# Uncertainty and modelling cost based methodology for modelling choices in multiscale structures

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Choices made in the design phases of multiscale structures are guided by the integration of knowledge on parameters at different scales of observation of the structure. These choices are often based on many experimental and predictive campaigns which increase modelling costs. The work developed here integrates the consideration of uncertainties in order to rationalise the cost of modelling (predictive and experimental) while controlling uncertainty over those parameters that are of interest for the structure scale. The methodology is applied to the study of a thick composite pressure vessel to be used for hydrogen storage.

Design method, Uncertainty, Multiscale modelling

## 1. Introduction

The cost of decisions taken during the different design phases affects a large proportion of the cost of the life cycle of a product. To reduce decisional risk, many experimental, analytical, numerical or semi analytical models are incorporated into the modelling process to guide the designer's choices [1]. During the preliminary design phase or as part of a product redesign, many concepts are envisaged relating to sizing or choice of materials. Improvements in predicting the behaviour of these systems are dependent on integrating knowledge into the models. This integration is carried out at different scales of the structure (not always representative) by means of complex and costly experimental modelling campaigns. One of the problems facing the designer is based on the right trade off between improving the quality of the prediction and increasing modelling costs. Different studies put managing uncertainty in product design at the different phases of the design process [2]. Many studies also propose decision support methodologies in design integrating the consideration of uncertainties into the resolution of optimisation problems [3 ,4]. In order to consider uncertainties, there are issues that have to be dealt with such as identifying their nature, their representation and their propagation in the associated models. In the literature, different studies differentiate between aleatory and epistemic uncertainties in their approaches to representation and propagation [1, 5]. Probabilistic approaches, used in this work, are based on a representation of uncertainty specific to each parameter across all of the studied interval. When using these approaches, uncertainties over the models' output parameters are assessed based on the variability of the input variables and the models used [6]. To do this, sources of uncertainty are represented by means of different interpretations described in the works of Sudret [7] according to information available on the uncertain parameters. These uncertainties are then propagated in the models using sampling methods [8]. The aim of this study is to develop a method to assist design under uncertainties to guide the designer in choosing combinations of predictive and experimental models so that levels of uncertainty and modelling costs are controlled and adapted to the advancement of the design process. After first focusing on considering uncertainties in the method developed here, the results are applied to a case study of a thick composite pressure vessel for hydrogen storage [6].

## 2. Methodology structure

The study structure for this work is a thick carbon fibre composite wounded pressure vessel designed to ensure a minimum burst pressure. Figure 1 shows a breakdown of the studied vessel into different observation scales.
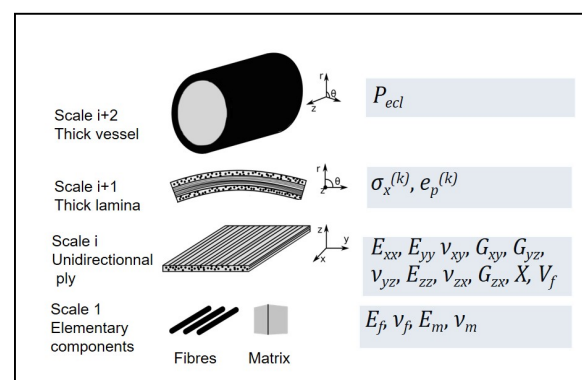


**Figure 1.** Outline of experimental and predictive modelling.

The developed methodology is based on the definition of different sets of vectors. The set $X=[x_1,...,x_S]$ contains vectors $x_i$ of parameters obtained at each ith scale from experimental test campaigns or geometric parameters, involved in characterising the burst pressure of the vessel. The set $M\{X\}=[m_1,...,m_S]$ includes vectors $m_i$, of predictive and experimental models defined at each ith scale to determine parameters of the set $X$. The set $W\{M\}$ contains vectors $w^j$ called modelling paths defined by a combination of models (predictive or experimental) selected in $M\{X\}$, at different scales, to define each parameter of $X$ involved in

determining the burst pressure of the vessel $P_{ecl}$. A change of model along a path results in a new modelling path being defined in $W\{M\}$. Thus, the search space contains a multitude of modelling paths.

## 2.1. Uncertainty and modelling costs methods

The designer's decision making process is based on:

- consideration of aleatory uncertainties $U\{X\}$ over the parameters of the set $X$. Representation and propagation are described by a frequentist interpretation of the probabilistic approach. Distribution analysis was used to propagate all information on the uncertainty of the input variables via the total description of the distribution envelope using probability density functions.
- consideration of epistemic uncertainties $U\{M\}$ over the models $m_i$ of the set $M\{X\}$. In addition to propagating uncertainties associated with the input variables of the set $X$, each predictive model presents an epistemic uncertainty defined from the Mean Squared Error (MSE) [9] between a reference distribution and the results obtained by the model.

Uncertainty across all parameters is propagated using probability density functions represented by normal laws obtained by Monte Carlo sampling. Epistemic and aleatory uncertainties are aggregated to ensure they are carried along the modelling paths by representing terms linked to the variance by normal distributions with zero mean and variance corresponding to the square of their standard deviation [10]. Each modelling path $w^j$ of the set $W\{M\}$ conveys an uncertainty about the burst pressure $u^j(P_{ecl})$.

- defining the cost of the models in order to assess the cost of modelling path. Fuzzy logic [11] was used with logical rules implemented using the Mamdani inference method [12]. The defuzzification was carried out using the barycentre method [13]. The cost of the models used is determined so that each modelling path presents a cost associated with the experimental and predictive modelling of the parameters. Total cost of the analytical models is based on two criteria: the number of input parameters in the model and the number of operations carried out. Calculating the cost of experimental models is based on calculating the cost of the treatment model (similar to calculating the cost of analytical models) and calculating the cost of the experiment. This cost takes into account the complexity of setting up the test pieces, the quantity of test pieces, the complexity of the equipment used. Finally, the vector $c[W]$ contains the j variables $c(w^j)$ defining modelling path costs.

The Figure 2 summarises the process of search for solutions consisted of solving a multiobjective optimisation problem.

The methodology is applied to determine optimised modelling paths $w^j$ that will minimise uncertainty over the burst pressure $u^j(P_{ecl})$ of the vessel and minimise the cost of modelling $c(w^j)$.

## 2.2. Overview of mechanical properties required

At each scale, the parameters involved in determining the burst pressure of the vessel $P_{ecl}$ are defined (Figure 1). Burst pressure is calculated using a fibre direction failure criterion in each ply of the stratification. This criterion requires knowledge of the fibre direction stress $\sigma_x^{(k)}$ in each ply of the stratification, calculated using the predictive model proposed by Xia et al. [14], and the fibre direction stress at failure, written $X$. When using the thick model, all the elastic properties of the unidirectional plies $E_{xx}$, $v_{xy}$, $G_{xy}$, $G_{yz}$, $v_{yz}$, $E_{zz}$, $v_{zx}$, $G_{zx}$, $E_{yy}$ must be determined in the different axes. The experimental modelling in this study is based on

experimental tests carried out on: UD plates wound, specimens obtained from wound cylinders with 310 mm diameter (Cyl. Φ310) and 32 mm diameter tubes (Φ32 tube) [15].
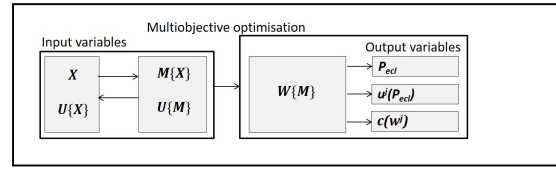


**Figure 2.** Multiobjective optimisation process

The different models used are summarised in Table 1. The stratification and the inner diameter are fixed by the specifications. Ply thickness $e_p^{(k)}$ is obtained from two models: one where ply thickness is constant in the stratification and one which considers that the thickness of each ply is variable [16]. The fibre volume fraction $V_f$ is approximated using three techniques: chemical dissolution (ch. diss.), supercritical solvolysis (solv.) and image analysis measurements (img. anal.) of stratified plates [16]. Models that consider or disregard the volume fraction of porosities are included. The effect of the porosity rate on the elastic properties of the plies is taken into account by applying an adjustment to the elastic modulus $E_m$, the Poisson's ratio $v_m$ of the matrix, and the fibre direction stress at failure of unidirectional ply $X$ [16]. The reference path, identified in Table 1, is based on experimental and predictive campaigns validated in the work of [16] to define the vessel [15, 16].

**Table 1**
Experimental and predictive modelling of parameters

| Parameters | Analytical modelling | Experimental modelling | | |
|---|---|---|---|---|
| $E_f$, $V_m$ | Database [16] * | | | |
| $E_m$ | Database | Nanoindentation [16] * | | |
| $E_{xx}$ | Chamis [17] | Plate [15] * | Cyl. Φ310 [15] | |
| $E_{yy}$ | | Plate * | Cyl. Φ310 | Φ32 tube [15] |
| $E_{zz}$ | Chamis | RARDE [15] * | | |
| $v_{xy}$ | Chamis | Plate* | | |
| $G_{xy}$ | Chamis | Plate* | Cyl. Φ310 | Φ32 tube |
| $G_{yz}$ | Chamis * | | | |
| $X$ | Plate* | | | |
| $V_f$ | | img. anal. [16] * | solv. [16] | ch. diss. [16] |
| $V_p$ | None | img. anal. * | | |
| $\sigma_x^{(k)}$ | Xia [14] * | | | |
| $e_p^{(k)}$ | | constant [16] | variable [16] * | |
| $P_{ecl}$ | Failure criteria [16] * | | | |

* reference modelling path choices

## 3. Results

### 3.1. Obtaining the Pareto front

The search space includes all possible modelling paths for defining the burst pressure of the vessel. The genetic algorithm NSGA-II (Fast Nondominated Sorting Genetic Algorithm) was used to determine the optimised modelling paths that make it possible to minimise uncertainty over burst pressure and modelling cost. This algorithm is based on elitism and nesting processes [18] and its effectiveness in problems with two objectives has been demonstrated in several studies [19, 20]. The configuration of the NSGA-II genetic algorithm is based on a population composed of 80 generations of 100 individuals. Crossover probability is fixed at 85% and mutation probability at 7%. For more in-depth information, the choice of the number of individuals, the number of generations, crossover probability and

mutation probability are discussed in several studies [20, 21]. In the proposed methodology, uncertainty over the burst pressure is obtained by calculating the root mean square error (RMSE) between the distribution obtained on the burst pressure at the end of each modelling path and that obtained when using the reference modelling path identified in Table 1. Thus the RMSE indicator contains two pieces of information: the coefficient of variation which characterises the aleatory and epistemic uncertainty carried by the modelling path and the deviation from the mean which characterises the deviation between the average obtained for the burst pressure values at the end of a modelling path and that obtained by the reference path. Figure 3 presents all the modelling paths that were evaluated by the NSGA-II algorithm according to their modelling cost. The cost shown in Figure 3 is calculated in relation to the cost of the reference path and the RMSE indicator is adimensional, using the average burst pressure for each modelling path. Ten optimised modelling paths were identified on the Pareto front. The reference modelling path has a high cost and a burst pressure with an average value of 2540.9 bars, with a coefficient of variation of 2.1%.
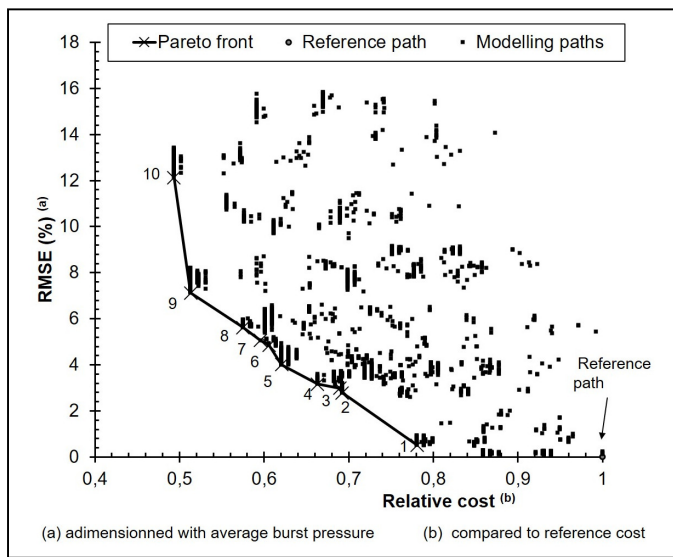


**Figure 3.** Pareto front obtained by minimising modelling cost and uncertainty (RMSE) on the burst pressure of the vessel.

### 3.2. Determining efficient knowledge integration

Table 2 presents the modelling choices made from the 10 modelling paths on the Pareto front and the values of costs associated with each modelling path. Analysis of knowledge integration focuses on 4 key discriminating parameters in determining the burst pressure: longitudinal Young's modulus of the plies $E_{xx}$, out of plane Young's modulus $E_{zz}$, porosity rate $V_p$ and ply thickness $e_p^{(k)}$. The results obtained show that path 10, 50% less expensive than the reference path, requires very little experimental development, the average burst pressure determined by this path is 2853 bars (+12.3%/reference) with a coefficient of variation of 7.2%. With a similar modelling cost, path 9 integrates the consideration of variable ply thickness, which improves the burst pressure prediction compared to path 10. The average pressure calculated by path 9 is 2710 bars with a coefficient of variation of 5.5%. The integration of the experimental tests on the longitudinal Young's modulus of the plies $E_{xx}$ allows a significant reduction in the coefficient of variation on the burst pressure (2.1% vs. 5.5%) for the group of three modelling paths (6, 7, 8). The choice from these experimental models (based on tensile tests on wound UD plates or on specimens obtained from large diameter cylinder) does not

significantly influence the cost of modelling and the quality of the burst pressure prediction.

**Table 2**
Choice of predictive and experimental modelling of the Pareto front modelling paths

| | Path ID Parameters | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $E_{xx}$ | Plate | ✓ | | | ✓ | | | | ✓ | | |
| | Cyl. | | ✓ | ✓ | | | ✓ | ✓ | | | |
| | Chamis | | | | | ✓ | | | | ✓ | ✓ |
| $E_{zz}$ | RARDE | ✓ | | | | | | | | | |
| | Chamis | | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ |
| $e_p^{(k)}$ | variable | ✓ | | | | ✓ | ✓ | ✓ | ✓ | ✓ | |
| | constant | | ✓ | ✓ | ✓ | | | | | | ✓ |
| $V_p$ | Yes | ✓ | ✓ | ✓ | ✓ | ✓ | | | | | |
| | No | | | | | | ✓ | ✓ | ✓ | ✓ | ✓ |
| Cost Gain (%) | | 22 | 31 | 31 | 34 | 38 | 39 | 40 | 42 | 49 | 51 |

The savings made in these modelling paths are the result of using the transverse isotropy hypothesis and disregarding porosities. Path 5 uses predictive modelling for the longitudinal Young's modulus of the plies $E_{xx}$ which leads to an increase in the coefficient of variation and in the deviation from the reference mean, but this second deviation is offset by consideration of porosities. Modelling paths 2 to 4 form a group of paths with similar modelling costs. All these paths consider a constant ply thickness in the structure. In all these paths, the effect of the volume fraction of the porosities is considered in the modelling. These paths differ from path 1 as they determine the out of plane modulus $E_{zz}$ using the transverse isotropy hypothesis. The differences between these modelling paths are mainly focused on the experimental model used to define the volume fraction of the fibres $V_f$ and the longitudinal Young's modulus $E_{xx}$. The results show that these experimental models do not have a significant influence on the quality of the burst pressure prediction. Finally, for modelling path 1 the cost is 22% less than the reference and the propagated epistemic and aleatory uncertainty is similar to the reference (2.2% vs. 2.1%). The average burst pressure calculated for this modelling path is 2529 bars (-0.5%/reference). This modelling path takes porosities into account and the variable thickness of the plies in the structure. The out of plane Young's modulus $E_{zz}$ is obtained from an experimental model. The longitudinal Young's modulus for the plies $E_{xx}$ is modelled using experimental tests on wound plates. This drop in cost compared to the reference is possible due to a rationalisation of the experimental models used to calculate burst pressure, especially when using predictive models to characterise the Poisson's ratio in the plane and shear moduli. Results obtained by using the Pareto front show that the quality of the estimate of the burst pressure averages is improved by the experimental modelling of the out of plane Young's modulus $E_{zz}$, by considering the porosity rate $V_p$ and by the experimental modelling of variable ply thickness $e_p^{(k)}$. In addition, the level of epistemic and aleatory uncertainty over the burst pressure decreases with the experimental modelling of variable ply thickness $e_p^{(k)}$ and the longitudinal Young's modulus of the plies $E_{xx}$ without the need to resort to applying the model to sections of specimens which are more complex to prepare.

## 4. Composite vessel redesign

Modelling paths 1, 6 and 9 (Table 2) on the Pareto front were used in the redesign of the thick composite pressure vessel. The basic vessel with an inner diameter of 310 mm has the following stratification: $[(\pm15/\pm25/90_2/\pm35/\pm45/90_2)_7/90]$. The minimum

burst pressure of this basic vessel must be greater than 2300 bars. The redesign concerns vessels with inner diameters of between 220 mm and 380 mm, (volume of the vessel increased or decreased by 50%), and burst pressures between 1800 bars and 2800 bars. Four redesign case studies are defined (Table 3). Calculating the minimum burst pressure is based on the experimental and predictive modelling choices made in optimised modelling paths 1, 6 and 9 (Table 2). The cost of each optimised modelling paths 1,6,9, calculated on the basic vessel is retained in the redesign of the vessel. During the redesign process, the design parameter represents the number of groups of plies N in the stratification $[(\pm15/\pm25/90_2/\pm35/\pm45/90_2)_N/90]$ which will guarantee the minimum burst pressure required in each case study. Figure 4 shows the overestimate obtained in parameter N compared to the sizing solution obtained when using the reference modelling path.

**Table 3**
Case study to redesign a hydrogen pressure vessel

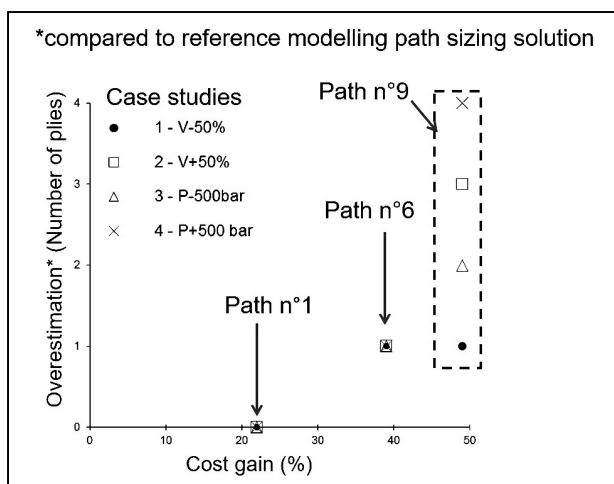| Vessel | Inner diameter | Minimum burst pressure | Redesigned vessel |
|---|---|---|---|
| Case study 1 | 220 mm | 2300 bars | V-50% |
| Case study 2 | 380 mm | 2300 bars | V+50% |
| Case study 3 | 310 mm | 1800 bars | P-500 bars |
| Case study 4 | 310 mm | 2800 bars | P+500 bars |



**Figure 4.** Stratification obtained in the redesign of the pressure vessel compared to the reference stratification.

Solution 1, which shows a 22% gain in the cost of modelling compared to the reference modelling path, delivers the same sizing proposals as the reference path in all the proposed redesign cases (volume 50% higher or lower and minimum burst pressure increased or decreased by 500 bars). Solution 6, where the modelling cost is 39% lower, delivers a systematic oversizing of a group of plies for each redesign case. This solution represents a good trade-off between modelling cost and precision in the prediction. Finally, solution 9 produces varying overestimates depending on the redesign case. These results are linked to the large number of predictive models assigned to this modelling path. The use of optimised paths in the pressure vessel redesign phase makes it possible to select design choices during the preliminary design phases while still guaranteeing low modelling costs and a controlled level of confidence regarding the parameters of interest.

## 5. Conclusion

The methodology developed here, and applied to the case study of a thick composite pressure vessel on which reference studies had been carried out [15, 16], made it possible to examine in further depth the means of integrating knowledge in order to model multiscale structures. The optimisation work rationalises the experimental and predictive modelling by reducing their costs, while at the same time guaranteeing a controlled uncertainty over the burst pressure of the vessel. Different modelling choices were selected for the redesign of the vessel with different trade offs between modelling costs and uncertainty. The optimised modelling paths result in sizing solutions suitable for vessel volumes 50% larger or smaller and for burst pressures 500 bars lower or higher. This methodology takes place in cases where the designer's knowledge of the parameters is high such as routine design or redesign process. Different representation of uncertainties and propagation methods will have to be developed in order to integrate lower levels of information on uncertain parameters corresponding, for instance, to upstream design phases or at the pre-project stage.

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