A CONTAINER DESIGN FOR A THERMALLY INDUCED DECONFINEMENT OF ENERGETIC MATTER

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SUMMARY: The transportation of dangerous energetic matter requires containers with various specifications in order to get the maximum security. The design of a suitable structure is based on a method in which the material particularities result from the container functions. In this paper, the interest of this type of method is studied. Thus, after a description of the methodological process, the example of the container is detailed. The successive steps of the conception leading to the final structure are explained. The numerical simulations allow the dimensions of the structure to be defined and the thermo-mechanical behavior of the container to be numerically simulated, particularly for the polymer filling the cells of the alveolar structure.

KEYWORDS: Design – Structure – Multimaterials – Thermal deconfinement – Selective reinforcement.

INTRODUCTION

The development of multimaterials in most domains of application has given rise during the last decade to several methodological approaches devoted to design structures in which different types of materials are involved [1-3]. Some methods focus on the coupling conditions of various material components by taking into account their incompatibilities induced for instance by thermal expansion mismatch or differences in stiffness and chemical activity. On the contrary, other approaches mainly aim at making a hierarchy in the structure functions in order to give them a suitable importance in the structure design and cost.

Combining the principles of the previous approaches, the objective of the method proposed and used in this contribution, is to generate a material design from mechanisms pointed out as possible responses to the structure functions requirements.
The application considered for applying the method concerns the transportation of dangerous energetic matter. More particularly, some kinds of transports require containers whose main

specifications are not only sufficient resistances to various types of mechanical loading at different temperatures and low weights, but also the ability to prevent the structure from detonation above a given temperature threshold or during accident.

Thus, the design of a suitable structure for such an application is based on three major requirements related to (1) the energetic matter deconfinement according to well defined conditions of temperature, (2) the shock waves destructuration when the structure is submitted to projectiles or collisions and (3) the resistance to internal pressure.

The aim of the present study is to show how the use of a methodological process is helpful for designing a structure in which each component particularly fits the specific application giving rise to a new multimaterial.

After describing the method, all the specifications of the structure will be detailed in order to enhance the influence of each function on the materials choice, and the structure design. Thus, concerning the deconfinement function which is of prime necessity, expectable mechanisms will be schematically depicted and discussed before choosing one of them and then, giving rise to a materials specification. Finally, after designing the multimaterial structure, its dimensioning will be approached through numerical simulation tests.

METHODOLOGICAL APPROACH

The conception method used here leads to design simultaneously the structure and its material. It is based on the following steps which schematically illustrate the design thought:

- firstly, a functional analysis of the concerned application allows the importance of each function to be estimated, giving rise to a hierarchy of functions,
- thus, the properties required to ensure these functions can be selected and quantified, allowing the material specifications to be defined,
- then, the structure and materials can be simultaneously defined while already thinking to a processing method for manufacturing the structure,
- consecutively, the characteristics of the whole structure can be predicted by computation from those of the material components with the help of models such as homogenization models,
- finally, the structure can be realized and tested.

The optimization of the conception requires iterative runs of part of these steps after numerical or experimental evaluations of the designed structure.

FUNCTIONAL ANALYSIS OF THE CONTAINER

Structure functions and constraints

Knowing that the container environment is not well defined yet, the multimaterial structure has been studied for a tubular structure, although the structure shape has to be considered as an important parameter which strongly influences the structure design and conditions of manufacturing. Thus, the present study deals with a 5 liter cylindrical vessel, whose wall thickness must not exceed 10 mm and whose main specifications are:

- undergoing an internal pressure of 3 MPa during 720 secondes,

- allowing the quick deconfinement of the contained energetic matter above 150 °C and consequently preventing the structure from explosion at any temperature,
- protecting the energetic matter from the shock waves which might induce the detonation if a mechanical aggression occurred,
- preventing the internal temperature from going out of the defined temperature range of storage or use (-20°C to +70°C) even if the external temperature decreases during some hours up to -40 °C,
- insuring the imperviousness despite the chemical aggressiveness of contained matters,
- keeping this imperviousness after an accidental impact,
- minimizing weight and cost, in particular by requiring only a simple manufacturing process.

The analysis of these functions leads to research various mechanisms allowing each function to be ensured separately or advantageously combined. This combination could be obtained either in a single material if it is possible or by coupling several materials according to a specific architecture, that is designing a multimaterial structure. As an example, the deconfinement function which is expected to influence most greatly the structure design, will be studied in the next section without considering in this first step the interaction and eventual coupling of the proposed deconfinement mechanisms with other functions.

Basic mechanisms of deconfinement

The thermal deconfinement of the structure means the container no longer offers any noticeable mechanical resistance to fluid flow above a threshold temperature fixed at 150 °C. To achieve such a function, various mechanisms can be put forward and schematically depicted as follows:

1. Security devices such as safety valves, release any excessive increase in internal pressure above 150 °C, thanks to a temperature dependent activation of the device and a sufficient exhaust flow for a small internal/external pressure difference.
2. The strong mismatch in the components thermal expansion coefficients (CTE) of a multimaterial container, is able to generate such high thermally induced stresses that the occurrence of multicrackings of one of the composite components, allows an effective deconfinement
3. The container envelope becomes so widely porous or exhibits so many low pressure induced perforations above the threshold temperature, that the structure no longer offers any impediment to rather weakly viscous fluid flow.
4. The container is made of at least two parts whose joint is abruptly weakened at the threshold temperature, leading to the container opening without necessitating any noticeable internal pressure.
5. A drastic drop in the mechanical performances of the container material enables an easy failure of the structure above 150°C under the action of a low internal pressure.

Prior to define material specifications for each of the previous mechanisms, computing roughly the material characteristics allowing the mechanisms to operate, and comparing the proposed solutions with other required functions, enables the elimination of two deconfinement mechanisms.
Mechanism 1 is often used for limiting container internal pressure, but must be more sophisticated in the present case. Indeed, the container has to undergo rather high internal

pressure in a wide temperature range around room temperature (-20 °C to +70 °C), but must release any internal pressure increase as soon as energetic matter temperature exceeds 150 °C. Complying these two conditions dictates the use of a temperature monitored valve which is more complex and expensive than a spring tare controlled valve. Furthermore, ensuring a sufficiently large section for fluid flow is an additional technological difficulty which finally led to leave this solution requiring the multiplication of the valves number.

Besides, mechanism 2 requires components with large CTE mismatch and significant stiffnesses in order to generate sufficiently high thermally induced stresses at 150 °C. More, the less expansible component must be brittle enough to enable the structure damage and destructuration without additional effort. Preliminary numerical assessments related to various types of material lead to consider that one ceramic component should be chosen which is not compatible with the need of imperviousness after collision. Thus, this second solution has been left.

On the contrary, mechanisms 3, 4 and 5 were thoroughly studied and appeared to be combinable according to a composite structure described in the next section.

MATERIAL ARCHITECTURE AND SPECIFICATIONS

Composite design

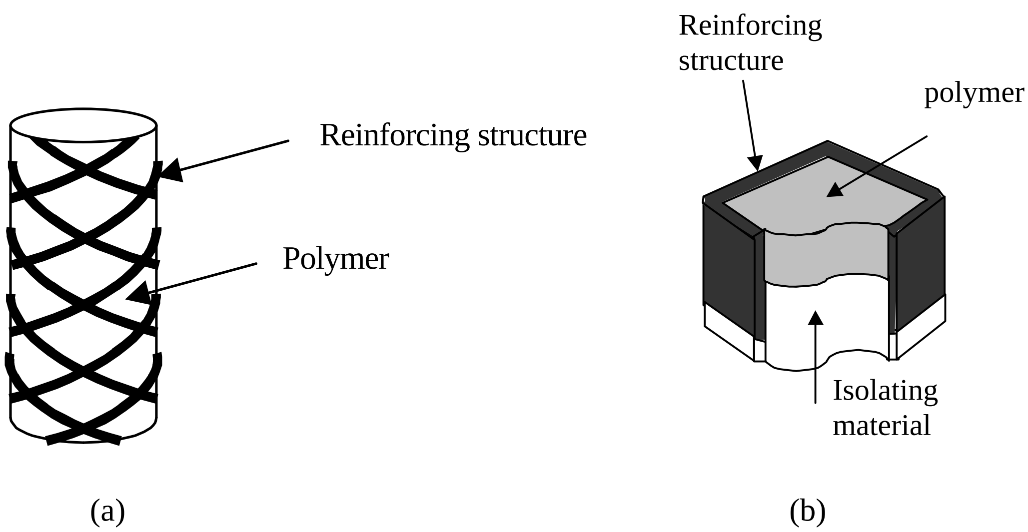

Fig. 1: Schematic representation of the proposed alveolar container structure
(a) general feature
(b) materials in the thickness

The combination of the last three deconfinement mechanisms previously proposed can be achieved thanks to the design of a composite structure consisting in a wound net made of fibrous yarns whose mesh is filled up by an easily melted material. This conception schematically illustrated in Fig. 1a is able to comply mechanism 3 since the filling material melting at 150 °C enables the contained energetic matter to flow through the rather wide-mesh net. Besides, the poor transversal resistance of the wound fibrous yarns is able to initiate the container opening as expected according to mechanism 4, provided the longitudinal yarns stiffness decreases strongly at the threshold temperature. More, if this decrease in stiffness is accompanied by a drop in yarns strength at the deconfinement temperature, mechanism 5 is able to operate for low internal pressure. Thus, the redundancy of deconfinement mechanisms can be considered as an additional security factor and gives more possibilities for complying the other container functions.

For instance, the cellular design of the container envelope with thin and stiff fibrous yarn divisions surrounding compliant cells as illustrated in Fig. 1b, is particularly favorable to the destructuration of shock waves induced by a projectile. Also, the presence of a fibrous reinforcement dedicated to undergo rather high internal pressure at low temperatures, makes easier the choice of a suitable material for the cells which have not to support the main loading. Therefore, the proposed conception is able to comply the major container functions provided to find materials exhibiting the precise specifications required by each component of the designed structure.

Components specifications and choice

The properties required by the container fibrous architecture can be defined as follows:

- at temperatures lower than 70 °C, fibers must be rigid enough compared to the other components in order to support in their longitudinal direction most of the structure loading related to the maximum internal pressure (3 MPa),
- consequently the fibers strength must be sufficiently high, at temperatures lower than the threshold, to minimize the cell divisions thickness and thus offering the smallest section to projectile impacts,
- for the lowest temperatures of use (around -20 °C) fibers must not be brittle in order to preserve the structure containing function after an accidental collision,
- deconfinement mechanisms 4 and 5 require a drastic drop in fiber longitudinal mechanical performance at temperature of about 120-150 °C,
- mechanism 4 also requires at 150 °C significant load transfer critical lengths between fibers, that is transversal bonding sufficiently weak to enable a container opening along one of the fibrous divisions.

The whole previous specifications turns the material choice into polyethylene fibers whose characteristics given by manufacturers are often different from those reported in literature [4]. Thus, until further mechanical tests are performed on the related polyethylene fibers in a wide range of temperature, underestimated values will be deliberately used in numerical simulations of the designed container behavior.

Concerning the cells, the filling material must exhibit the following properties:

- a solid/liquid transition in a narrow temperature domain close to 150 °C,
- a good creep resistance at temperature lower than 70 °C,
- a low rigidity to facilitate shock wave destructuration in interaction with the fibrous divisions,
- a significant resilience up to temperatures as low as -40 °C,
- the lowest possible thermal diffusivity,
- imperviousness and chemical inertia in relation to the contained energetic matter would permit to do without liner.

Again, these specifications turns the material choice into thermoplastic polymers, which still renders difficult to meet the last requirements. As a consequence, the thermal resistance and imperviousness functions of the container envelope have been separated from the other functions, giving rise to a thin internal metallic liner for ensuring the imperviousness and a thermal barrier made of tangled short insulating ceramic fibers.

At this stage of the methodological approach and before going into more details about materials nature and structure definition, numerical simulations of the roughly designed container behavior were performed in order to validate the first steps of the approach and to guide a more precise specification of the conception.

NUMERICAL SIMULATIONS OF THE CONTAINER BEHAVIOR

Knowing that the first approach of the container design has been based mainly on the deconfinement and shock waves destructuration functions, the container resistance to the maximum internal pressure (3 MPa) at temperatures of use (-20 °C to 70 °C), was the primordial function to be validated first.

On the one hand, the ability of the container fibrous net to undergo the maximum internal pressure loading was estimated by considering the container envelope deformations as identical to those occurring with an homogeneous envelope. On the other hand, the heterogeneity of the structure conception was taken into account through the numerical simulation of the polymer cell deformations.

Fibrous net dimensioning

The structure parameters optimization which will have to be done before realizing and testing the container, could be prepared while validating the alveolar conception. The parameters which are most strongly influencing the container behavior, were pointed out among the following parameters defined on the representative element of the multimaterial envelope. During this step, it is worthy to keep in mind the envelop is assumed to be homogeneously deformed (Fig. 2):

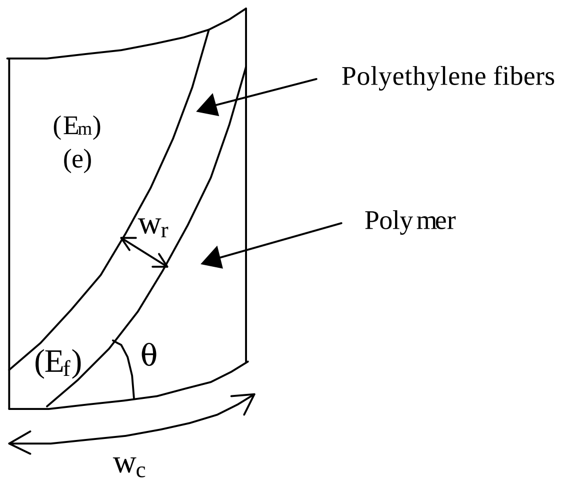

Fig. 2 : Container representative element used for the numerical simulation

The dimensioning parameters of the container representative element (CRE) are :

- w_c the width of the CRE,
- θ, the winding angle,

- w_r, the width of the reinforcing fibrous divisions,
- e, the thickness of the polymer in each cell,
- E_m and E_f, respectively the fibers and polymer rigidities.

Although the cylindrical container structure has been considered as quasi infinite in length in order to ignore any bottom effect during this first approach, the loading induced by the internal pressure was assumed biaxial to simulate the behavior of a closed container.

The influence of the previous parameters considered as variables, upon the container behavior, was evaluated through the following functions considered as the container response:

- σ_{eq}, the Von Mises stress in the polymer cells,
- σ_{fl} and σ_{ft}, respectively the longitudinal and transversal stress in the fibers.

In order to point out the most influent parameters, a design of experiment technique was used [5,6]. The extreme values given to the variables previously defined, that is the dimensioning parameters of the container, are reported in Table 1.

	w_c (mm)	**θ (°)**	**w_r (mm)**	**e (mm)**	**E_m (GPa)**	**E_f (GPa)**
Minimum	12	45	2	2	0.5	40
Maximum	24	65	10	4	3	80

Table 1: Extreme values given to the parameters

Assuming the function can be represented by first degree polynomial leads to write for instance σ_{eq} as Eqn 1:

$$\sigma_{eq} = \sigma_{eq}^{*} + \sigma_{eq}^{w_c} \cdot X_{w_c} + \ldots \qquad (1)$$

where the extreme values of w_c lead to give X_{w_c} the values -1 and 1. Thus, the influence of w_c on σ_{eq} can be given by $\frac{\sigma_{eq}^{wc}}{\sigma_{eq}^{*}}$.

Computing the container response for these extreme values leads to the following average values of the related functions:

$\sigma_{eq}^{*} = 26$ MPa $\sigma_{fl}^{*} = 67$ MPa $\sigma_{f}^{*} = 15$ MPa

The main results of these numerical experiments are reported in Table 2 and show the importance of the most influent parameters with respect to the response average values considered as references.

Matrix (Von Mises stress)	**Fiber**	
	Longitudinal direction	**Transverse direction**

Young modulus of the matrix (27%)	Width of reinforcement (36%)	Width of reinforcement (40%)
Width of the CRE (23%)	Width of the CRE (23%)	Width of the CRE (36%)
Thickness of polymer (19%)	Winding angle (18%)	Winding angle (23%)

Table 2: Most important parameters and their relative influence

The main conclusion we can draw from these results is that the most important dimensioning parameter is the cell size, since w_c greatly influences the three calculated stresses. Also, it is worthy of note, the fibrous divisions width is the major parameter to consider for adjusting the conditions of container opening according to mechanism 4.

In order to obtain an acceptable stress state when a 3 MPa internal pressure is applied, w_c has to be as low as possible. However, the width of the fibrous divisions must be chosen simultaneously with w_c. As a matter of fact, a structure with small cells, and wide reinforcement, leaving few space for the matrix, must be avoided in order to keep the alveolar feature of the structure. So, a medium value of w_c is fixed, and w_r is then determined to prevent the structure from a fracture under a 3 MPa internal pressure. It must be noted that the stresses in the fibers longitudinal direction are far from their expected strength. So, dimensioning the fibrous net is ruled by the stress level in the fibers transverse direction.

The determination of w_r is coupled with another geometric parameter. Indeed, the transverse stress also depends on the winding angle. Unlike w_r, the choice of an extreme value of θ does not affect the cellular structure. Thus, the maximum winding angle, leading to the minimum transverse stress, is applied. The last geometric parameter, e, is chosen high enough to give the matrix a relatively low stress.

The only parameters that have not been fixed yet are relative to the mechanical properties of materials. Unlike the previous geometric parameters, these material ones cannot be controlled easily, and depend on manufacturing conditions. That is why, on the one hand, the fibers characteristics are underestimated when, on the other hand, the matrix properties are relatively high for the considered class of material. Thus, the simulations are performed for unfavorable cases.

Finally, the following values have been chosen for the structure :

w_c = 18 mm
w_r = 4 mm
θ = 65°
E_f = 40 GPa
E_m = 1 GPa
e = 3 mm

It must be noted these parameters values are still opened to modifications if further simulations or the experiments show the impossibility of the designed container to cope with the whole functional requirements.

Polymer cells deformations

Now, the container envelope will note be considered any more as deforming homogeneously, since the question is to study the behavior of the polymer filling the alveolus inside the fibrous divisions. Obviously, the low rigidity of the filling polymer gives rise to radial displacements more significant at the center of the cell than at the edges as shown in Fig. 3. The corresponding combination of tensile and flexural stresses, must be small enough to undergo at temperatures lower than 70 °C the maximum internal pressure without any blistering effect and high enough at 150 °C to cause the extrusion of the filling polymer through the reinforcing structure.

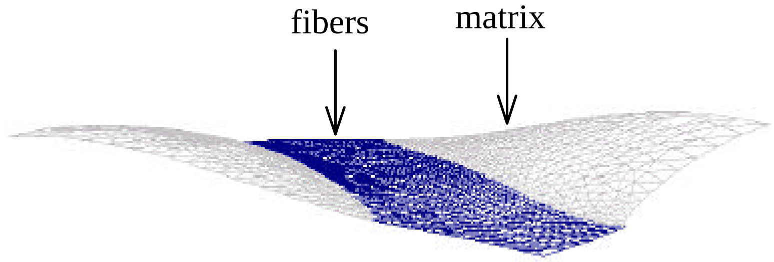

Fig. 3 : Deformation shape of the CRE

The amplitudes of the CRE radial displacements can be also visualized as shown in Fig.4.

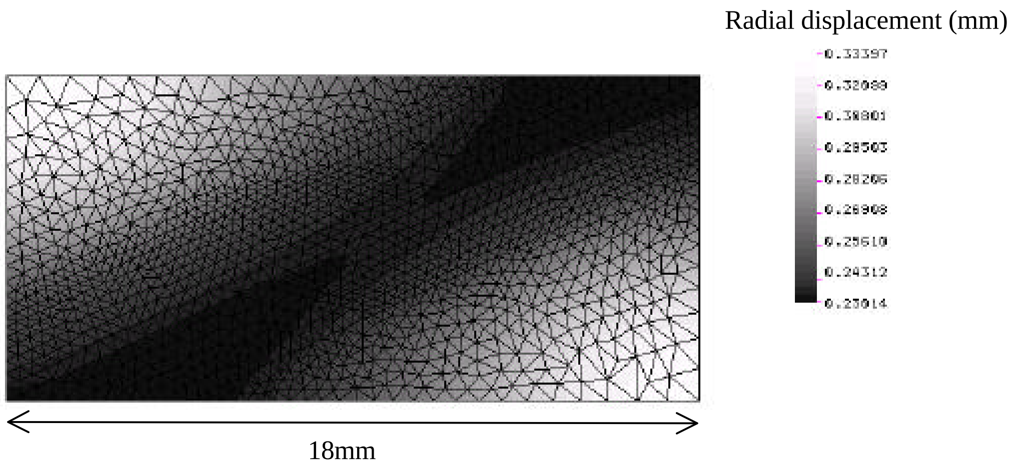

Fig. 4 : Radial displacement for a 3 MPa internal pressure

This simulation shows that, according to the hypotheses which have been made, particularly considering the filling polymer as quasi elastic at room temperature, the related displacements remains small. However, further investigations have to be performed with the filling polymer vicoelastic characteristics determined in a wide range of temperature (RT-150 °C).

CONCLUSION

A container devoted to the transportation of energetic matter was designed using a method according to which the structure and the material are defined simultaneously.
The functional analysis of the container has allowed the definition of requirements among which the deconfinement of energetic matter is the predominant function.
The research of various mechanisms allowing such a deconfinement has given rise to a combination of three different mechanisms of container collapse.

Complying these mechanisms and other container functions have required a combination of materials through the conception of an alveolar structure.
The validation of the conception and a first determination of the structure dimensions have been dealt with numerical simulations through the design of experiments method.
However, the simulation of the deconfinement mechanisms need further investigations concerning the polyethylene fibers properties and the polymer matrix characteristics in a wide range of temperatures.

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