DEFLAGRATION-TO-DETONATION TRANSITION DUE TO A PRESSURIZED RELEASE OF A HYDROGEN JET. FIRST RESULTS OF THE ONGOING TAU-NRCN-CEA PROJECT.

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ABSTRACT

A sudden release of compressed gases and the formation of a jet flow can occur in nature and various engineering applications. In particular, high-pressure hydrogen jets can spontaneously ignite when released into an environment that contains oxygen. For some scenarios, these high-pressure hydrogen jets can be released into a mixture containing hydrogen and oxygen. This scenario can possibly lead to a wide range of combustion regimes, such as jet flames, slow or fast deflagrations, or even hazardous detonations. Each combustion regime is characterized by typical pressures and temperatures, however, fast transition between regimes is also possible.

A common project between Tel Aviv University (TAU), Nuclear Research Center Negev (NRCN) and Commissariat à l'Energie Atomique et aux énergies alternatives (CEA) has been recently launched in order to understand these phenomena from experimental, modelling and numerical points of view. The main goal is to investigate the dynamics and combustion regimes that arise once a pressurized hydrogen jet is released into a reactive environment that contains inhomogeneous concentrations of hydrogen, steam, and air.

In this paper we present the first numerical results describing high-pressure hydrogen release obtained using a massively parallel compressible structured-grid flow solver. The experimental arrangements devoted to this phenomenon will also be described.

1.0 INTRODUCTION

A sudden release of compressed gases and the formation of a jet flow can occur in nature and various engineering applications. In particular, high-pressure hydrogen jets can spontaneously ignite when released into an environment that contains oxygen [1]. This scenario can lead to a wide range of combustion regimes, such as jet flames, slow or fast deflagrations, or even hazardous detonations. Each combustion regime is characterized by typical pressures and temperatures, however, fast transition between regimes is also possible.

Better understanding of these complex phenomena is essential for prevention and mitigation of hydrogen explosions. Such accidental explosions can occur in industrial hydrogen storage facilities, hydrogen pressure vessels designated for fuel cell applications, and nuclear reactors. For the latter, in case of a severe accident in the primary cooling circuit of nuclear power plants (NPP) the water coolant evaporates and steam reacts with the fuel cladding (Zircaloy), leading to production of hydrogen. Consequently, the pressure inside the reactor vessel increases, and the mixture of hydrogen and steam can either leak slowly into containment atmosphere, or suddenly release as a turbulent jet, accidently or in purpose. An ignition event, either due to autoignition or other ignition sources, can quickly develop into an internal hydrogen explosion, as occurred in Fukushima Daiichi nuclear power plant ([2], [3])

The most destructive type of such an explosion is the one produced by a detonation wave. In many cases, the formation of a detonation is due to a process known as Deflagration-to-Detonation Transition (DDT). In this process, a deflagration wave (flame) accelerates and transitions into a detonation wave. DDT usually occurs in confined geometries due to flame interaction with obstacles. However, it has been

recently demonstrated that the effect of turbulence alone can lead to DDT, even under completely unconfined conditions [4].
A common project between Tel Aviv University (TAU), Negev Nuclear Research Center (NNRC) and Commissariat à l'Energie Atomique (CEA) has been recently launched in order to understand these phenomena from experimental, modelling and numerical points of view. The main goal is to investigate the dynamics and combustion regimes that arise once a *pressurized hydrogen jet is released into a reactive environment that contains inhomogeneous concentrations of hydrogen, steam, and air*.
From the phenomenological point of view, we deal with two distinct phenomena. The *first* is the species distribution, including flammable gases, inside a relatively big volume, which is a slow process and requires a particular models and algorithms adapted to Low-Mach flows. The *second* represents the high-pressure jet release inside the previously formed flammable mixture, which is a very fast process involving not only formation of complex shocked flows but also a diffusive chemical reaction and the following flame propagation. The main challenge is to explore the transition between all the combustion regimes, namely, jet flame, deflagration, and detonation. A single computational code cannot model all these phenomena due to disparity in length and time scales. From the modelling side, we therefore decided to use two codes having different models and algorithms.
The initial species concentration field in the high-fidelity simulations, prior to the jet release, will be evaluated based on Large Eddy Simulation (LES) and Unsteady Reynolds Average Navier-Stokes (URANS) methods. These simulations will replicate a slow hydrogen leakage scenario in a large-scale facility. High-fidelity massively parallel simulations, using the explicit in-house code, will capture the jet auto ignition, the flame acceleration process, and the possible transition into a detonation wave due to turbulence-induced DDT.
Before performing the scenario-type computations, an extensive code validation against experimental results is required. Moreover, the experimental work dedicated to a pressurized hydrogen jet release into a reactive environment is necessary due to the lack of the data in the open literature. This work will be carried out during the project and the related results will serve for the code validation.
This paper describes ***(a)*** the systematic approach of our codes validation, and ***(b)*** the preparative steps for the on-going experimental work.

2.0 MAIN VALIDATION RESULTS.

First, we present some of the results dedicated to the validation of the code dealing with species distribution inside a gas volume. Second, validation related to a high-pressure hydrogen jet release is introduced, followed by jet-ignition phenomenon simulations.

Slow Leakage Simulations

We have developed new simulation capabilities of a slow jet leakage via the open-source Computational Fluid Dynamics (CFD) software package OpenFOAM. We decided to validate our solver against the classical experimental work of Deri et al. [5], which involves turbulent jet erosion of a stably stratified gas layer in a small-scale test facility. The test section consists of a parallelepiped transparent box (Figure 1, left) which is 1.29 m tall with a square 0.92 x 0.92 m section. The experiment was performed at the room pressure and temperature.
The helium is injected from the two facing horizontal nozzles located on the lateral edges at 0.3 m from the roof (d_{inj} = 4 mm). The air is injected from the vertical nozzle at the middle of the bottom plate (D_{inj} = 20 mm).
At the beginning, the facility is full of ambient air. Then, 9.1 g of helium is introduced via the two horizontal helium inlets; this phase takes 300 s. The air injection takes 300 s starting at t = 360 s (i.e. one minute after the helium injection). A local Froude number is commonly used in the open literature to treat jet/stratification interaction phenomena. It is defined as:

$$Fr = \frac{U_{ref}}{N\,L} \tag{1}$$

where U_{ref} is an estimation of the fountain velocity at the interaction height, L is the local fountain length scale (Figure 1, right) and $N = 2\ s^{-1}$ in the experiments. The experimental data corresponding to $Fr = 1.09$ are chosen here for comparisons. The results are presented in terms of dimensionless density $(\rho_{ref} - \rho)/\rho_{ref}$, where ρ_{ref} is the density of pure air at the laboratory conditions. The local density ρ depends on the helium fraction via the Dalton's law.

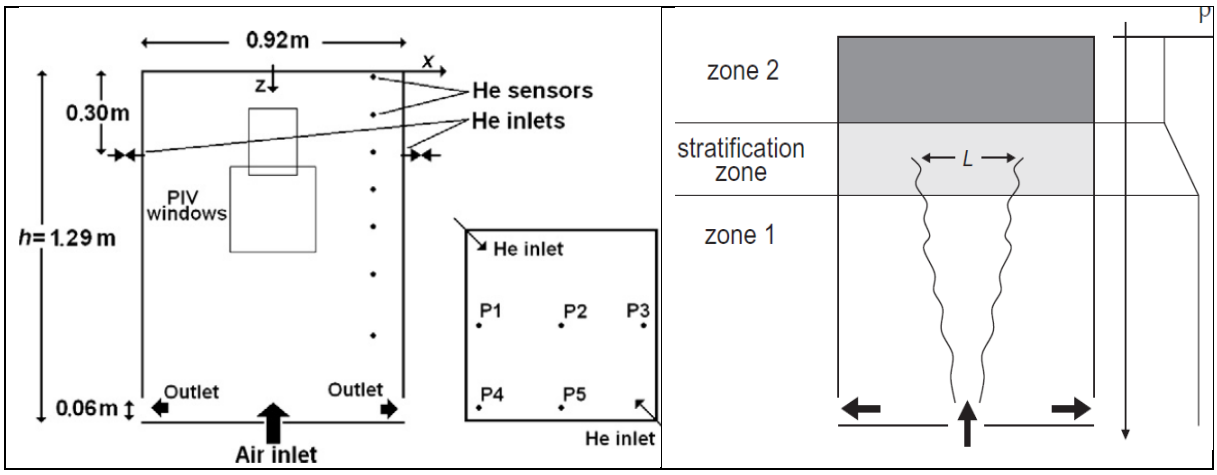


Figure 1. Front and top sketch of the experimental layout (left); sketch of the experiment (right). Scanned from [5].

We have chosen to utilize the rhoBouyantReactingFoam solver, coupled with a *k*-ε URANS approach, for modelling this problem. However, the original solver is only applicable for laminar and turbulent Schmidt numbers that equal unity. Thus, we extended the solver to take into account the effect of arbitrary Schmidt numbers, which is highly important for accurately solving the slow jet leakage problem. Additionally, we have implemented a source term for buoyancy effects in the ε-equation which promotes turbulence production in unstable stratification or decays the turbulent kinetic energy in stable stratification. The initial and boundary conditions were carefully chosen based on the experimental results by [5], and a 2-D axisymmetric grid was generated. We have executed simulations for different Froude numbers and carefully compared our simulation results against the experimental results of [5]. The grid convergence study has been carried out, which involved coarse and fine grids with 11,549 and 46,376 cells, respectively. Figure 2 presents the dimensionless density as a function of time at different heights and for the two grids. Our solver results are validated against the experimental results of [5], for a Froude number of 1.09 with excellent agreement.

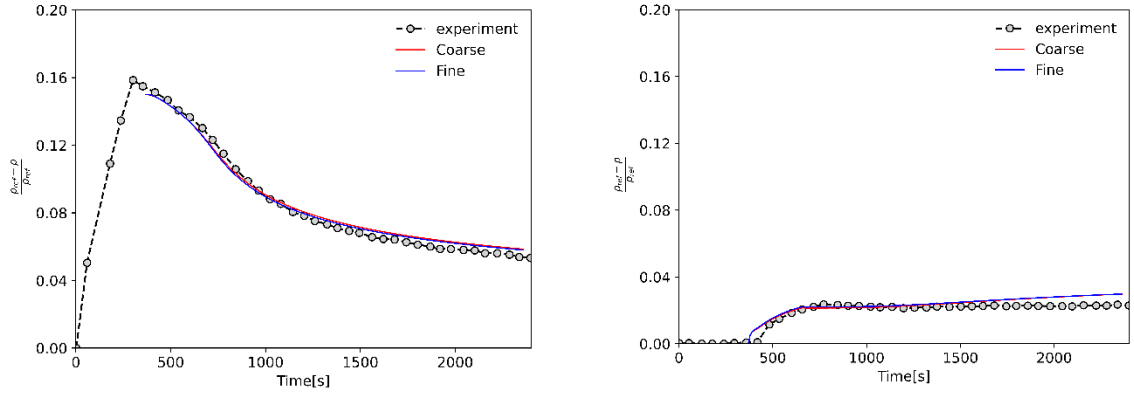


Figure 2. Validation of OpenFOAM solver against experimental results of [5]. The dimensionless density as a function of time for coarse and fine grids at heights of: z=0 m (left) and z=0.8 m (right).

Pressurized Jet Release Simulations

We set-up and conduct pressurized jet release simulations via our massively parallel in-house code Athena-RFX++. Moreover, we further extend our solver for a 2-D axisymmetric grid. First, we carefully tested our new solver and validated its accuracy against a pressurized jet release simulation of hydrogen into hydrogen from the literature [6]. The simulation setup is based on the assumption of chocked conditions and a constant mass flux at the inlet. Figure 3 presents a comparison between our simulation and the simulation of [6] by showing the Mach number as a function of distance at different time instants. A good agreement is achieved between the two simulations.

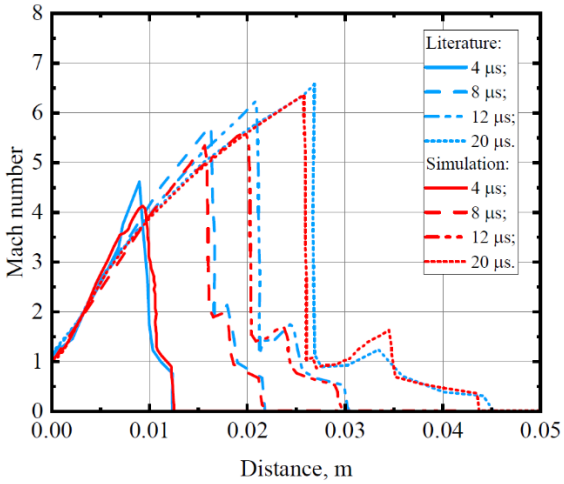


Figure 3. Validation of the 2-D axisymmetric solver, our simulation results (Athena-RFX++) against the simulation results of [6]: The Mach number as a function of the distance from jet opening for different time instants.

Second, the influence of the boundary condition at the inlet on the jet evolution has been investigated [7]. Thus, two computational models were devised: a) Full scale model that includes both the high- and low-pressure zones, see Figure 4. b) A simplified approach, where only the low-pressure zone is solved, and the high-pressure zone is modeled via a chocked flow inlet condition.

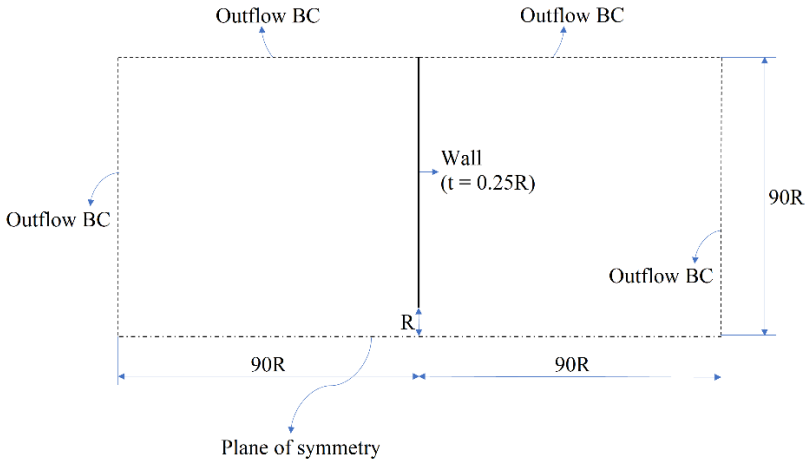


Figure 4. Computational domain for the pressurized jet release full-scale simulation showing the high-pressure zone (left) and low-pressure (right) divided by a thin wall with a slit. The details about the boundary conditions and geometry are clearly outlined.

A qualitative comparison of the synthetic Schlieren images of the jet obtained from the two simulations at t = 20μs is presented in Figure 5 (top). The left-hand side shows the synthetic Schlieren image of the jet obtained from the full-scale computation and the right-hand side shows the synthetic Schlieren image of the jet obtained from the choked-inlet simulation. In both the simulations, flow structures, such as the lead strong shock wave, contact surface, Mach shock, and the transversely-expanding barrel shock are well resolved. However, unlike the full-scale computation, in the case of steady state choked-inlet flow, the barrel shock is detached from the slit exit. Therefore, it is shown in Figure 5 (top) that the jet expands more rapidly in the axial direction in case of the choked-inlet. This is illustrated in the comparison of the pressure shown in Figure 5 (bottom). The results correspond to the values of pressure along the jet-axis in the regions corresponding to Mach shock, contact surface (where ignition is most likely to occur), and the lead shock wave. Therefore, not accounting for the transient effects of the flow at the inlet leads to a faster expanding jet, which is the case for the steady-state choked-inlet computation. Furthermore, it can lead to wrong predictions of the different flow structures, and possibly, the jet-ignition characteristics. Further details can be found in [7].

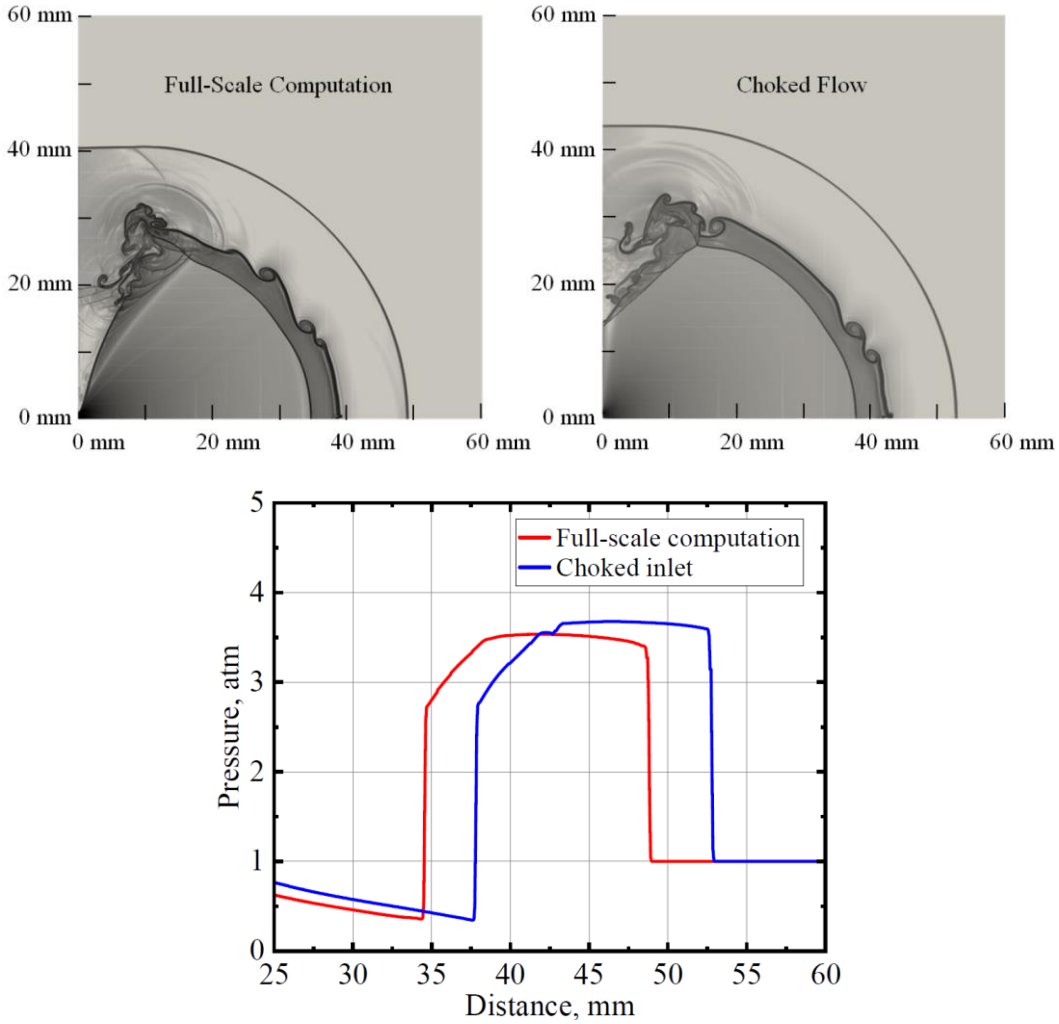


Figure 5. Pressurized jet release simulations – Full-scale vs. chocked inlet: Synthetic Schlieren images of the jet structure at t=20 µs. The full-scale computation result is on left, whereas the choked flow computation result is on the right (top). Comparison of the predicted pressure by full-scale and choked-inlet simulations along the jet axis at t=20 µs (bottom).

Hydrogen Jet Ignition Modelling and Chemical Reaction Model Calibration.

Particular attention should paid to the modelling of hydrogen jet ignition. In the framework of the current project, the initial results on this subject have been obtained and described in [8]. Here we present some of the results for completeness; further details can be found in [8].

The C++-based open-source code - Ember, see [9], is utilised for conducting numerical simulations of a 1-D transient reactive diffusion-layer ignition. This code is originally designated for modelling 1-D laminar strained flames and provides superior performance for reactive-flow simulations with large multi-step chemical kinetic models.

The governing equations are the 1-D transient low-Mach number conservation equations of energy and species. Note that as we are studying a stagnant reactive diffusion layer (in the frame of reference of jet), see also [10], the velocity is zero, and thus we can solve the problem without the continuity and momentum equations. In particular, we focus on conditions that are relevant to scenarios of a pressurized jet release into a diluted oxidizing environment. Thus, the diffusion layer mimics the conditions for diffusion ignition at the jet head, where one side contains fuel and the other contains oxidizer. In our simulations we assume that there is no expansion or strain as we are interested in capturing the problem fundamental dynamics.

For all the simulations, the same boundary conditions are implemented. However, for each simulation, the initial conditions are varied based on the ambient conditions. This allows us to calculate the initial conditions on the fuel and oxidizer sides of the diffusion layer via a 1-D shock-tube problem [11], [12] that is solved by the software package Cantera [13] and therefore mimic conditions similar to a pressurized jet release at the early stages before significant expansion occurs. For all the cases, we use a representative pressure ratio of 700 between the fuel (driver section) and atmospheric ambient (driven section) both with an initial temperature of 293 K. The domain size is 2 mm and the interface between fuel and oxidizer is located exactly in the middle. We utilize a uniform grid with 1200 cells, which was found sufficient for the solution convergence. Also, a time step of $1.0 \times 10{-}10$ s was found sufficiently small for accurately capturing the changes in reaction, diffusion, and convection terms for all the tested cases. Each simulation is carried out until ignition is achieved. For all the simulations, we use the chemical mechanism by Burke et al. [14], which is designated for high-pressure hydrogen-air chemical reactions. In addition, as previously mentioned, we are using mixture averaged diffusion coefficients, which were found to yield almost indistinguishable results in comparison with the much more computationally expensive multi-component diffusion coefficients.

The initial temperature of the gases on both sides of the diffusion layer and the pressure at the diffusion layer are shown in Table 1 for each case, i.e., different low-pressure gas. The low-pressure-gas mixture that contains the highest mole percentage of N_2 is a mixture that contains 6% of O_2 and 94% of N_2. As previously mentioned, the high-pressure gas is pure H_2 in all the cases.

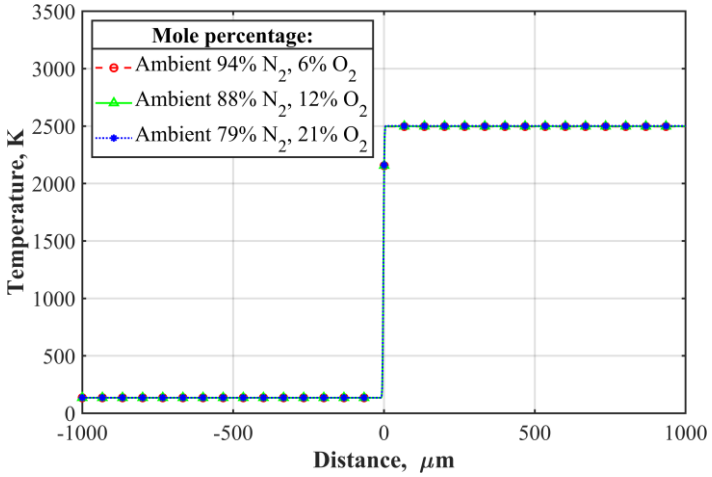
Table 1. Initial temperature and pressure profiles at the diffusion layer for diluted air side obtained from the shock-tube solution for a pressure ratio of 700.

Ambient composition	H_2 **temperature**, K	**Air temperature**, K	**Initial pressure**, atm
21% O_2, 79% N_2	135.2	2501	54.5
12% O_2, 88% N_2	134.9	2498	54.1
6% O_2, 94% N_2	134.7	2496	53.9

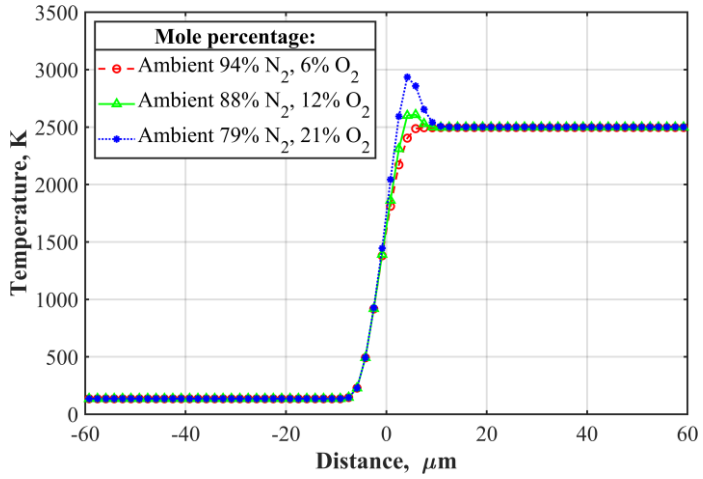
On the ambient side, the pressure is 1 atm. Three different cases for the ambient side conditions are considered. The first is 6% $O_2$with 94% N_2, the second is 12% $O_2$with 88% N_2, and the last is undiluted air with 21% O_2 and 79% N_2, as shown in Table 1. The N_2 dilution on the air side has a negligible effect on the initial conditions, see Table 1. For instance, for 21% O_2 the pressure at the diffusion layer is equal 54.48 atm, and for the 12% O_2 case, a value of 54.1 atm is obtained. For the last case, the pressure in the diffusion layer is 53.85 atm. Hence, the differences between the initial temperature profiles are also very small. This is not surprising as N_2 and O_2 have similar molar weights. Next, we present and analyse temperature profiles during the ignition process.

The temperature profiles are shown in Figure 6. At the first time step, as previously mentioned, the initial profiles are almost identical, see Figure 6a. The dilution effect of the nitrogen on the air side did

not affect the speed of sound, which leads to almost the same shock-wave strength, thus the initial states of the air sides are almost the same (Figure 6a). After 0.06 μs, self-ignition has occurred for the pure air case and the diluted case with 12% O_2. This is clearly seen by the temperature rise shown in Figure 6b. It can be noticed that the pure-air case undergoes self-ignition first; however, it seems that the time difference between the self-ignition processes for the pure-air case and 12% O_2 case is small. Figure 6c shows that the self-ignition has also occurred for the case with 6% O_2 at 0.50 μs. In summary, it is observed that although the last case contained only 6% of O_2, this amount did not delay significantly the self-ignition process in comparison with the undiluted case.



(a)



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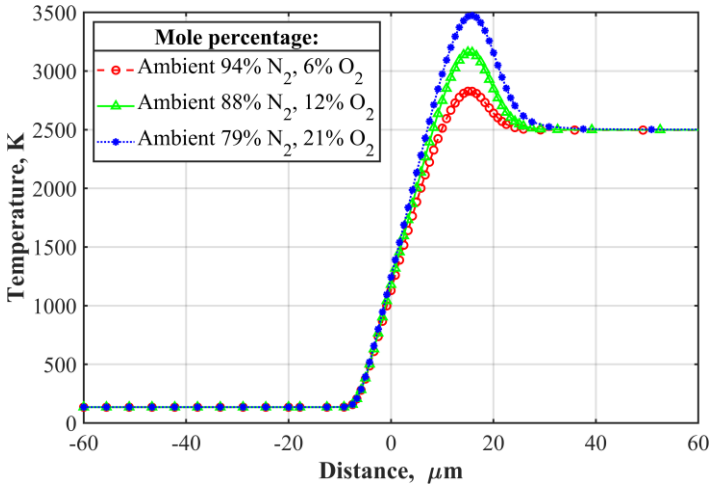

(c)

Figure 6. Temperature profiles in the diffusion layer region at (a) t=0 μs, (b) t=0.06 μs, and (c) t=0.50 μs.

We demonstrate that nitrogen dilution increases the ignition delay time. As nitrogen dilution of the ambient side does not affect the resulting shock wave strength significantly, the difference in the ignition time delays between the cases is solely due to the lower oxygen content. Nevertheless, the difference in the ignition time delays is not very significant.

3.0 PRELIMINARY WORK RELATED TO JET IGNITION EXPERIMENTS

The experimental work will be performed inside the SSEXHY facility located at CEA (Saclay, France). The SSEXHY combustion tube [15] features a stainless steel obstructed duct designed to study the acceleration mechanisms of premixed hydrogen/air flames. The tube includes four interchangeable sections connected by flanges. Each section is 1310 mm long with an internal diameter of 120 mm. Two blank flanges can be used to seal the combustion tube at its extremities. A picture of the experimental device is shown in Figure 7.

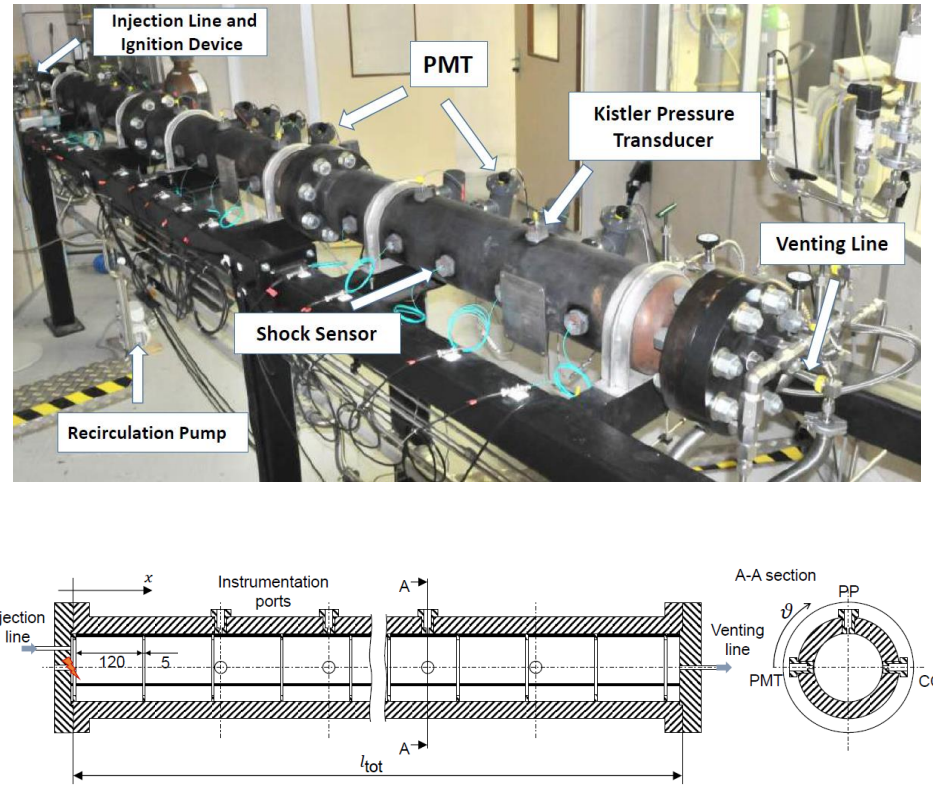

Figure 7. Picture of SSEXHY Tube having 3 sections and showing different instrumentations (top); schematic of the Tube (bottom). Sizes are given in mm. PMT=”PhotoMultiplier Tube”, CC = “Shock Sensor”, PP = “Pressure Transducer”.

One of the standard sections will be replaced by the viewing section and CEA has started to prepare the SSEXHY experimental facility for the project experiments. The work carried out concerns three main areas:

- the further development and qualification of the viewing section;
- the design and the manufacture of the system to produce the pressurized jet;

- the implementation of an adapted metrology to follow the time and space evolution of the phenomena.

For the viewing section, the finalised design shown in Figure 8 includes two quartz windows of size 20 cm x 12 cm. The production is now in progress and the device should be available in the first half of 2023 for the qualification tests.

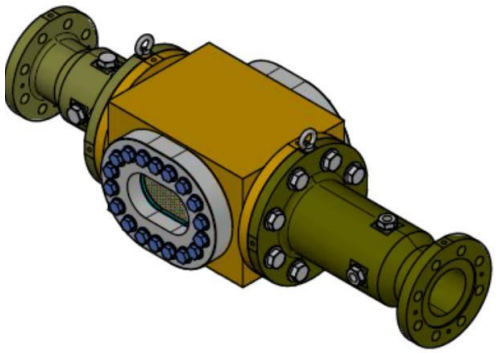

Figure 8. General view of the design of the viewing section to be installed for the project in the SSEXHY experimental device.

For the high-pressure gas injections, we propose to install inside the tube a small tank equipped with a rupture disk to produce the pressurized jet and to properly locate the pressurized release with respect to the viewing section. The description of this device is provided schematically in Figure 9 and a picture of the assembly under test is provided in Figure 10. It allows to control from outside of the SSEXHY tube with gas supply (helium or hydrogen), pressure measurement, draining or vacuuming. Then, a cylindrical tank of ~0.3 liters is installed in the tube with at its end a flange whose closing cap is provided with an orifice of given diameter. Several caps with different diameters are available.

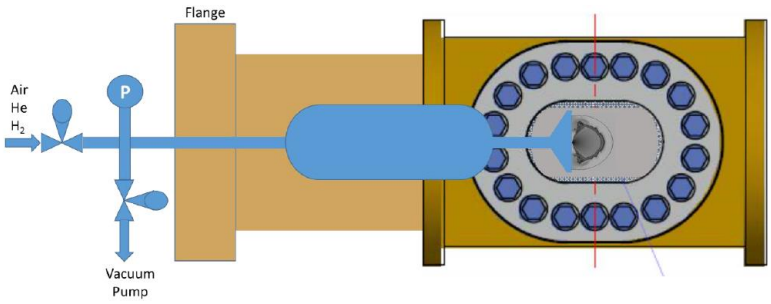

Figure 9. Schematic description of the new device envisaged to produce the pressurized jet of helium or hydrogen.

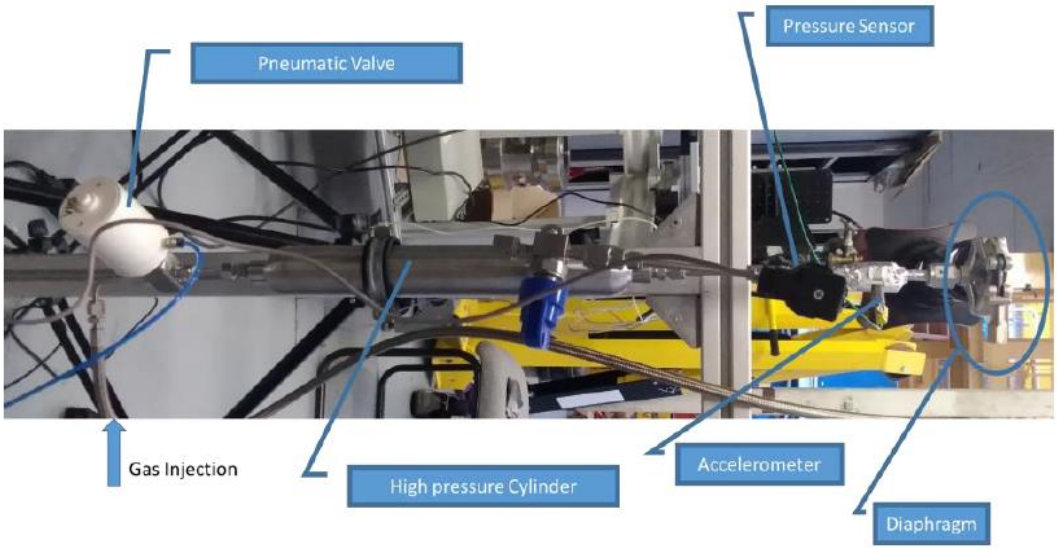

Figure 10. Photo of the device mounted during the pre-test of the open-air rupture.

The envisaged test sequence is as follows:

- the diaphragm is positioned on the selected cap for the test;
- the injection system is reassembled inside the SSEXHY tube and connected to the selected gas supply, the vacuum pump and the pressure sensor;
- the SSEXHY tube and the injection system are evacuated;
- the SSEXHY tube and the injection system are filled under atmospheric pressure (the mixture in the SSEXHY tube may or may not be flammable and the mixture in the injection system may be composed of air (for the pre-tests), helium or hydrogen for the tests;
- the pressure in the injection device is suddenly increased with the driving gas to break the diaphragm and generate the pressurized jet;
- the cameras and measuring devices (pressure, photomultiplier, etc.) are triggered when the diaphragm bursts, using an accelerometer.

For the disk rupture, we tested the use of an aluminium tape with a star marking to locate the rupture. The reproducibility seems to be adequate after the first tests but further tests are necessary to control this parameter.
For the instrumentation of the tests, the CEA worked on the installation of a Schlieren device in full diameter to obtain a proper viewing of the transient phenomena following the rupture of the diaphragm and the propagation of the waves in the mixture located downstream. The studied set-up is very classical and described in many publications, a picture of this set-up is provided on Figure 11.
We work with two parabolic mirrors of 12 inches in diameter and two plane mirrors of the same size. High-Power LED (Thorlabs) provide the light source. For the camera, we performed tests with the high-speed cameras of the laboratory and with commercial high-speed cameras. The selected test is a shock wave exiting a shock tube (1 inch in diameter) and produced by an air overpressure. These tests allowed us to evaluate the recordings of different high-speed cameras with frame rates ranging from 50 kfps to 5 Mfps. Examples of the viewing are provided in Figure 12. We can clearly distinguish an initial shock wave taking spherical form as well as a contact line separating the compressed air. The laboratory is acquiring some of these cameras and their use will therefore benefit the metrology of the project.

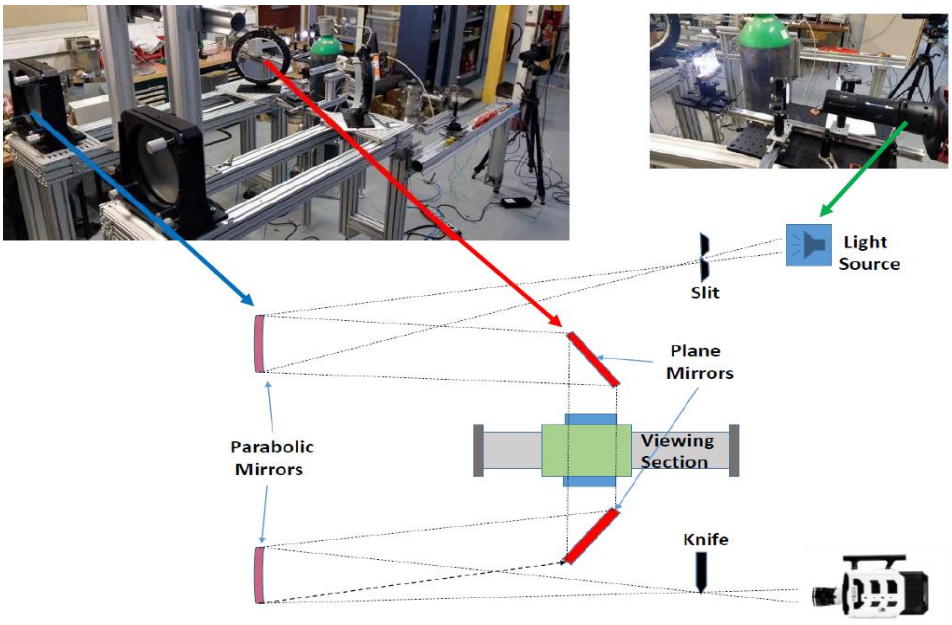

Figure 11. Z-Schlieren assembly designed for viewing.

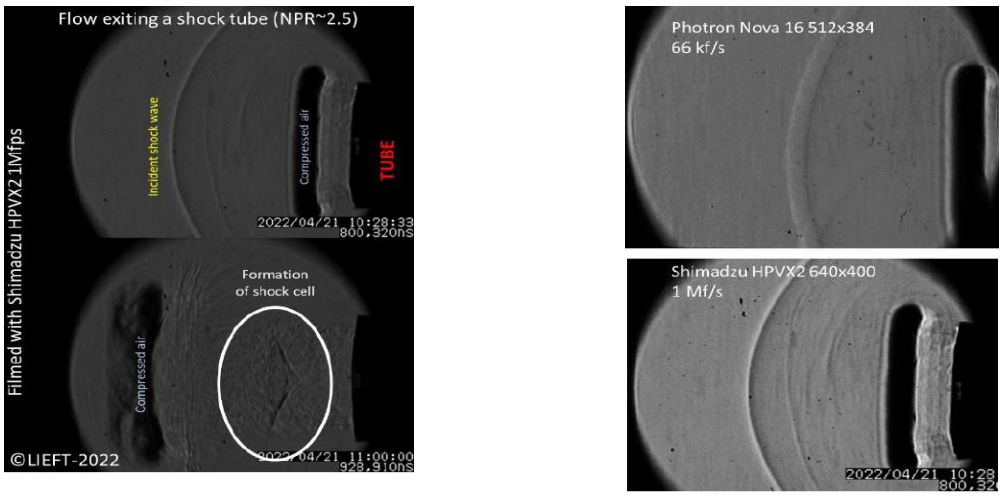

Figure 12. Schlieren images of a shock wave and the material wave from a tube into infinite medium made with different high-speed cameras.

3.0 CONCLUSIONS.

A common project between Tel Aviv University (TAU), Negev Nuclear Research Center (NNRC) and Commissariat à l'Energie Atomique (CEA) has been recently launched in order to understand the phenomena of high-pressure hydrogen jet release and injection from experimental, modelling and numerical points of view. The main goal is to investigate the dynamics and combustion regimes that arise once a pressurized hydrogen jet is released into a *reactive* environment that contains inhomogeneous concentrations of hydrogen, steam, and air.

In this paper we described the numerical codes validation against related experimental results. First, some of the numerical solutions dealing with light gas erosion by a vertical air jet are compared to their experimental counterparts. The grid sensitivity study has been performed showing a good agreement Second, validation related to a high-pressure hydrogen jet release is introduced, followed by jet-ignition phenomenon simulations. The importance of correct boundary conditions is highlighted; not accounting for the transient effects of the flow at the inlet leads to a faster expanding jet, which is the case for the

steady-state choked-inlet computation. This can lead to wrong predictions of the different flow structures, and possibly, the jet-ignition characteristics.
The initial steps of experimental work dedicated to a pressurized hydrogen jet release into a reactive environment are presented in the paper. This included a set of experiments using Z-Shclieren technique revealing high-speed shocked flow structures.
The future work is divided into two major tasks: (a) further codes validation followed by large-scale slow hydrogen leakage URANS and LES simulations, and (b) qualification tests of the visualisation section installed in SSEXHY facility followed by pressurized jet release into reactive mixture experiments.

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