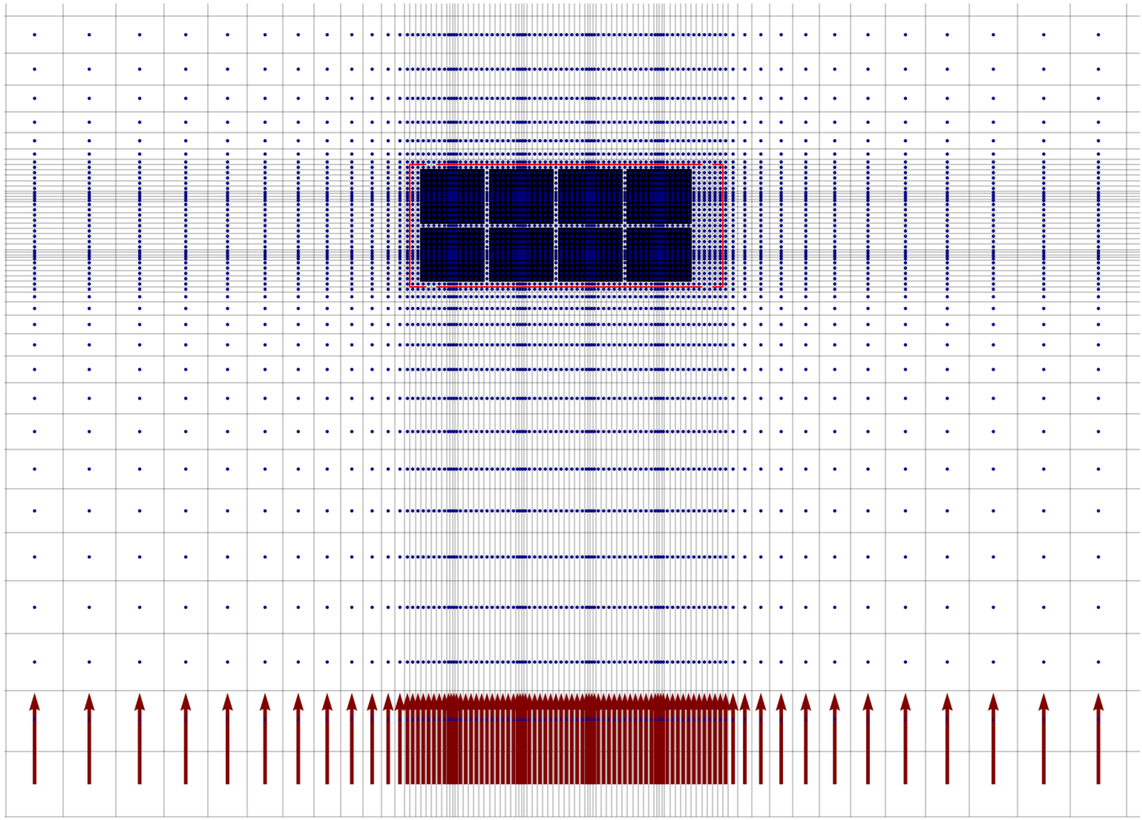
Pulsed release scenario



Analysis and Results

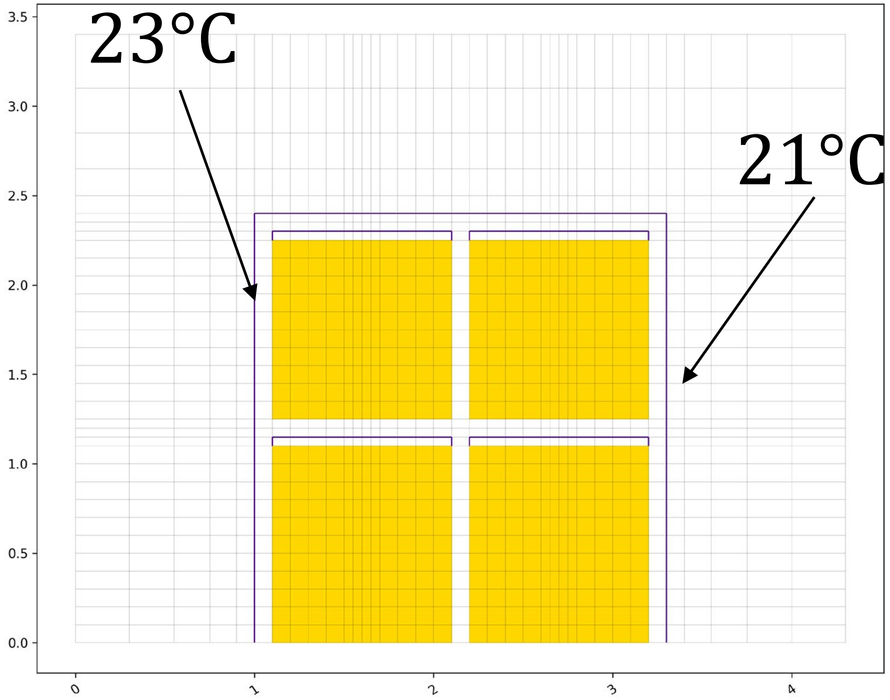
Wind scenario

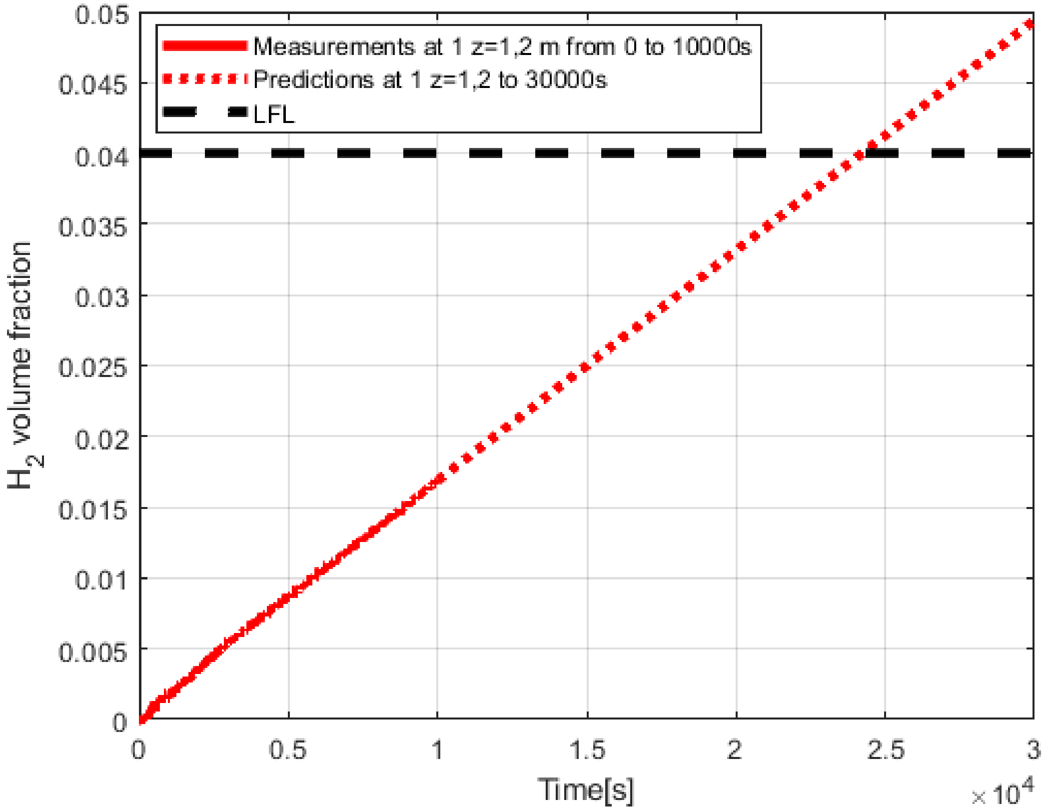




Analysis and Results

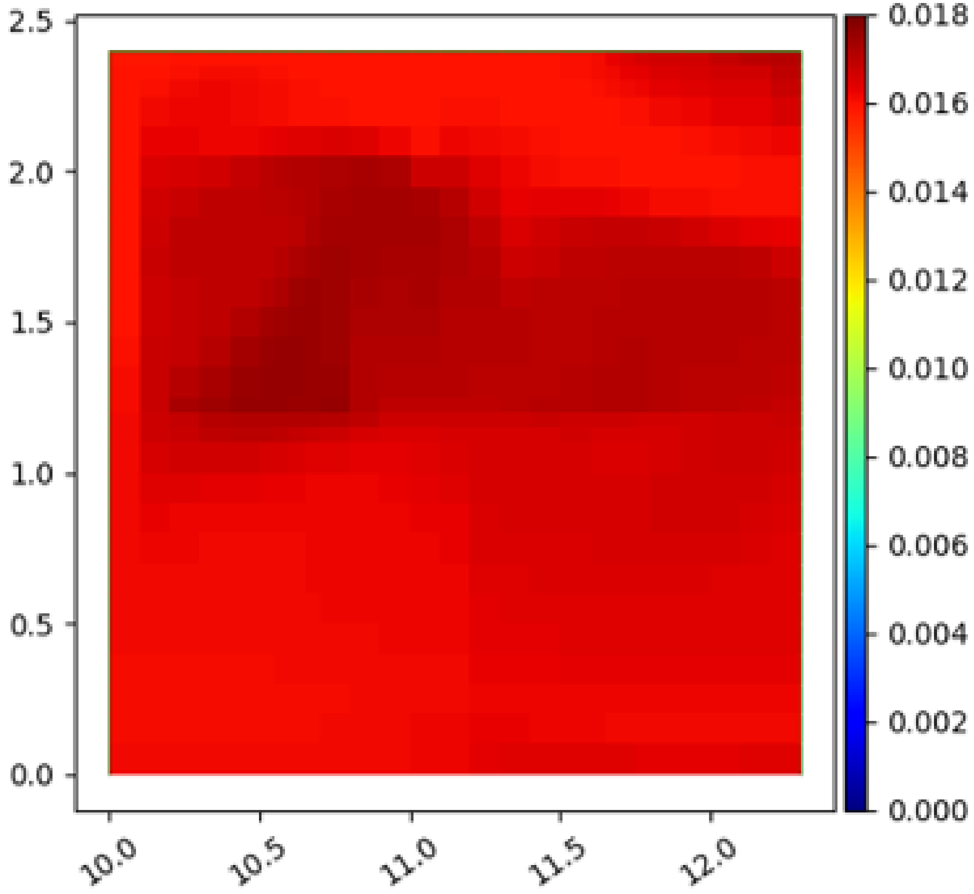
Sun scenario

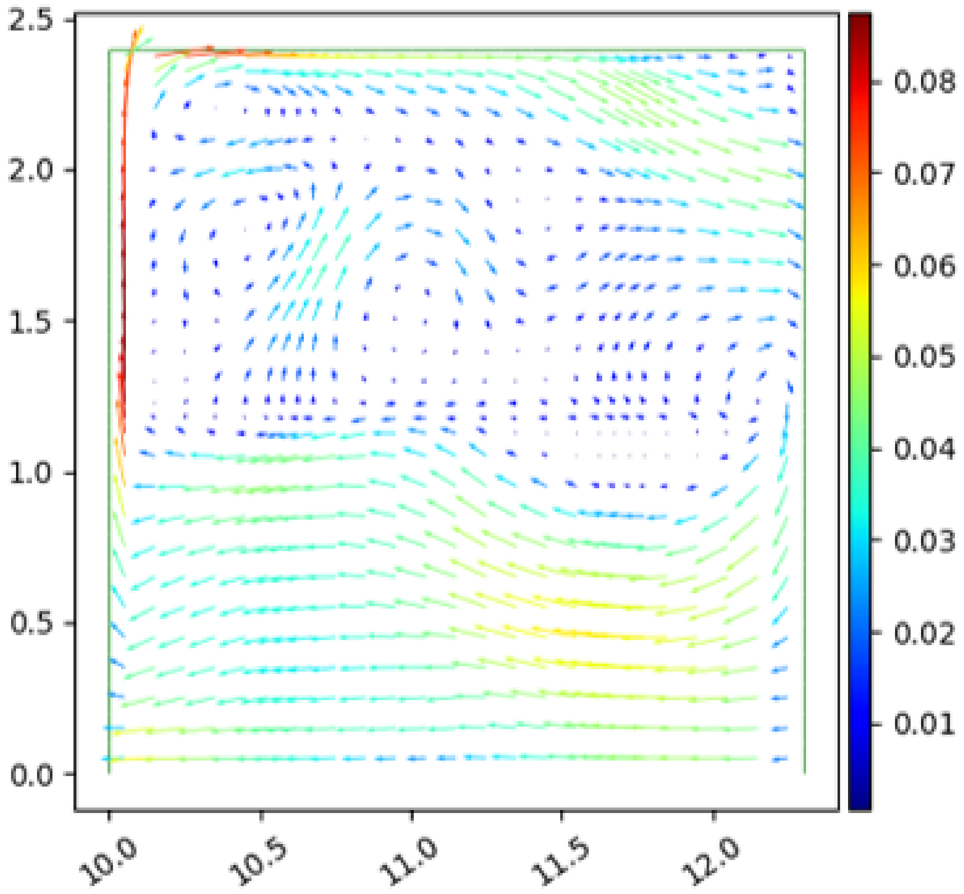




Analysis and Results

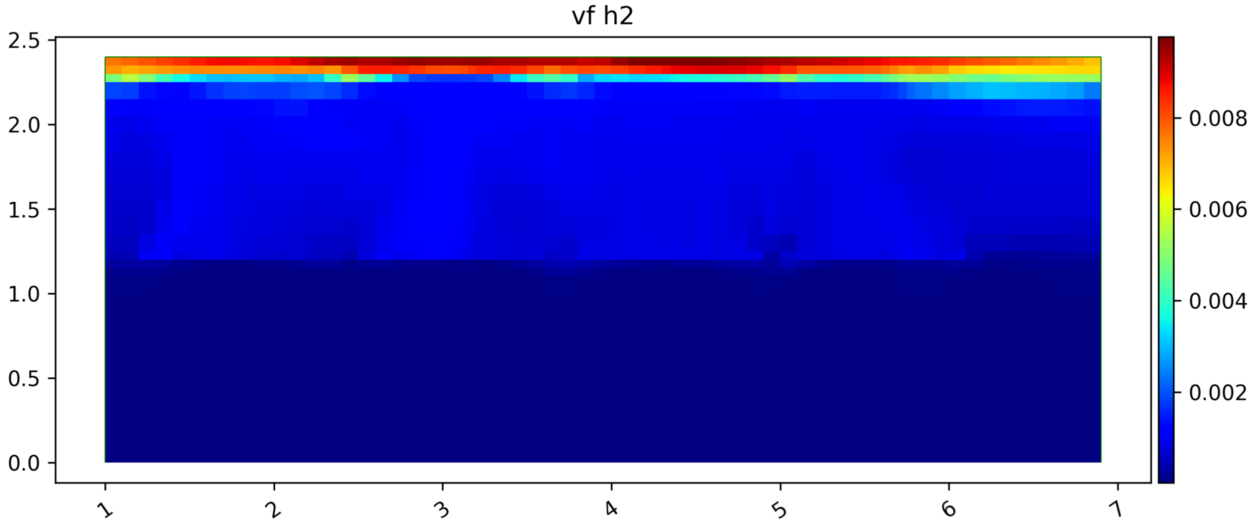
Sun scenario

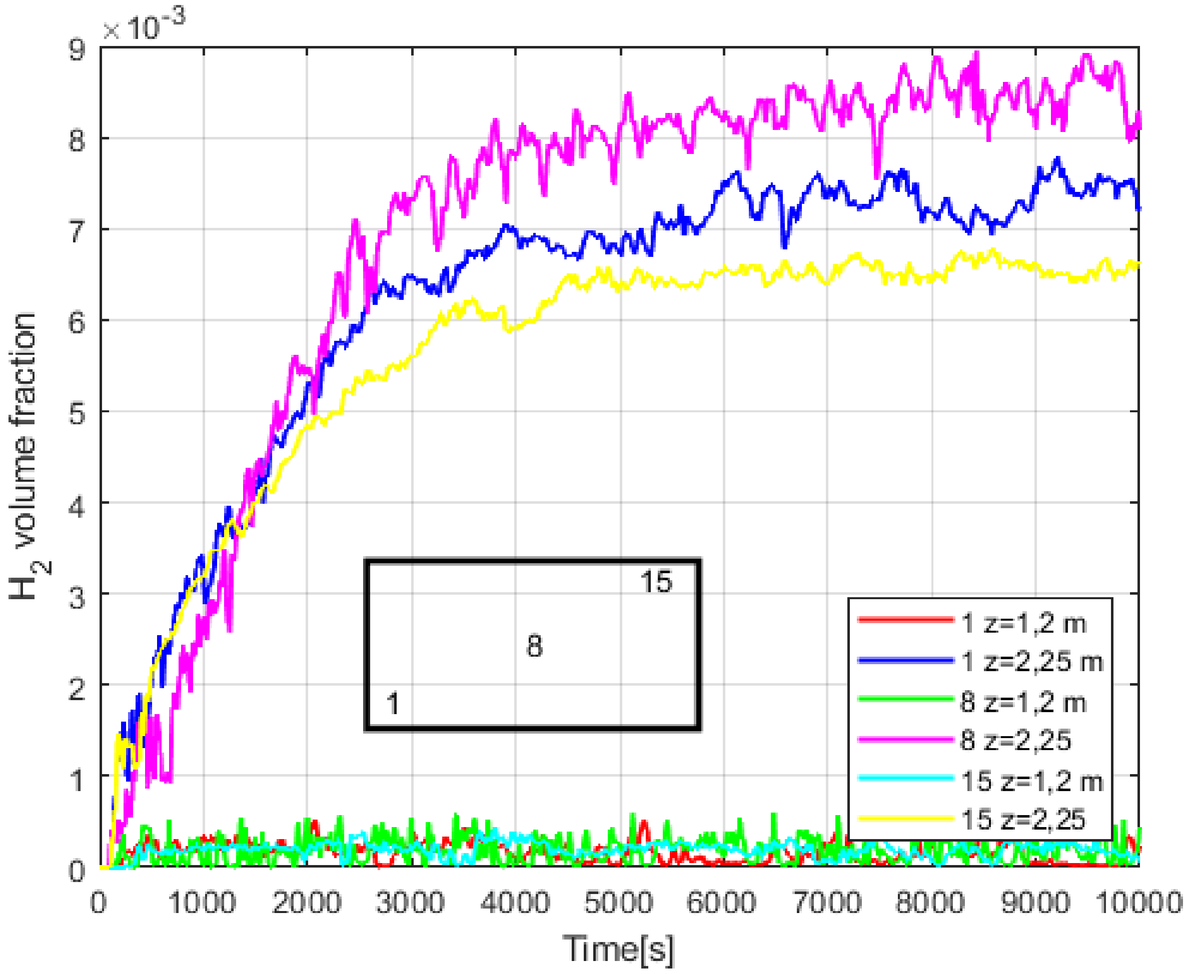




Analysis and Results

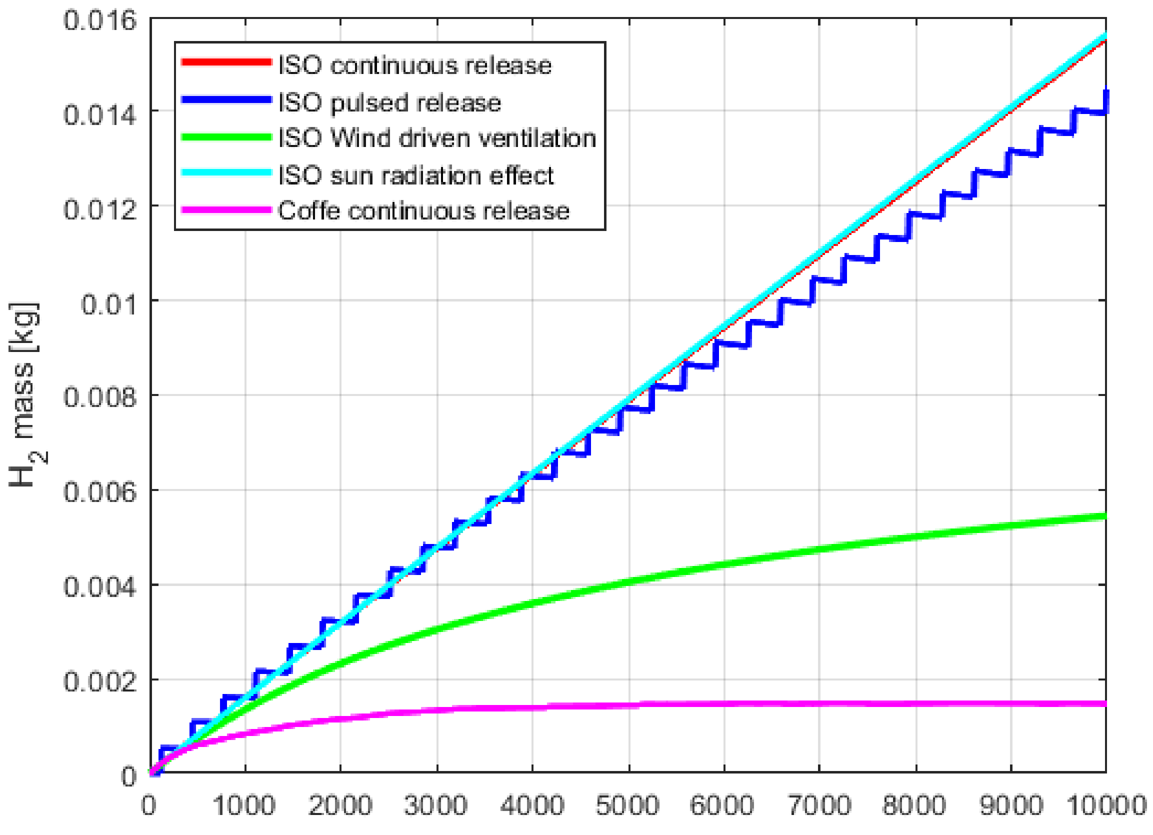
Coffee container





Analysis and Results

- To evaluate the effective ventilation of all scenarios, the total mass within the container was also calculated.
- After 10000s, 16g of hydrogen are released by IBCs.
- The poorest ventilation is achieved with the effect of the sun.



	Continuous	Pulsed	Wind	Sun	Coffee
Vented H_2	0,43g	1,6g	11g	0,38g	14,5g

Contents

Summary

- A conservative CFD analysis was done on the release of hydrogen in a confined space.
- Release of hydrogen occurs inside a 20ft container from 16 IBCs.
- Safety valves model was developed to simulate the pulsed release of hydrogen.
- Wind, sun and different configuration of the container effects on the venting of hydrogen were investigated.
- The main objective of the analysis was to ensure that an explosive environment does not form inside the outer container.

Conclusions

ISO Container

- The distribution of hydrogen in the case of continuous release (“reference case”) is stratified, and the lower flammability limit is reached after 15,000 seconds in the upper part of the container.

- Safety valves promote both improved mixing and better ventilation compared to the reference case. The flammability limit is reached after 30,000 seconds.

Coffee Container

- Hydrogen is locally accumulated in the upper part of the container. The specific configuration of the container allows for better ventilation compared to the ISO-type container.

Conclusions

Based on the assumptions made about wind and solar radiation, it can be stated that:

- Wind, incident in the direction of the ventilation openings with an intensity of 1 m/s, enhances natural ventilation and prevents the formation of a flammable environment.

- Solar radiation, assumed as a temperature difference between the container walls, promotes strong mixing, lowering hydrogen concentration values, but does not eliminate the risk of flammability. Furthermore, it does not provide advantages to ventilation.