SIMULATION OF BURST OF HYPERBARIC HYDROGEN TANKS IN FIRE CONDITIONS

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Abstract
The exploitation of the benefits of hydrogen energy at large scale needs the understanding of the degradation mechanisms of storage subjected to severe conditions, fire for example. In a first stage of the European project FireComp, studies on the thermal-mechanical behaviour of the materials used for hydrogen storage have been performed. A second stage tackles the modelling of the coupled thermomechanical mechanisms and their consequences on the mechanical strength of samples and storage vessels subjected to this type of loading. Two different approaches have been selected: on the one hand, a Progressive Failure Analysis (PFA) directly relates the material strength and stiffness of the material to the temperature and, on the other hand, a Continuum Damage Mechanics (CDM) approach controls the evolution of internal damage variables in the framework of the Thermodynamics of Irreversible Processes. Both types of modelling are compared to experiment, at sample and storage scales.

1. Introduction

Use of hydrogen energy at a large scale necessitates mastering the reliability of storage at very high pressure. Type-IV tanks (made of a polymer liner for tightness, metallic bosses for connectivity and a wound composite shell for structural strength) are nowadays considered as a mature way. In order to better characterize the conditions that need to be achieved to avoid a failure of the composite pressure vessel subjected to a fire, the FireComp project (a three year FCH JU funded pre-normative research project) aims to model the thermo-mechanical behavior of such high pressure storage. The FireComp project brings together partners from diverse expertise: a Gaseous Compressed Hydrogen technology integrator as a coordinator (AIR LIQUIDE), a pressure vessel supplier (HEXAGON), a leading actor in international Standards, Codes and Regulations development (HSL), experts in industrial risks (INERIS), experts in thermal radiation and mechanical behavior of the composite (CNRS (Pprime & LEMTA), Samtech), experts in thermal degradation and combustion of composites, numerical simulation (Edinburgh University and Samtech) and an expert in European R&D collaborative project management (ALMA).
Experimental work has been done at the sample scale [1,2] in order to improve the understanding of heat transfer mechanisms and the loss of strength of composite in fire conditions and to provide information for modelling of the thermo-mechanical behavior of structures made of this material (epoxy resin and T700 carbon fibres). This communication deals with the numerical tools implemented by the partners Samtech and CNRS to simulate (i) the residual strength of samples first subjected to fire, (ii) the time to burst of pressurized type IV cylinders in fire conditions. The partner INERIS performed bonfire tests on real tanks. These experimental data allow validating the modelling tools incorporated in Finite Elements softwares.
First, the thermomechanical damage models are briefly presented. In a second part, they are used to simulate the behavior of samples subjected first to fire and then to a mechanical load. These

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simulations are a preliminary step to validate the models. At last, fully coupled FE computations on real tanks are run to calculate the time to burst of pressurized vessels in fire.

2. Models for thermomechanical behaviour

Two different approaches have been implemented to model the mechanical and thermal behaviour of composite:
- a continuum damage mechanics approach (damage model by Ladeveze [3]) in which the damage state is given by a set of damage variables which evolve according to the thermal and mechanical loading.
- an approach by Progressive Failure Analysis, in which the strength and the stiffness of the material are progressively reduced as soon as a damage criterion (namely, Hashin criteria [4]) are reached.

In each case, the mechanical properties are temperature-dependent. The experimental data [1,2] are used for validation.

2.1. Continuum Damage Mechanics

One of the approaches selected in this project for modeling the damages inside the plies (intra-laminar damages) is based on the continuum damage mechanics approach initially developed in [3], in which the laminate is made of homogeneous plies and damage variables impacting the stiffness of each ply are associated to the different failure modes, representing the fiber breaking, matrix cracking and de-cohesion between fibers and matrix. The model is native in LMS Samcef and there is no need for additional plug-ins/user-routines to solve the progressive damage problem. All the temperature dependent material parameters can be defined in the input file, and the material model is evaluated at the Gauss points, inside the finite elements. Three damage variables are used, which vary from the undamaged (0) to the fully damaged state (1), namely:

- d_{11} represents the stiffness reduction due to fiber failure.
- d_{22} represents the loss of cohesion between the fibers and the matrix.
- d_{12} represents the matrix damage, i.e. the cracking of the matrix.

23 parameters have to be identified, for a given temperature: 9 elastic constants, 10 damage related parameters, 4 plasticity parameters.

The tests performed on samples subjected to a mechanical load and a fire exposure [1] clearly evidenced the negligible role of the stress on the heat transfer. As a consequence a sequential thermo-mechanical solution procedure was implemented. Because it was observed, that above the glass transition temperature, the material was as good as completely damaged, only temperature dependence is taken into account and no charring dependence is implemented for the mechanical model.

First a thermal analysis is run, using the thermal properties identified by the partner University of Edinburgh [2]. The temperature is calculated for the charring material, using the thermal boundary conditions (convection, radiation, combustion of pyrolysis gas). The temperature field is stored in a result file, which will be re-read by the mechanical calculation.

The mechanical damage model is temperature dependent, and the material model is evaluated using the temperature distribution at a given time instance. The temperature field at a given time instance is obtained by interpolating in time between the calculated (and stored) temperature fields from the thermal analysis. This means that the time step between the thermal and mechanical calculation does not have to be identical.

The above described approach has one drawback, namely if the temperature decreases the elastic properties will again increase. This model should therefore only be used with non-decreasing temperatures. This limitation is not fundamental and the model can be easily extended.

2.2. Progressive Failure Analysis

With a view to perform simulations on large structures (wound composite tanks) and to save computation run time, a Progressive Failure Analysis has also been chosen, that is simpler than a

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CDM model. This method has been successfully implemented by Gentilleau *et al.* [5], who dealt with the thermomechanical behavior of hyperbaric tanks. In the same way as these developments, the approach presented here only uses tools as simple as possible, which can be found in the standard version of the Finite Element software Abaqus.

Tests clearly show the different types of behavior of the wound composite, according to the loading direction (linear elastic in the direction of the fibers and in the direction perpendicular to the fibers, elastic-plastic under shear stress). This anisotropy is introduced by using a Hill criterion, only selecting the shear stress components. The plastic-like behavior is then implemented via tables "yield stress vs. plastic strain" identified from tension tests performed on ±45° samples. In order to take into account the progressive degradation observed for this type of tests, the stiffness reduction is related to the cumulative plastic strain, given by the hardening curve. This constitutive relation is modeled by the means of a "User Field" subroutine in Abaqus, which allows to index one (or more) field to the variables of the model. In this case, this field contains the equivalent plastic strain which plays the role of damage variable. The shear moduli are then given as a function of the cumulative plastic strain in a table. It is a simple way to build a damage model, but it avoids integrating complex evolution laws at each Gauss points and building intricate Jacobian matrices.

Regarding the directions "fiber" and "normal to fiber", the corresponding parameters in the Hill criterion are set to zero in order to avoid any nonlinear behavior in these directions. The brittle behavior is dealt with by the means of Hashin-like criteria (failure occurs as soon as the stress in the direction parallel or perpendicular to the fiber reaches a given strength). In order to avoid numerical difficulties (in terms of convergence in particular) due to the brutal failure assumed by these criteria, a progressive degradation is introduced in these directions: the stiffness in the direction affected by damage is not immediately set to zero but is more progressively reduced.

Unlike CDM approaches, no damage variable (in its thermodynamic meaning) is used. However, some indicators play the role of damage variables.

- the cumulative plastic strain: for ±45° samples, a direct link between the irreversible strain and the stiffness degradation can be highlighted. The plastic strain plays thus a double role (plastic strain and damage indicator)
- the ratio stress / strength: in the direction parallel or normal to fiber (brittle behavior), the damage level can be related by the ratio of the stress in the considered direction and the corresponding strength. If this ratio reaches a given value, damage appears and progressively evolves towards its maximum value (noted d_{max}).

14 parameters have to be identified: 4 elastic constants, 5 strength values for the Hashin like criteria, 3 maximum values for damage level, 1 maximum plastic strain (for ±45° samples), 1 hardening curve (for ±45° samples).

Starting from the hypothesis of the negligible role of the stress on the heat transfer, a successive solving of the heat equation and of the mechanical behavior is implemented. The mechanical behaviour and the heat equation are solved simultaneously: the latter (starting from the thermal properties determined at the previous step) provides the updated value of the temperature, whereas the former gives the stress components, the damage levels (from the strengths depending on the temperature T_n determined at the previous step) and then the stiffness. From the updated temperature T_{n+1}, the thermal (conductivity, specific heat) and mechanical properties (stiffness, strength) are modified. The procedure then returns the updated mechanical stress and strain. Regarding the composite degradation due to charring, it is assumed to be temperature-driven: as soon as the temperature reaches a critical temperature (350°C, measured from TGA tests), the mechanical properties are set permanently to a low value.

3. Sample scale: simulation of residual strength

As a preliminary validation of the approaches outlined in the previous section, tensile tests on specimens ±45° (EC45) first subjected to fire are simulated. The purpose is to verify that the char can be considered as a fully damaged material. The specimens are cut in large hydrogen storage, so that they are quasi-flat. The experimental data are detailed in [1]: the specimen is first subjected to an

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incident flux of 35kW/m^2 during a given time and then subjected to tension. In order to reproduce the actual tensile test, the sample FE geometry is a parallelepiped made of 6 layers (45°/-45°/45°/-45°/45°/-45°) of dimensions 300mmx25.5mmx6.35mm. The fixed grip of the tension set-up is represented by a constraint (no displacement) applied along 44mm. The mobile grip is represented in the same manner: an increasing displacement is applied at the other end. The parallelepiped is meshed with continuum 3D linear finite element with temperature-displacement coupling and full integration. The work [1] provides the char thickness according to a given incident energy. A partition of the sample is performed: the mechanical properties of char are assumed to be very low, whereas the stiffness and the strength of the rest of the sample remain equal to their initial values (Figure 1). This hypothesis is justified by the fact that the resin decomposition in the char also affects the load transfer to the fibres: without resin, the fibres no longer play their role of reinforcement

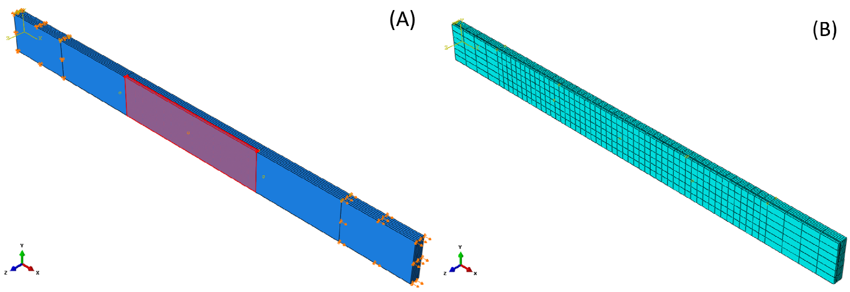

Figure 1. Modelling of sample EC45 by FEA; (A) Partition composite (blue) and char (red) and Boundary conditions. (B) Mesh of sample

Figure 2 shows the results of the simulation of the tensile test up to fracture by the Progressive Failure Analysis. The dashed lines represent the experiment and the solid lines the simulation. The number XXX in the caption EC45-XXX represents the experimental fire exposure duration (and is then related to the char thickness). A good correlation can be observed between simulation and experiment for all exposure conditions. Similar simulations have been performed for 90° and quasi-isotropic samples. These results prove (i) it is reasonable to consider the char as a composite material with no stiffness, (ii) the Progressive Failure Analysis is able to accurately simulate the non linear mechanical behaviour and the fracture of the EC45 sample (as well as other types of specimen).

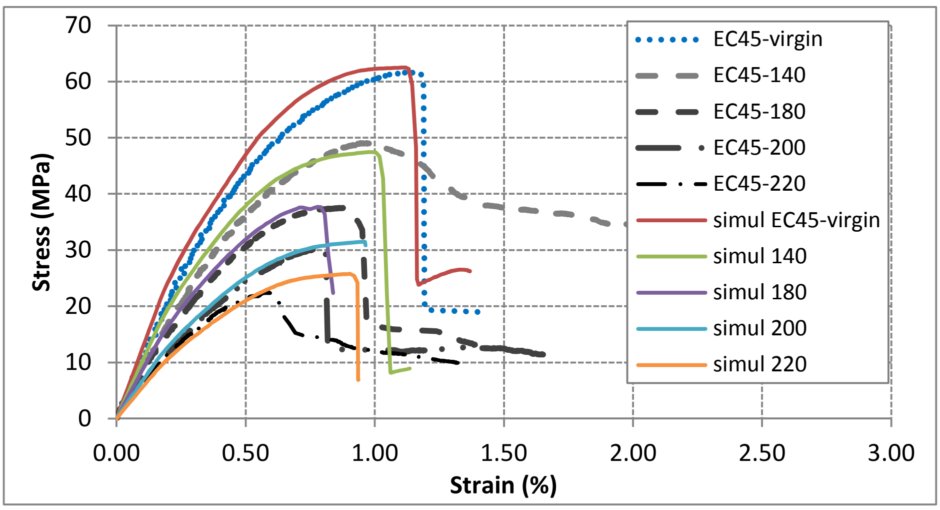

Figure 2. Simulation (solid line) and experiment (dashed line) of tensile test for EC45 after exposure duration of 140, 180, 200 & 220 (s) - Stress (MPa) vs. Strain (%)

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4. Vessel scale: simulation of time to burst

The previous section only deals with “uncoupled” simulations: the sample is first subjected to fire, and in a second step to a tensile test. This section addresses the specific issue of the thermomechanical coupling: the objective is to simulate the thermal and mechanical behavior of the pressurized vessels (with an inner operating pressure of 700 bar) and an incident flux and to compare the results to the experiments performed by the partner INERIS, in particular the time to burst.

4.1. Simulation by Continuum Damage Mechanics

The full cylinder has been modeled in 3D. The reason for this choice is to have the possibility to apply a 3D heat load. In Figure 3 the finite element mesh of the cylinder (only half of the model) is shown. A constant lay-up is chosen along the length of the cylinder, resulting in a constant thickness composite shell. Although this is not always realistic, it is assumed that the cylinder would burst in the center section and that the design of composite at the dome would not have a major influence on the burst pressure.
The domes of the cylinder are modelled using 6051 volume elements, and the liner is modelled using 4711 elements. The composite shell is constructed by extruding the outer surface of the liner and applying the actual layup, resulting in a constant thickness composite shell. For the extrusion a discretization was chosen, which resulted in two plies per element (in the thickness direction). This resulted in a total of 122.960 volume elements for the composite shell.

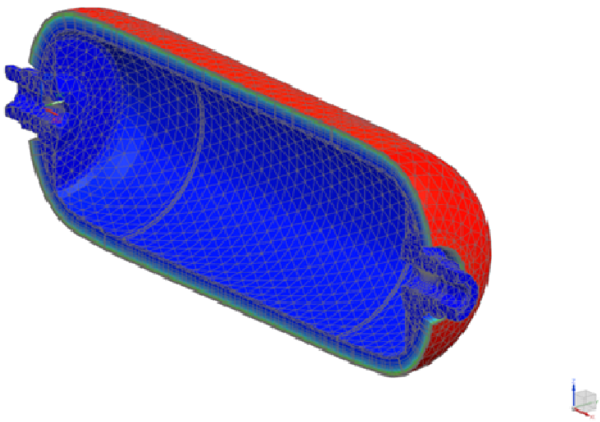

Figure 3. FE mesh of the cylinder, only one half shown (constant lay-up)

The loading of the cylinder consists of three components, namely a fixation, an applied inner pressure (700 bar) and an applied heat flux. For one boss the movement in the three directions is fixed, while for the other boss only the movement in the Y- and Z-direction is fixed, allowing an elongation of the cylinder. The thermo-mechanical analysis consists of two separate analysis steps. The first one is a thermal analysis (using Samcef), in order to calculate the temperature distribution as a function of time. Measurements performed by INERIS showed that the resultant heat flux was around the 100 kW/m^2 level. Because the actual heat flux is not known exactly, it was decided to perform two calculations where we use an applied heat flux of 100 kW/m^2 and 200 kW/m^2 respectively, and model the re-radiation (ε=0.91) with the environment (15°C), and the natural convection (Churchill and Chu correlation, h~8W/(m^2.°C)). The duration of the calculation was chosen around 600 s, in order to be longer than the actual time to burst. The second calculation is a mechanical calculation, where first a

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constant pressure of 700 bar is applied, after which the temperature field from the previous calculation is applied.

During the first step the pressure (700 bar) will be applied from zero until the working pressure, after that the temperature field will be applied, and the calculation continued until burst. In Figure 4 we show the radial displacement of the centre of the cylinder as a function of time.

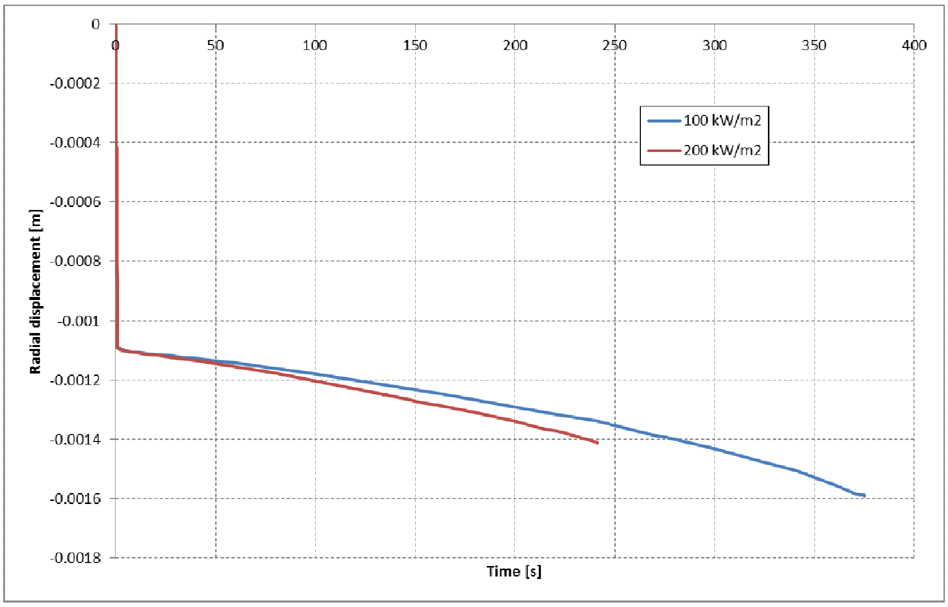

Figure 4. Radial displacement as a function of time for different heat loads.

What we can see is, that the cylinder will deform quickly due to the application of the pressure, after which it will further deform as a function of the temperature applied during the further duration of the calculation. The cylinder will slowly damage due to the pressure and the temperature until it will finally burst. The results are summarized in Table 1. When we compare the time to burst at 700 bar and 200 kW/m^2 with the measured results we are within 1.5% difference.

Table 1. Time to burst (Continuum Damage Mechanics)

	700 bar	Experiment
100 kW/m^2	361 s	238 s
200 kW/m^2	241 s	

4.2. Simulation by Progressive Failure Analysis

In this approach it has been chosen to take advantage of the symmetries of the problem: the geometry is axisymmetric (only a slice of the vessel is represented) and only one half of the tank is modeled (Figure 5). A symmetry condition (no displacement in the Y-direction on the right end) is applied.

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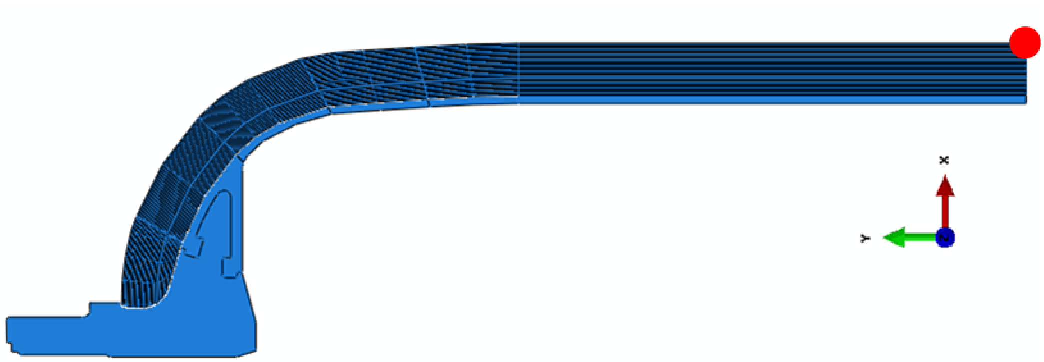

Figure 5. FE geometry (constant lay-up)

This geometry is meshed with axisymmetric elements, a constant lay-up (as for the CDM approach) is assumed. Thanks to this axisymmetry assumption, the number of elements is limited and the computation time reduced: 6851 for the boss and the liner, 15713 for the composite (the thickness of each composite layer contains one element). The chosen boundary conditions consider that the tank is maintained at its both ends: the end of the boss is clamped.
The simulations run in this part are composed of two steps: in the first one, an inner pressure of 700 bar is applied. In the second one, the inner pressure is maintained constant and an incident flux is applied homogeneously on the outer surface of the vessel. The simulation runs until the radial displacement increases rapidly (this happens when the first fibers break). The radiative transfer at the tank surface is taken into account by setting the emissivity to 0.91. No convective transfer has been taken into account.
As the actual flux received by the vessel is not available, two different simulations have been run, the one considering a value of 100 kW/m^2, the other 200 kw/m^2. When the vessel is subjected to the incident flux, the temperature progressively increases in the composite shell (rapidly at the top of the shell, slowly close to the liner). The stiffness in the fiber direction (which ensures the mechanical strength of the tank) undergoes two different regimes: (i) until 350°C it decreases slowly, (ii) as soon as the temperature reaches 350°C (beginning of combustion), it sharply drops and becomes almost zero at 450°C. This stiffness reduction redistributes the stress to the colder layers which undergo a higher load level and break when the hoop stress is equal to 2450 MPa. This damage mechanism leads to the following time to burst (Table 2):

Table 2. Time to burst (Progressive Failure Analysis)

	700 bar	Experiment
100 kW/m^2	228 s	238 s
200 kW/m^2	195 s	

The simulation performed by the PFA method is quite satisfactory (deviation of only 4% in the case of a flux of 100kW/m^2, 18% for 200kW/m^2). The time to burst simulated with the constant lay-up approach only slightly depends on the incident flux. Indeed, the very low conductivity of the material homogenizes the temperature in the composite thickness and the temperature values for 100kW/m^2 and 200kW/m^2 are very close in the composite shell. This result validates the “temperature-dependent” method: the temperature is the pivotal variable which governs the burst mechanism. Once the temperature is known, it is sufficient to link the mechanical properties to the temperature.

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5. Conclusion

The FireComp project aims at simulating the mechanical strength of vessels subjected to an inner pressure and fire. Two different approaches (Continuum Damage Mechanics and Progressive Failure Analysis) have been compared and have been found to provide satisfactory results at sample scale as well as at vessel scale. These methods have opposite advantages and drawbacks:

- The Continuum Damage Mechanics approach is written in the framework of the Thermodynamics of Irreversible Processes, damage effects are controlled by the evolution of damage internal variables, an abundant literature has proved its ability to simulate very different loading cases; however, the integration of nonlinear equations is a computer time consuming process (although this limit is not prohibitive).
- The Progressive Failure Analysis method does not define damage variables, the mechanical properties are related to the temperature in a tabulated way. It is not based on thermodynamic principles. However, it takes into account the main damage mechanisms found in composite materials and needs a reasonable number of parameters to identify. Its simplicity allows to quickly provide numerical results when simulating complex structures.

These simulations may be improved by complementary experimental inputs. For example, considering a homogeneous incident heat flux is a strong assumption that influences the time to burst. The mechanical strength of the vessel also depends on the stiffness reduction due to temperature and combustion. If these data are known between 20°C and 150°C and beyond 350°C, the range 150°C-350°C should be further investigated.

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