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Experimental and Numerical Evaluation of Transient Temperature Distribution inside a Cylinder during Fast Filling for H_2 Applications

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1 Introduction

For practical use in near-term applications as transition and automotive markets, high pressure compressed gas storage of hydrogen remains a robust technology whose feasibility has been already demonstrated for working pressure up to 700 bar (European project Storhy for instance [1]). Safety issues are of critical importance in the context of hydrogen energy and must be clearly addressed. To guarantee the integrity of pressure vessels during successive refuelling processes in service, standards have been defined for vehicular applications which limit the gas temperature within the cylinder to 383 K and the gas pressure to 1.25 times the cylinder's design pressure.

Challenge consists in improving the efficiency of refuelling process while ensuring the safety of cylinders. In order to evaluate thermal and mechanics effects or damages on wall structure, a key issue is at first to give an accurate estimation of the temperature evolution at the surface of the interior cylinder wall and to highlight the hot spots where the temperature rises to a maximum associated with a the time of exposure.

To address this question, both experimental and numerical works may be found in the literature. To evaluate temperature distribution within the cylinder wall, a simple approach consists in coupling a single gas temperature evolution prediction and a one-dimensional conduction calculation within the wall (e.g. [2]). Such a method was also applied in Air Liquide R&D [3] and allowed to understand the influence of filling parameters such as initial conditions, targeted pressure and geometry of the cylinder as the ratio between the length and the diameter. Experimental studies using measurement devices placed inside the vessel have been also carried out, allowing evaluating the temperature in few points (e.g. [3], [4], [5]) or in a more extended region using a large matrix of sensors [6]. Two-dimensional CFD simulations with *Fluent* Software have also been also performed by the authors on a test corresponding to 350 bars for a filling duration inferior to one minute [7].

This paper proposes an accurate evaluation of transient temperature distribution within the gas during fast filling process with nitrogen gas. This experimental work has been coupled with numerical simulations on 2D and 3D geometries including the calculation of thermal conduction inside the walls.

In a first part, the experimental setup and devices are presented and main results are addressed. In a second part, the numerical settings of CFD calculations are described and first results are discussed in regard to measures.

2 Experiments

The instrumented cylinder is a 46L type 4 cylinder whose wall consists in a plastic liner (here polyethylene) and fully wrapped with a carbon-epoxy composite. The cylinder features are given Table 1.

Table 1: Cylinder characteristics (* with boss).

Working Pressure (bar)	Mass (kg)	Length* (m)	Diameter(m)	L/D ratio
200	18	1.47	0.235	6.2

To facilitate the instrumental device development, the gas used here is nitrogen and not hydrogen, which would have imposed heavier leak prevention and safety procedures, without being necessary to achieve the experiments objectives to understand the physics of fast filling. The experimental bench is composed of a nitrogen buffer at a pressure of 100 to 200 bars depending on test, a regulator, a calibrated throat, a long duct, a cylinder and a data acquisition system. The regulator decreases the pressure the buffer pressure to 100 bars. Two diameters have been considered (6 mm and 1 mm) leading to filling rates equal to 150 bar/min and 21 bars/min and corresponding to durations of around 30 s and 2 min 30s to reach a targeted pressure inside the cylinder of around 50 bars. The overall experimental bench is illustrated Fig 1 (left). The reproducibility of measures has been also investigated. Table 2 presents examples of experimental conditions for the two calibrated throat diameters.

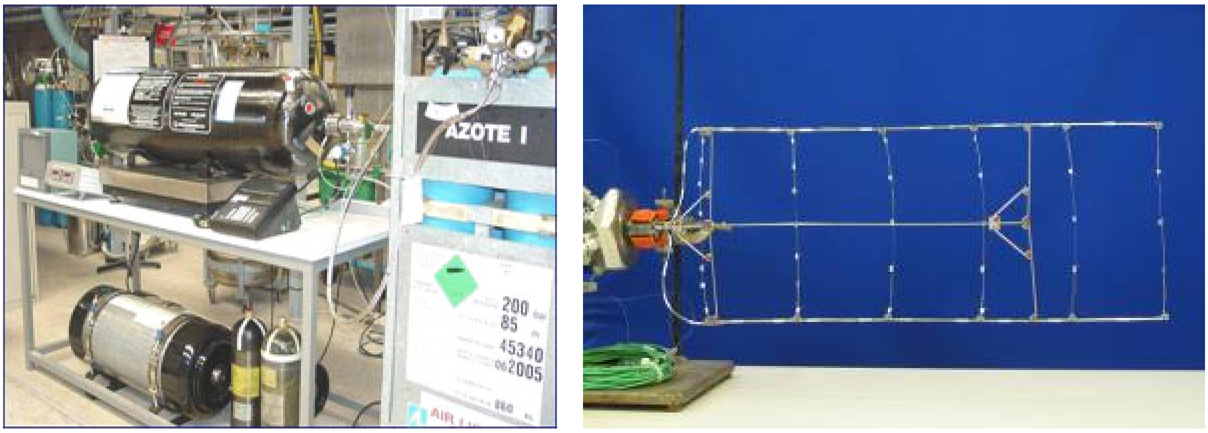


Figure 1: Experimental facilities in CRCD (left: experimental bench, right: second thermocouples matrix introduced at the bottom of the cylinder).

Table 2: Tests conditions.

Test	Throat diameter (mm)	P Buffer (barg)	P after expansion (barg)	P_i cylinder. (barg)	P_{final} (barg)	Charge duration (s)	Filling rate (bar/min)	T amb (°C)
#1	6.0	160	100	0.0	50	19.95	150	21.4
#2	1.1	185 - 190	100	0.0	50	141.40	21	22.3

Two experimental devices have been successively used to measure the temperature distribution in the vertical plane of the cylinder. These devices are composed of type K thermocouples with a diameter of 0.25 mm. The measure uncertainty is +/- 2.5 K and the time sampling during the filling is set to 50 ms. Note that on these tests, filing has been made horizontally. The large number of sensors (57) allows to accurately following the temperature evolution at any point of the interest zone. A view of the matrix #2 is given Figure 1 (right) and a schematic representation of sensors locations obtained with the two devices is given Figure 2.

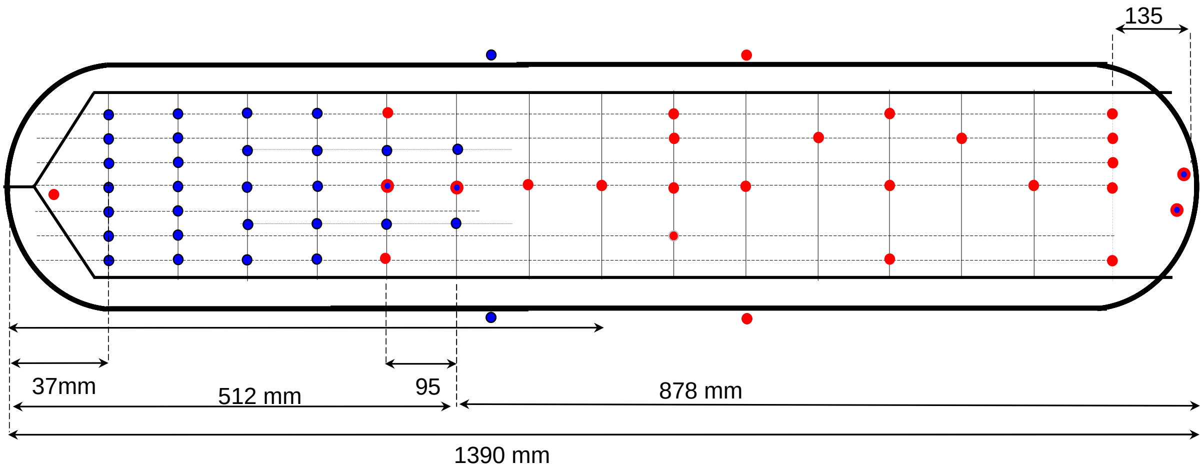


Figure 2: **Matrix of sensors installed within the cylinder (in red: first device, in blue: second device, points in blue and red correspond to covering points). Note that gas entrance is placed here on the right.**

2.1 Physics of fast filling

The gas entrance is depicted by a jet whose regime evolves during the filling time. Indeed, the instantaneous nozzle pressure ratio which drives the jet behaviour decreases during filling process as internal pressure increases. Therefore, an under-expanded regime is expected at the beginning and an over-expanded one at the end of the filling time. Hence, the jet characteristics (length, velocity and turbulence level) are directly correlated to the filling rate for which corresponds a given filling duration. Note that the jet confinement in the vessel leads to recirculation zones all around the jet. Moreover, depending on the jet and cylinder lengths, a flow zone characterized by very low Reynolds numbers may extend from the end of jet zone to the cylinder bottom. This zone may be seen as a stagnation zone where buoyancy effects may initiate free convection mechanism.

2.2 Experimental results and discussion

Figure 3 depicts the temperature evolution during filling for the sensors located along the jet direction. It shows clearly two distinct transient regimes. In a first zone going from the gas entrance to approximately a distance of x / L = 2/3 (corresponding to sensor #105), the temperature at any location increases continuously during time and reaches a maximum at the end of time filling. This observation is in accordance with measures from the literature

[3, 4, 5, 6] and calculations obtained with zero-dimensional models [2, 3] and also three-dimensional calculations [7].

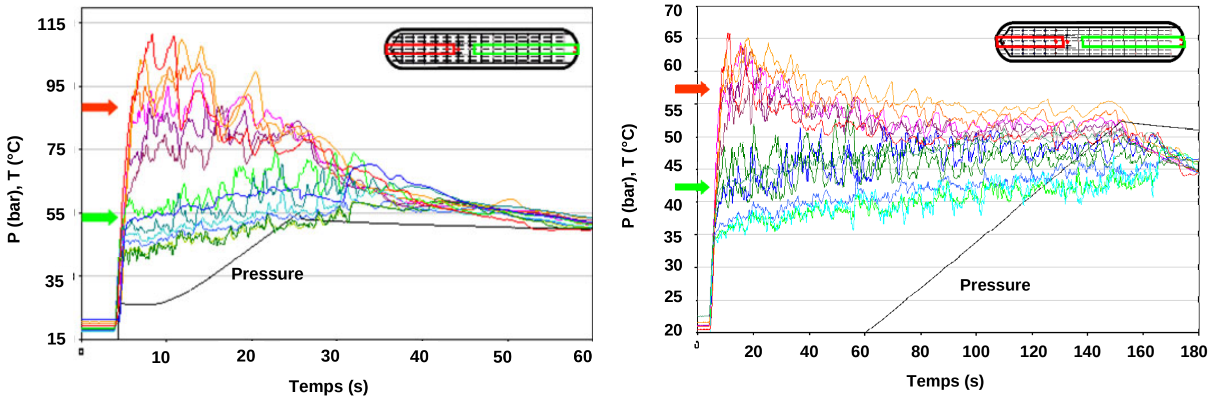


Figure 3: Temperature evolution along the cylinder centreline during fast filling (left: for a filling rate of 150 bar / min ; right: for a filling rate of 21 bar / min).

In a second zone located at the cylinder bottom, the maximum temperature at each position is observed very quickly (before 5 s for a filling rate of 150 bar/min and before 20 s for 21 bar/min) and one can observe a constant cooling thereafter to recover a quasi homogeneous temperature at the end of filling period.

Moreover, a longitudinal temperature gradient is also clearly highlighted. This gradient is not constant along the longitudinal distance: the smaller gradient is observed within the jet and the greater at a distance between the two zones previously mentioned (i.e. at a distance such as x / L is around 2/3).

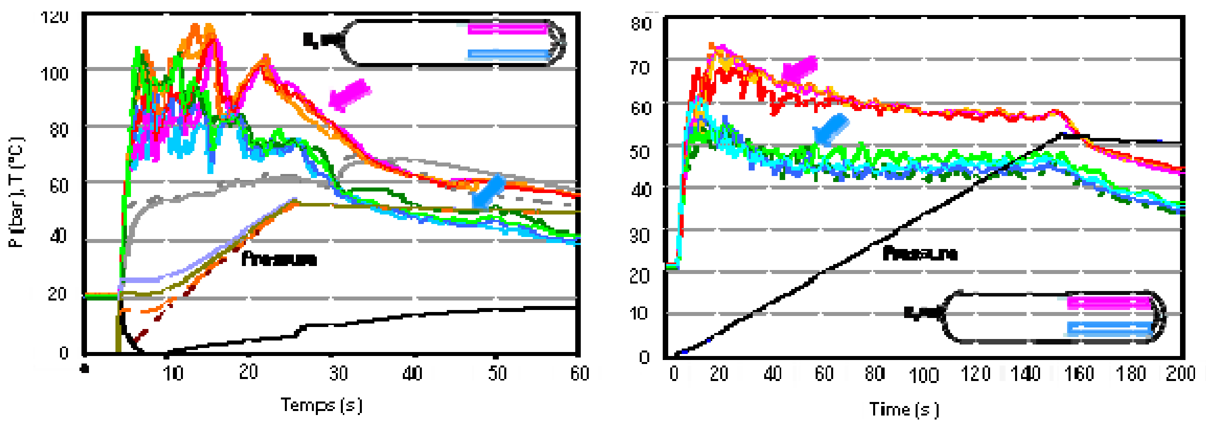


Figure 4: Temperature evolution at sensors located along the wall, in red on the left-figure (left: for a filling rate of 150 bar / min ; right: for a filling rate of 21 bar / min).

Figure 4 shows the temperature evolution on sensors located on two longitudinal lines at a same radial distance from the centreline but one at the top of the cylinder and the second below. All these sensors belong to the second region where higher temperatures are reached. Stratification in the transverse direction appears clearly with a constant difference of

15°C between the two levels for the lowest filling rate. This observation suggests that transient free convection mechanism appears in that region.

3 CFD Numerical Simulations

3.1 Numerical setup

CFD (Computational Fluid Dynamics) simulations have been carried out to reproduce the test #1 (150 bar / min). Both 2D axi-symmetric and 3D geometry for the half-cylinder have been handled (Figure 5). The mesh for the 2D geometry contains 20000 hexahedrons control volumes. This mesh is suitable to reproduce the expanded jet inside the cylinder and to predict the temperature evolution in the first part of the cylinder where buoyancy effects are negligible. The 3D mesh contains 1 million control volumes. The compressible pressure-based solver is used with a realizable k-ε turbulence closure model. For time discretization, implicit formulation is used with an optimized time-stepping strategy to reduce the computational time without impairing the solution's accuracy. The walls are taken into account and thermal conduction is resolved inside. Usual thermal exchange coefficients are defined for outside natural convection with air whereas coupled heat exchanges are handled by the solver inside the vessel. At inlet condition, a total pressure ramp is imposed according to experimental measures.

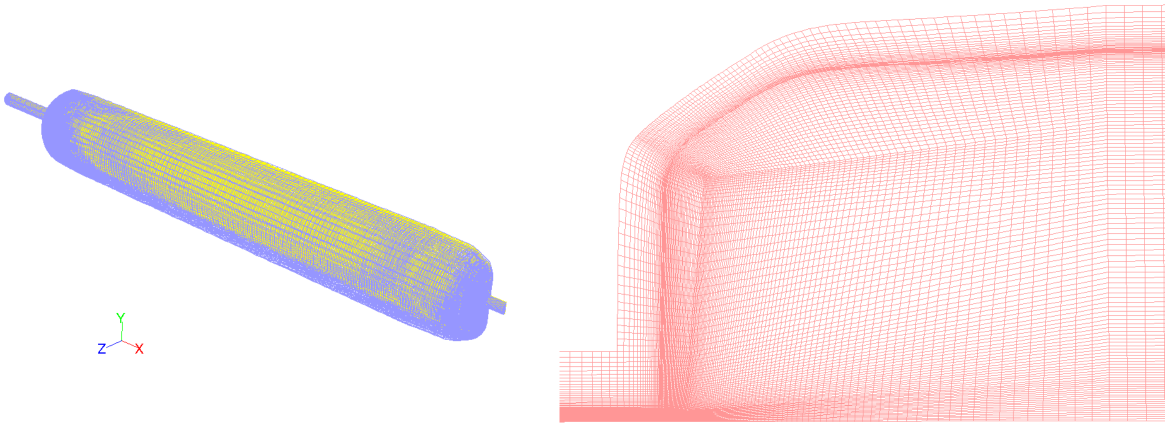
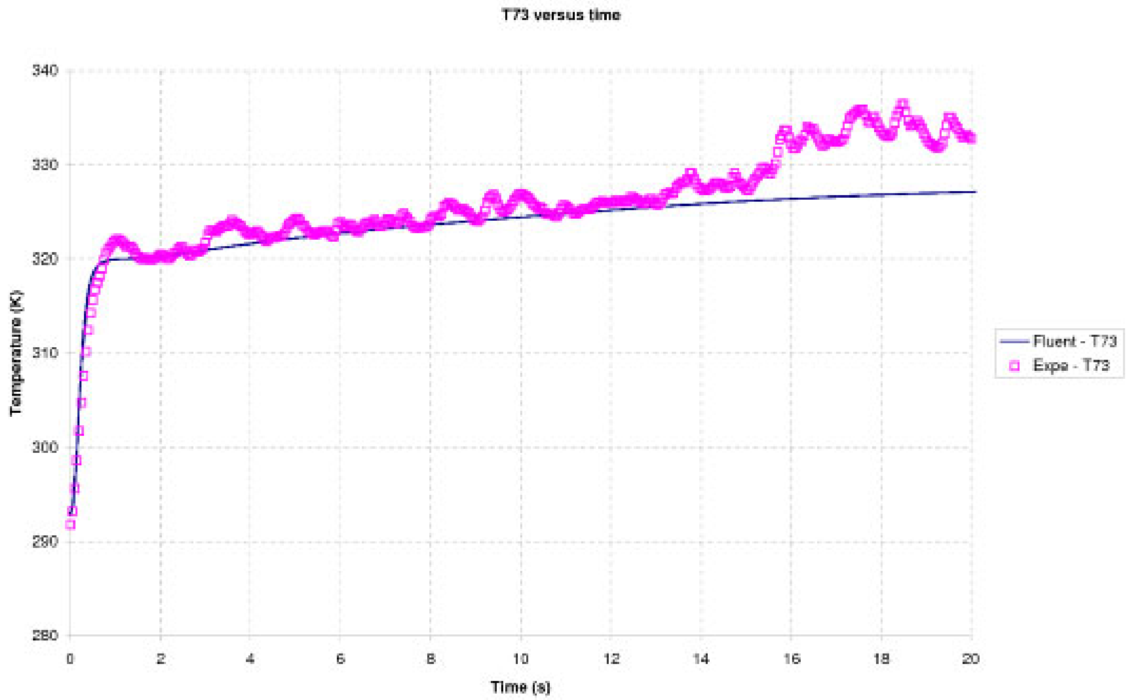


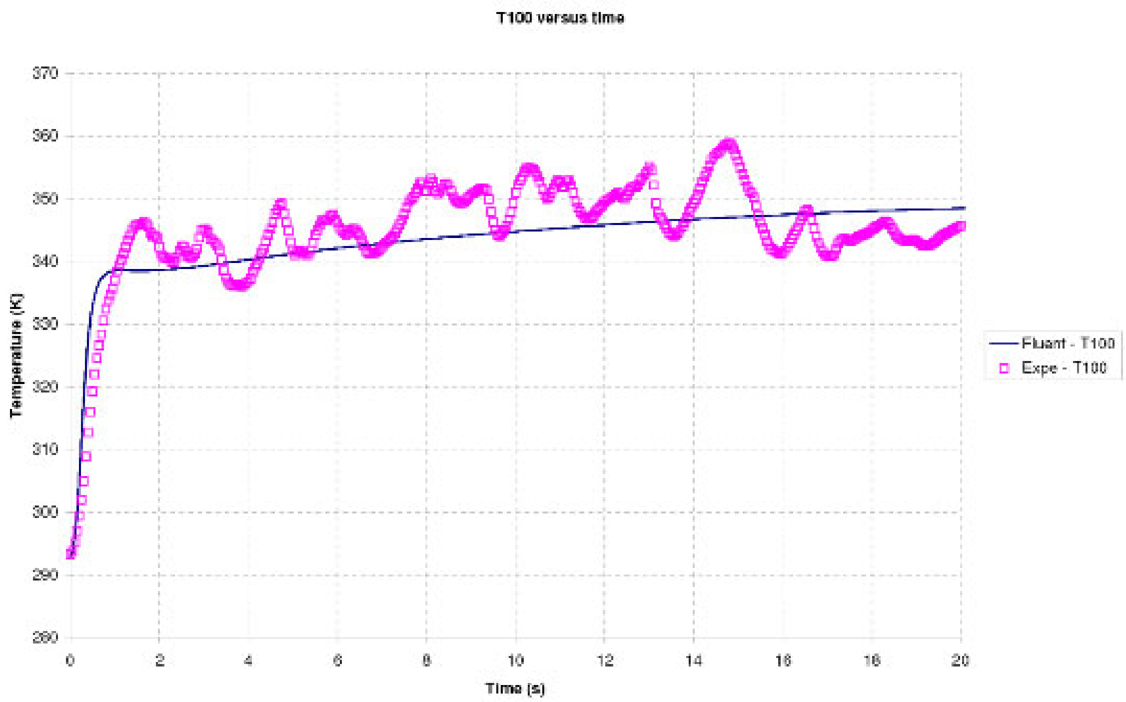
Figure 5: Mesh visualization for the 3D geometry (left) and zoom on near-field jet region (right) in a cut plane.

3.2 Main results

For 2D simulations, typical flow patterns are well reproduced with the development of an under-expanded jet extending to half the cylinder length surrounded by recirculation zones. The predicted temperatures inside the jet and more downstream are in relative good agreement with measures collected on matrix #1. An example is given Figure 6. However, comparisons made more downstream for the matrix #2 (note shown here) confirm that a simple 2D axi-symmetric approach is inappropriate to reproduce the thermal effects at the cylinder bottom. Indeed, neglecting free convection phenomena leads to a significant overestimation of temperature rise in that region and including buoyancy effects in 3D simulations should improve the results in future work.



a)



b)

Figure 6: Temperature evolution during filling up to 20 s at sensors #73 (a) and sensor #110 (b) for a filling rate of 150 bar/min.

4 Conclusions

This paper presents a large part of ongoing work at AIR LIQUIDE R&D on the understanding and evaluation of transient temperature distribution during filling process of high pressure gas cylinders and for two filling rates. The originality of the study consists in the geometric features of cylinder whose large scale ratio leads to the establishment of a secondary zone at the bottom of the cylinder in which free convection mechanism appears, even for very fast filling process. This zone is the place of a significant temperature rise up to about 100°C during a few seconds. The numerical study performed with Fluent CFD tool for a 2D axi-symmetric problem gives a relatively good agreement with measures for the prediction of transient temperature distribution in a first part of the cylinder where buoyancy effects remain negligible. Challenges ahead are to perform 3D simulations to understand natural convection establishment and better predict the temperature distribution at the bottom of the cylinder. Furthermore, and once the gas phase behaviour simulation would be considered validated against experimental work, it will be part of future work to extend the focus of the numerical study to the prediction of transient thermo-mechanical cycles in the cylinder structural shell.

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