OSIRHYS IV project: Qualification and optimization of 700 bar composite pressure vessel

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Abstract
The present study is the part of French funded project: OSIRHYS IV. It is dedicated to the study of uncertainties and approximations of high pressure vessel composite design and calculation. The goal of OSIRHYS IV project is to develop and validate models and methods for composite high pressure design and optimization with behavior uncertainties knowledge. Introduction of probabilistic variables into the model allow to provide interesting information about how this parameter affect the tank behavior. The qualification process involves a comparison between experimental and numerical results on a tank which are also presented in this study.

1. Introduction

Hydrogen is an alternative to traditional energy sources like oil and natural gas. It offers great advantages as no greenhouse gas emission. For more than a decade, this way has been the focus of research and development efforts. Hydrogen storage stays a key issue for the high scale deployment of fuel cell applications. Different ways exist to store hydrogen, such as liquid storage tank at cryogenic temperature [1-3], polymer and composite foam [4,5], metal hydrides [6] and gaseous high pressure storage vessel [7,8].

The gaseous hydrogen storage at high pressure with type IV vessels (with a polymeric liner fully-wrapped with a fiber-resin composite) is considered as the most appropriate at least for short term. To be efficient, this storage must be done at high pressure (above 350 bar and up to 700 bar for on-board applications). Recent developments on 700 bar type IV vessels have demonstrated very promising results (high cycling resistance, burst pressure, hydrogen tightness, gravimetric and volumetric storage capacities…).

To reach commercial deployments, this technology needs research and development to cut costs and improve performance, reliability and durability of current high pressure vessels. The composite shell allows withstanding high mechanical stresses due to internal pressure. An optimization of composite structure will allow reaching a significant cost reduction of hydrogen cylinders. An improvement of numerical simulation is needed because today most of the engineers work with simplified models frequently not fully representative.

Nowadays, it can be found some studies on the numerical modeling of composite pressure vessel [9-12] but the comparison of the results with detailed experimental database and the estimation of computational error are not common. OSIRHYS IV is a project supported by the French Research National Agency (ANR) through “Hydrogène et Piles à Combustible” program (HPAC program). The purpose of this project is to clarify uncertainties and approximations of high pressure vessel composite design and calculation. The project is dedicated to enhance the whole conception and simulation chain. It aims at improving material and process (filament winding) characterization and at establishing a strong and shared database between all project partners. The goal of OSIRHYS IV project is to develop and validate models and methods for composite high pressure design and optimization with behavior uncertainties knowledge.

The qualification process involves a comparison between experimental and numerical results on a tank. This paper will focus on the comparison of the type IV hydrogen high pressure storage vessel experimental and numerical behavior under different thermal conditions (from -40°C to 85°C).

In a first section, a presentation of the tank and of the modeling of its geometry is done. Another section focuses on the composite material behavior law developed in the project in order to take into account matrix and fiber damage with probabilistic approach. Effect of temperature is also introduced into the model. In a third section, the numerical results obtained, using the composite behavior law developed during the project, were compared to several experimental results obtained at room temperature by various sophisticated techniques. In the end, the influence of temperature on burst behavior was investigated with using numerical simulations and compared to experimental results.

2. Design, geometry and finite element modelling

The tank modeled in this study is 700 bar type IV hydrogen high pressure storage vessel. Type IV high pressure storage vessels are made of metal bosses to ensure the tank connectivity, a polymer liner whose main function is the tightness, and a wound composite shell to provide mechanical strength. In this study, the bosses of the 2L tank are made of 316L stainless steel, the liner is made by reactive rotomolding of PA6, and the composite shell is a wound composite carbon epoxy prepreg.

The composite shell is of vital importance with respect to security because it ensures the mechanical strength. The difficulty in accurately analyzing the behavior of filament wound structures derives from the varying orientation of the wound filaments throughout the structure. The geometric complexity of this composite shell is important: the shape of domes varies significantly depending on the fiber angle in the cylindrical part and the winding pattern. It influences the whole structure behavior, so it is necessary to predict at best its response during pressurization.
To implement a simulation of the mechanical behavior of the tank, it will be modeled with the “Abaqus” finite elements software and the “Wound Composite Modeler” specific plugin. With this plugin the composite shell is modeled layer by layer: each layer is generated from the contour of the previous layer, except for the first layer which is generated from the liner contour. All helical layers have a helical winding pattern described by the following equation:

$$\theta(R) = \sin^{-1}\left(\frac{R_0}{R}\right) \pm \delta\left(\frac{R - R_0}{R_{tl} - R_0}\right)^n \quad (1)$$

Here, R is the radial distance from the center line to a point in the layer, R0 is the radial distance from the centerline to the turnaround point, and Rtl is the radius at the dome-cylinder tangent line, and δ is the difference in degrees between the frictionless wind angle (input for the layer) and the wind angle calculated by the first term of Equation 1. A frictionless winding pattern is obtained by choosing $\delta = 0$. If friction is accounted for, $\delta \neq 0$, then the wind angle distribution will vary.

As the layer traverses the dome to the polar boss, the thickness of the helical layer gradually builds up as described by Equation 2.

$$t(r) = \frac{t_{tl} \cdot \cos(\theta_{tl})}{\cos(\theta_r)} \cdot \frac{r_{tl}}{r + 2 \cdot BW \cdot \left(\frac{r_{tl} - r}{r_{tl} - r_0} \right)^4} \tag{2}$$

θ_{tl} is the wind angle at the tangent line, θ_r is the wind angle at radius, t_{tl} is the thickness at the tangent line and BW is the helical band width.

Input data of the plugin are the fibers angle and the thickness of each layer. The position of the end of each layer was readjusted using tank radiography. These adjustments can be achieved by varying the gliding coefficient of the fiber yarn. The gap between liner part and composite part highlight by X-ray observations is modeled. A void between the two parts is created and a perfect contact with no friction is added.
Figure 1 shows the boundary conditions applied to the model. An internal pressure varying from 0 bar to 2000 bar is applied on all internal faces of the tank (bosses and liner). Displacements of one extremity of the tank are set to zero (top of a boss). Axial and radial displacements are measured in FE simulation as shown in Figure 1.

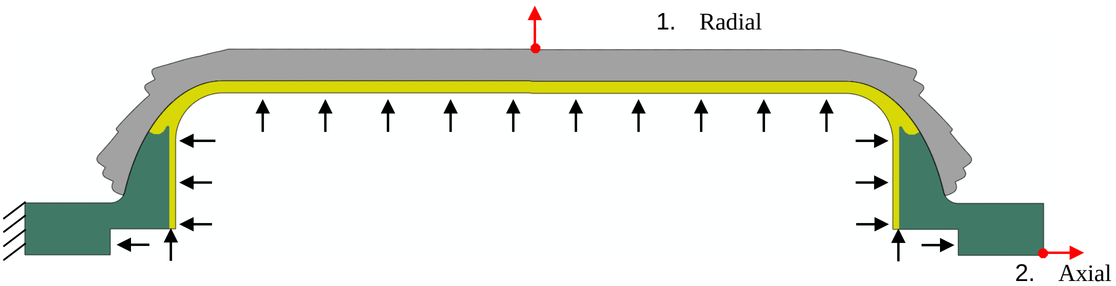

Figure 1. Tank modeling and boundary conditions

3. Composite material behavior law

The mechanical behavior law detailed in this section is based on the work presented in [12] where a coupled anisotropic thermo-mechanical behavior law is presented. In this work, only matrix cracking is taken into account. The non-linear shear behavior is not modeled because of the low shear stress values reached in a high pressure tank. In addition to the initial damage variable d_m (Eq. 3) relative to matrix cracking, another damage variable d_f (Eq. 4) is added to model fiber breakage.

Triangular law used in [12] is replaced by exponential law in order to be smoother and so to improve numerical convergence.

$$d_m = \begin{cases} 0 & if\ \varepsilon_{22} < \varepsilon_{22R}(T) \\ 1 - exp\left(\frac{(\varepsilon_{22R}^2(T) - \varepsilon_{22}^2)}{\alpha_m(T)}\right) & else \end{cases} \quad (3)$$

$$d_f = \begin{cases} 0 & if\ \varepsilon_{11} < \varepsilon_{11R} \\ 1 - exp\left(\frac{(\varepsilon_{11R}^2 - \varepsilon_{11}^2)}{\alpha_f(T)}\right) & else \end{cases} \quad (4)$$

where ε_{11R} (T) and ε_{22R}(T) are strains threshold for damage initiation, α_f(T) and α_m(T) are parameters governing damage evolution.
Once a damage initiation criterion is satisfied, material stiffness coefficient is degraded (figure 2). The damage variable associated with the failure mode vary from 0 (undamaged state for the mode corresponding to this damage variable) to 1 (fully damage state for the mode corresponding to this damage variable).

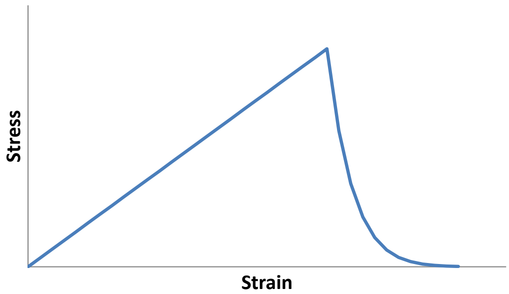

Figure 2. Example of behavior obtained with the implemented law

The composite elastic matrix can be written as the matrix in Eq. (3)

$$C = \begin{bmatrix} (1-d_f)C_{11}(T,TVF) & (1-d_f)(1-d_m)C_{12}(T) & (1-d_f)C_{13}(T) & 0 & 0 & 0 \\ (1-d_f)(1-d_m)C_{12}(T) & (1-d_m)C_{22}(T) & (1-d_m)C_{23}(T) & 0 & 0 & 0 \\ (1-d_f)C_{13}(T) & (1-d_m)C_{23}(T) & C_{33}(T) & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44}(T) & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55}(T) & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66}(T) \end{bmatrix} \quad (5)$$

where $C_{ij}(T)$ are the elastic stiffness coefficients, T is the temperature, d_m and d_f are the damage variables defined in Eq. 3 and Eq. 4.
Each layer of a wound structure is made of intertwining of fiber yarn with –θ and +θ angles. Thus, the behavior of a layer C_{ply} has been determined by a homogenization process applied on stiffness matrix (Eq. 6)

$$C_{ply}(T, d_m, d_f, TVF) = \frac{C_\theta(T,d_m,d_f,TVF) + C_{-\theta}(T,d_m,d_f,TVF)}{2} \quad (6)$$

where C_θ and $C_{-\theta}$ are the stiffness matrix of an elementary ply C rotated by an angle θ and –θ.

Variability of fiber breakage and fiber volume ratio are taken into account with the implementation of random variables determined experimentally. Weibull law is used for fiber breakage and Gaussian law is used for fiber volume ratio.

Elastic parameters of the composite materials are summarized in table 1.

	-40°C	25°C	85°C
E_1^0 (GPa)	136.85	134.22	115.06
E_2^0 (GPa)	9.596	8.175	1.182
E_3^0 (GPa)	9.596	8.175	1.182
ν_{12}^0	0.292	0.362	0.759
ν_{13}^0	0.292	0.362	0.759
ν_{23}^0	0.307	0.38	0.5
G_{12}^0 (GPa)	5.526	4.697	0.54
G_{13}^0 (GPa)	5.526	4.697	0.54
G_{23}^0 (GPa)	3.671	2.962	0.394

Table 1: Carbon fiber – epoxy wound composite material parameters

4. Comparison of experimental results and numerical results

In this paragraph, burst behavior of tank is studied and compared to experimental data. In a first step, experimental and numerical displacements curves for a burst test are compared (Figure 3).

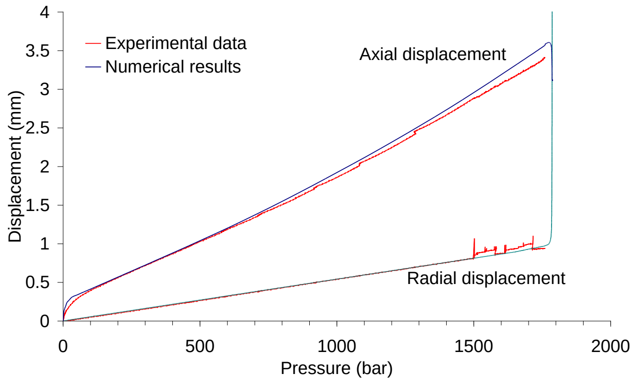

Figure 3. Numerical and experimental comparison of axial and radial displacement for burst test

Two burst modes can be defined for high pressure storage vessel:

- Dome burst (figure 4-a) – radial failure
- Cylindrical part burst (figure 4-b) – axial failure

For a safety reason cylindrical part burst is privileged because of the bosses/domes are not projected in this case. One can see in figure 3 that burst mode is a burst in cylindrical part, i.e. metallic boss goes inside the tank and are not ejected outside the tank.

(a) (b)

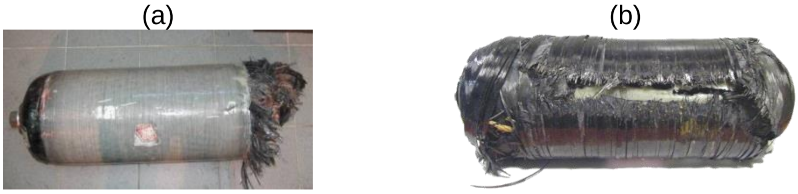

Figure 4. Vessels burst mode: dome burst (a) and cylindrical part burst (b)

Figure 5 shows that the end of curves (around burst pressure) is modified in function of random variables (FVR and fiber breakage). In this case, numerical burst pressure can be expressed as the pressure for which an inflection point of displacement curves is observed. Burst pressure is very well estimated (burst pressure is 1.3% overestimated): the average numerical burst pressure is 1775 bar whereas experimental average burst pressure is about 1756 bar.

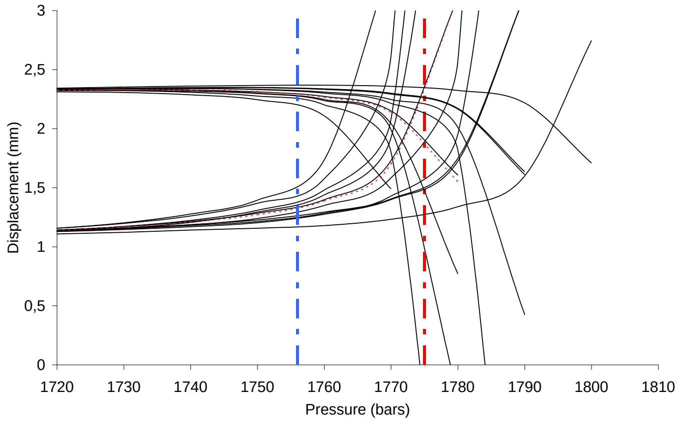

Figure 5. Numerical axial and radial displacement curves at burst for different probabilistic values

Simulated curves fit very well experimental ones. Radial displacements are linear in both cases. Axial displacements first exhibit a very strong non linearity, which is quite good captured by the numerical model. This non-linearity came from the gap between liner part and composite part which is progressively closed at the beginning of pressurization. Another non-linearity much more progressive appears progressively from a pressure of about 500 bar. Numerical model reproduces this non-linearity which is due to bosses plasticity and matrix damage (Figure 6). Matrix damage is located in helical layer of cylindrical part of the tank.

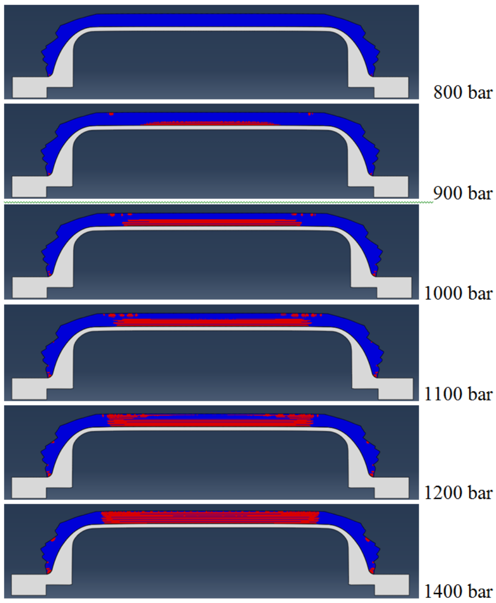

Figure 6. Evolution of matrix damage in composite tank

The good correlation observed with this model validate the hypothesis that shear non-linearity and delamination have no influence on tank behavior since project partners who take into account this phenomenon in their model obtained the same result.

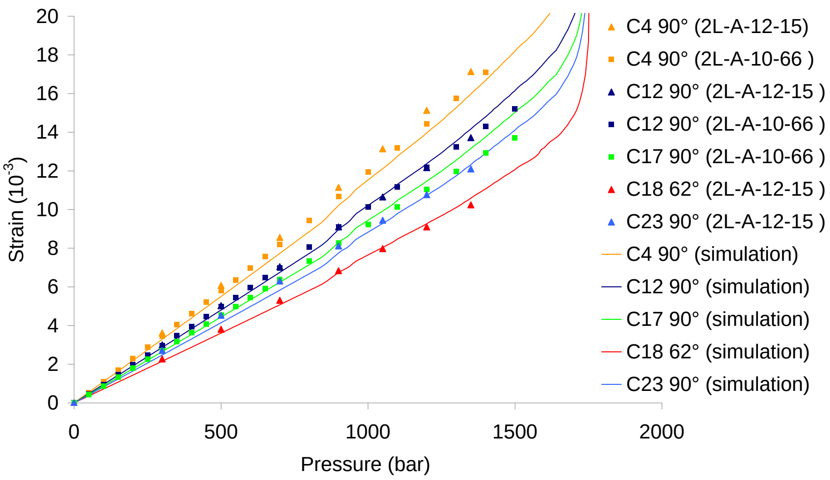

Figure 7. Comparison of optical fibers strain measurements and numerical results.

Optical fibers have been put inside several layers during the manufacturing process and allow an accurate strain measurement inside the tank. A comparison with fiber Bragg grating measurements and strain gauge measurements have been performed and show that these optical fibers are non-intrusive and do not influence tank behavior. Optical fibers measurements can also be used to validate the model (Figure 7) and exhibit a good correlation between strain measurements and numerical results.

5. Conclusion

Composite overwrapped pressure vessels of Osirhys IV project have been modeled in Abaqus finite element software. A composite behavior law has specially been implemented to take into account matrix cracking and fiber breakage effects. This law also account for material variability for fiber volume ratio and fiber breakage with the implementation of random variable for each calculation.

Results obtained with this model are compared to experimental results performed during the project. Global displacement and burst pressure are very well estimated by the numerical model. Strain measurements done with continuously sensitive optical fiber are also compared with numerical results and show a very good correlation.

Acknowledgements

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References

[1] P. Ifju, D. Myers and W. Schulz. Residual stress and thermal expansion of graphite epoxy laminates subjected to cryogenic temperatures. *Composites Science and Technology*, volume 66:2449-2455, 2006.

[2] L. Williams and D. Spond. A storage tank for vehicular storage of liquid hydrogen. *Applied Energy*, volume 6:99-112, 1980.

[3] D. Zellouf, J. Goyette, D. Massicotte, et al. Ultrasonic inspection of composite hydrogen reservoirs using frequency diversity techniques. *Ultrasonics*, volume 39:203-209, 2001.

[4] S. Levesque, M. Ciureanu, R. Roberge, et al. Hydrogen storage for fuel cell systems with stationary applications - I. Transient measurement technique for packed bed evaluation. *International Journal of Hydrogen Energy*, volume 25:1095-1105, 2000.

[5] M. Melnichuk, G. Andreasen, H. L. Corso, A. Visintin, and H. A. Peretti. Study and caracterisation of a metal hydride container. *International Journal of Hydrogen Energy*, volume 33:3571-3575, 2008.

[6] G. A. Banyay, M. M. Shaltout, H.Tiwari, et al. Polymer and composite foam for hydrogen storage application. *Journal of materials processing technology*, volume 19:102-105, 2007.

[7] S. Villalonga, F. Nony, C. Magnier, J. L. Yvernes, C. Thomas, B. Delmas and P. Mazabraud. Composite 700 bar-vessel for on-board compressed gaseous hydrogen storage. In *Proc. of 17th International Conference on Composite Materials*, Edinburgh, UK, 2009.

[8] N. Takeichi, H. Senoh, T. Yokota, et al. Hybrid hydrogen storage vessel, a novel high-pressure hydrogen storage vessel combined with hydrogen storage material. *International Journal of Hydrogen Energy*, volume 28:1121-1129, 2003.

[9] A. Onder, O. Sayman, T. Dogan, N. Tarakcioglu. Burst failure load of composite pressure vessels. *Composite Structures*, volume 89:159-166, 2009.

[10] D. Chapelle, F. Thiebaud, D. Perreux. Analysis and modeling of the burst pressure of high pressure hydrogen tanks. In *World Scientific Publ Co Pte Ltd*, Singapore, 2009.

[11] P. Xu, J. Y. Zheng, P. F. Liu. Finite element analysis of burst pressure of composite hydrogen storage vessels. *Materials and design*, volume 30:2295-2301, 2009.

[12] B. Gentilleau, F. Touchard, J. C. Grandidier. Numerical study of influence of temperature and matrix cracking on type IV hydrogen high pressure storage vessel behavior. *Composite Structures*, volume 111:98-110, 2014.