
A preliminary investigation of robust design and uncertainty quantification within the life cycle energy optimisation methodology

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The Life Cycle Energy Optimisation (LCEO) methodology aims at finding a design solution that uses a minimum amount of cumulative energy demand over the different phases of the vehicle's life cycle, while complying with a set of functional constraints. This effectively balances trade-offs, and therewith avoids sub-optimal shifting between the energy demand for the cradle-to-production of materials, operation of the vehicle, and end-of-life phases. The present work describes the inclusion of robust design aspects and uncertainty quantification into the LCEO framework. In particular, uncertainty is introduced through the assumption that the material and energy properties of a subset of the optimisation's candidate materials are described by statistical distributions as opposed to a priori fixed values. Subsequently, the nature of the LCEO-associated optimisation problem is changed from deterministic to stochastic. This change is handled by defining a multilevel representation hierarchy, and using the Multilevel Monte Carlo (MLMC) approach in the optimisation process to evaluate the expected compliance of a given design with the transport-related functional requirements. The extended framework is applied to the robust design optimisation of a subsystem of a vehicle model which is both mechanically and geometrically constrained. The ability of the LCEO methodology to include robust design aspects early during the vehicle design process, while simultaneously handling functional conflicts, to result in a robust life cycle energy optimal design is demonstrated. Furthermore, the performance increase obtained by the use of the MLMC approach instead of the classical Monte Carlo approach within an optimisation under uncertainty framework is illustrated.

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1. Introduction

Between 2009 and 2017, the fleet average CO₂ emissions from new cars have decreased by 18.6% [1], with these improvements being mostly the result of changes targeting the vehicle's propulsion system [2] and lightweight design [3]. However, several studies have underlined the necessity to take into consideration the entire life cycle of vehicles when addressing their environmental impact through incremental design alteration or radical architecture change [3, 4, 5]. Furthermore, most of the existing methodologies that support such engineering design activities have a re-active character [6]. They are often applied to assess the environmental performance of a limited subset of design alternatives, and only use the environmental performance indicators as criteria in a down-selection process [5] rather than main design drivers. These obstacles limit their ability to lead to the emergence of radically new vehicle concepts.

The life cycle energy optimisation (LCEO) methodology [6] has been proposed as a systematic approach that yields concrete design choices while addressing the critical conflict between functionality and environmental impact [7] existing in vehicle engineering design. The methodology is intended to enable early-stage life cycle energy (LCE) efficient vehicle design through solving an optimisation problem with the LCE as its objective function, while the functional requirements that the design is subject to are implemented as optimisation constraints.

Previous work on the LCEO methodology has concerned: the introduction and the formalisation of the methodology, and the investigation of the impact of the inclusion of the production and use-phase energies [6]; the impact of end-of-life (EOL) modelling [8]; the functional extension of the framework through the preliminary examination of the effect of vehicle shape and aerodynamic drag estimations [9]; as well as the expansion of the framework to enable vehicle production system design optimisation [10].

Beyond widening the area of applicability of the framework and uncovering fundamental links between the very mechanisms enabling the embodiment of the LCE optimal designs and the vehicle's life cycle parameters, the aforementioned works also underscore the high dependency of the optimal solutions on a number of parameters. Some of these parameters are characterised with a high level of uncertainty, whether intrinsically or due to the circumstances of conceptual vehicle design. For instance, EOL parameters are characterised with a high level of uncertainty as they are related to the lifespan of vehicles and their future use; while the uncertainty of the use phase-related energy estimates is due, in part, to the use of relatively lower fidelity models. The *epistemic uncertainty* introduced by such models is related to the so-called design paradox [11]: the amount of vehicle-specific knowledge is at its lowest when it is most needed, that is during the conceptual stage. Furthermore, due to the intrinsic variability of manufacturing – and EOL – processes, *aleatoric uncertainty* is expected in such quantities as the material properties.

Thus, in order to identify solutions – or classes of solutions – to the LCE optimisation problem that remain stable within a reasonable range of variation of these aforementioned parameters, it is necessary to include aspects of robust design and uncertainty quantification within the LCEO methodology. This is particularly relevant for cases including vehicle, or vehicle subsystem, models that are characterised by large design landscapes, and that are therefore more likely to feature large variations in optimal design outcomes based on changes in the optimisation parameters; and remains relevant for smaller models as it allows for the quantification of the impact of parameter uncertainty on the mechanisms enabling the optimal solutions.

This paper constitutes a first proof of concept of the introduction of uncertainty quantification within the LCEO framework. Therefore, it only targets one of the dimensions of the larger robustness problematic and does not aim at providing a comprehensive treatment of the latter within the LCEO methodology. In particular, this work targets the introduction of uncertainty in some of the parameters influencing the mechanical performance of a subset of the constitutive materials of a vehicle subsystem. This uncertainty may stem from the intrinsic variation in production processes, or even more so from mixing recycled materials with the virgin material stock. Indeed, the properties of the vehicle's constitutive materials can be significantly degraded depending on the EOL processing options considered.

The consideration of uncertainty in the mechanical parameters of the constitutive materials alters the nature of the optimisation problem at hand. The latter becomes constrained by a stochastic system of partial differential equations rather than a deterministic one. This is handled by using the non-intrusive, and relatively more computationally efficient, Multilevel Monte Carlo (MLMC) [12] approach in order to evaluate the verification of the functional transport-related constraints at any given design point during the optimisation loop.

The results show the gap in LCE between the deterministic solution and the robust formulation, as well as the performance increase obtained from the use of the MLMC approach instead of the classical Monte Carlo (MC) one within an Optimisation Under Uncertainty (OUU) framework. Furthermore,

a discussion of how additional aspects of robustness can be included in the LCEO framework is also provided.

Section 2 provides an overview of the LCEO methodology, as initially introduced in [6] and further elaborated in [8], as well as a brief description of the MLMC approach as introduced in [12]. Subsequently it presents the benchmark illustrative case study that has been established in previous works [6, 8, 9, 10, 13] and extends it to a stochastic formulation in order to accommodate the introduction of forward uncertainty quantification into the methodology. Following this, Section 3 presents some preliminary results that establish the optimality gap between the robust solutions and the deterministic ones and illustrates the performance increase associated with the use of the variance reduction scheme of the MLMC approach in lieu of the MC alternative. Finally, a summary outlook on the steps necessary to provide a more comprehensive treatment of uncertainty within the LCEO methodology is provided in Section 4.

2. Methodology

2.1 LCEO methodology

The LCEO method formally integrates environmental considerations into a design methodology through the formulation of a mathematical multidisciplinary design optimisation framework. The life cycle energy is used as the objective function to be minimised, as detailed in [6]. Functional requirements stemming from structural mechanics, and eventually other disciplinary fields, act as constraints on the design. Thus, this methodology does not compromise design requirements, but rather changes design variables so as to find the design solution which features the minimum life cycle energy use while fulfilling all the transport related functional requirements.

The life cycle energy is formulated as

$$E_L(X) = E_P(X) + E_U(X) + E_E(X), \quad (1)$$

where E_L is the life cycle energy, E_P is the production energy, E_U is the use-phase energy, E_E is the end-of-life energy, and X is the set of design variables.

The production energy is obtained from the embodied energy of the constitutive materials of a given design; while the EOL energy is obtained from the sum of two distinct contributions, and is expressed as

$$E_E(X) = E_{Pro}(X) + E_{Rec}(X). \quad (2)$$

$E_{Pro}(X)$ corresponds to the energy burdens and credits associated with the EOL processing of the material entering into the composition of the vehicle subsystem considered, while $E_{Rec}(X)$ corresponds to the corrected energy credits resulting from the EOL processing phase of the aforementioned vehicle subsystem [8]. A scenario-based approach is adopted for the treatment of the different material candidates entering into the composition of the vehicle subsystem, with more specific details about these scenarios being provided along with the description of the case study considered in this work in Section 2.3.1.

Finally, the use phase energy is obtained through multiplying the energy required to move the vehicle according to a prescribed drive cycle (New European Drive Cycle) by the number of such cycles during the entire use phase of a vehicle. The associated optimisation problem is expressed as

$$\min(E_L(X)), \quad (3)$$

subject to constraints of the form:

$$T_{(I)}(X) \leq 0, \quad (4)$$

$$T_{(E)}(X) = 0, \quad (5)$$

$$X_{min} \leq X \leq X_{max}. \quad (6)$$

Equation 4 corresponds to functional requirements expressed as inequalities, while Equation 5 refers to the functional requirements which are expressed as equalities. The last equation, Equation 6, is the set of design variable boundaries.

2.2 Multilevel Monte Carlo

The central idea of the MLMC approach is that Monte Carlo samples can be simultaneously and independently drawn on several approximations of the studied problem on a hierarchy of computational grids – or levels – with an associated decreasing sequence of mesh sizes $h_0 > h_1 > h_2 > \dots > h_L$ and an accordingly increasing number of degrees of freedom.

The linearity of the expectation operator $\mathbb{E}[\cdot]$ enables the expression of the expectation of a given Quantity of Interest (QoI) Q at the finest level, $\mathbb{E}[Q_L]$, to be rewritten as a telescopic sum of the expectation of the QoI at the coarsest level, $\mathbb{E}[Q_0]$, and a sum of correction terms adding the difference in expectation of the QoI between evaluations at the consecutive levels denoted by the subscript l :

$$\mathbb{E}[Q_L] = \mathbb{E}[Q_0] + \sum_{l=1}^L \mathbb{E}[Q_l - Q_{l-1}]. \quad (7)$$

Using sample average approximations, the MLMC estimator of $\mathbb{E}[Q]$ can be defined as the following:

$$\mathbb{E}^{MLMC}[Q_L] := \frac{1}{M_0} \sum_{m_0=1}^{M_0} Q_0^{(m_0)} + \sum_{l=1}^L \frac{1}{M_L} \sum_{m_l=1}^{M_L} (Q_l^{(m_l)} - Q_{l-1}^{(m_l)}). \quad (8)$$

where $Q_i^{(m_j)}$ refers to the j^{th} realisation of the QoI at the i^{th} mesh refinement level. Thus, the term $(Q_l^{(m_l)} - Q_{l-1}^{(m_l)})$ comes from two discrete approximations at two different refinement levels (l and $l - 1$) evaluated for the same samples. A presumption of this approach is that the mesh hierarchy provides errors and computational costs that respectively decrease and increase algebraically with h_l .

A computational complexity analysis of the error of the MLMC estimator shows that it is composed of a discretisation error and a statistical error. For a given error tolerance level, a splitting parameter can be introduced to split the tolerance requirements over both error sources. Subsequently, the optimal number of samples at different levels can be obtained by minimising the computational cost of the MLMC estimator subject to the accuracy constraint based on the statistical error; while a stopping criterion for the amount of levels to be added can be derived using the discretisation error constraint. More details about the MLMC algorithm can be found in [12].

2.3 Illustrative case study

This section reformulates the previously established LCEO benchmark problem [9] as a multilevel stochastic PDE-constrained optimisation problem with the QoIs intervening at the level of the design constraints. It also describes the simplifying assumptions made in order to compute the relevant QoIs more easily.

2.3.1 Description of the target vehicle subsystem

The MLMC augmented LCEO methodology is applied to the case study of the design of a vehicle component to illustrate the impact of uncertainty quantification into the framework. In particular, the vehicle component considered is the roof of a car, which has already served as a benchmark for previous LCEO studies [6, 8, 9, 10, 13]. The model considered here is two dimensional and relies on symmetry to reduce the size of the problem.

The car roof panel is assumed to be a sandwich panel consisting of three layers: two thin face sheets and a thicker core. This design choice introduces the face sheet layer thicknesses t_i , the core

layer thickness t_c and the material volume fractions $V_{i,j}$ as the design variables. The face sheets of the panel may be composed of a blend of carbon fibres (CF) and glass fibres (GF) as reinforcements to a thermosetting epoxy matrix. The core of the panel can be composed of a blend of polyvinylchloride (PVC), polyethylene (PET), and polyurethane (PUR). The material properties and embodied energies of these materials are provided in [6]. The hybridisation concept is used to allow for the continuous representation of the intra-layer material properties [14].

Two EOL scenarios are considered for the processing of the materials entering into the composition of the panel: a high and a low recycling scenario. In the first idealised reference scenario, it is assumed that little to no material property degradation takes place for CF and GF and that their resulting recyclates can entirely replace virgin fibres. On the other hand, in the second scenario, only a modest amount of recovered fibres is presumed to be able to be mixed with the virgin fibres. In order to limit the complexity of the study, the materials of the core layer are assumed to be incinerated with energy recovery in both scenarios. The processes as well as energy burden and credit values used in the optimisation are shown in Table 1.

Table 1: Overview of the two EOL scenarios modelled and the EOL credit and burden energy values used in the optimisation. Adapted from [8].

Nr.	Description	E_{Pro} [MJ/kg]					C_f		E_{Rec} [MJ/kg]	
		CF	GF	PET	PVC	PUR	CF	GF	CF	GF
1	CF Pyrolysis GF Shredding	30	0.17	-23.8	-22.9	-24	1	1	-286	-30
2	CF Milling GF Shredding	0.27	0.17	-23.8	-22.9	-24	0.3	0.3	-85.8	-9

Typical automotive design requirements that can be formulated on a vehicle's roof are related to loading cases in the event of the car rolling over [15], flutter behaviour under driving conditions [16] as well as fundamental sound transmissions properties. Therefore, two maximum displacement under load and two minimum frequency constraints are formulated on the panel. The maximum displacements allowed under local and global unit static pressures are set to $d_{1,max} = d_{2,max} = 2.5 \times 10^{-6}$; while the minimum frequencies for the first and second natural frequencies of the panel are set to $f_{1,min} = 330$ Hz and $f_{2,min} = 520$ Hz.

2.3.2 A multilevel stochastic formulation of the associated design problem

As a result of the application of the EOL processing alternatives presented in Table 1, as well as the inherent variability in production processes, the material properties of CF and GF can vary. In order to more accurately capture the impact of this effect on the optimal solutions, the material properties associated with these candidate materials are described through presumed probability distributions, instead of deterministically. Therefore, the LCEO problem presented in Section 2.1 becomes an optimisation problem constrained by a system of partial differential equations with random coefficients.

Consequently, the deterministic inequality constraints $d_i(X) \leq d_{i,max}$ and $f_i(X) \geq f_{i,min}$, for $i = 1, 2$, have to be reformulated as the chance constraints $P(d_i(X) \leq d_{i,max}) = 1$ and $P(f_i(X) \geq f_{i,min}) = 1$. However, the computation of such constraints can be challenging, and it is suggested here to relax them using statistics of the displacement and normal mode QoIs. Such a relaxation has been previously used in the context of reliability-based design optimisation of aircraft components [17].

The relaxed constraints for $i = 1, 2$ are formulated as

$$\mathbb{E}[d_i(X)] + n\sigma[d_i(X)] \leq d_{i,max}, \quad (9)$$

$$\mathbb{E}[f_i(X)] - n\sigma[f_i(X)] \geq f_{i,min}, \quad (10)$$

with n an integer and $\sigma[\cdot]$ the standard deviation operator.

The MLMC solver is used, in conjunction with a deterministic solver of the system of elastostatic equations implemented in FreeFem++ [18], in order to estimate the relevant statistics of the QoIs introduced in the relaxed constraints within the Differential Evolution population-based optimiser [19]. To this end, a mesh hierarchy is defined for the FEM model of the sandwich panel. In this work, a geometric mesh hierarchy is defined by taking $h_l = h_0\beta^{-l}$, where h_l is the mesh size at level l , h_0 the mesh size at the coarsest level and $\beta \geq 2$ is a constant integer.

3. Results

The preliminary results presented here are obtained for the inclusion of uncertainty at the level of the Young's modulus of the CF material candidate. It is assumed that the modulus follows the uniform distribution $\mathcal{U}(0.95E_N, 1.05E_N)$ centred around its nominal value E_N . The stochastic optimisation results are obtained for a relatively generous tolerance level of $\epsilon_{TOL} = 0.1$, $\beta = 2$ and $n = 3$. Both deterministic and stochastic results shown in Tables 2 and 3 are obtained for a total driving distance of 60,000 km, and are optimised for both EOL scenarios presented in Table 1.

Table 2: Deterministic optimisation results.

EOL Scenario	E_L [MJ]	m [kg]	V_{CF} [%]	V_{GF} [%]	t_1 [mm]	V_{PVC} [%]	V_{PUR} [%]	t_c [mm]
1	220	0.71	100	0	0.43	62	38	24.6
2	248	0.51	100	0	0.2	41	59	29.7

Table 3: Stochastic optimisation results.

EOL Scenario	E_L [MJ]	m [kg]	V_{CF} [%]	V_{GF} [%]	t_1 [mm]	V_{PVC} [%]	V_{PUR} [%]	t_c [mm]
1	222	0.81	100	0	0.44	92	8	22.9
2	250	0.58	81	19	0.22	46.3	53.7	30.8

Table 4: Typical number of deterministic model evaluations observed per mesh hierarchy level in the MLMC approach.

Mesh level	0	1	2	3
Number of model evaluations	868	50	50	1

A comparison between the stochastic and deterministic optimisation results presented in the aforementioned tables shows that the uncertainty characterising CF's Young modulus can be handled with a sub 1% LCE premium and with significant design changes. Indeed, the inclusion of robustness in the optimal designs leads to a mass increase of roughly 14% in both scenarios. However, this mass increase is arrived at differently depending on the EOL scenario considered.

In the first scenario, CF-associated uncertainty is neutralised by increasing the amount of CF used as well as increasing the amount of the stiffer PVC in the core of the panel. On the other hand, in the

second scenario, the same is achieved by replacing a fifth of the amount of CF with the previously unused GF.

These large variations in the optimal design with a relatively small impact on the LCE are likely the result of the multimodality of the design optimisation problem considered. However, it remains to be seen if this demonstrated flexibility would endure were the material properties of the other constitutive materials to also be described stochastically.

Finally, the performance of the MLMC approach can be illustrated by the break-down of model evaluations per mesh hierarchy level shown in Table 4. The latter shows that, for the design point considered, most of the FEM model calls are performed at the lowest level (0), and only one call is performed at the highest level (3). Conversely, fulfilling a similar tolerance level using the MC approach would typically require a number of model calls of the order of 10^3 at a mesh level comparable to mesh level 2 in Table 4.

4. Summary and outlook

In this paper, it was demonstrated on an illustrative case study how uncertainty can be systematically and efficiently included in the LCEO methodology to enable robust design aspects to be considered early during the vehicle engineering design process. This was achieved by capitalising on the relatively increased computational efficiency offered by the MLMC approach within an OUU context. The results of this study have shown that – under the assumption of the stochastic variation of the material properties of one of the constitutive materials of a vehicle subsystem – robust alternative LCE optimal designs can be obtained at a marginal LCE increase relative to the deterministic optimal solution. Additionally, these robust designs constitute a significant departure from the deterministic ones, with the design changes varying depending on the life cycle scenario considered.

Further work includes more rigorously handling the estimation of the higher order statistical moments of the constraints-related QoIs using estimators such as the ones introduced by Bierig & Chernov [20] or Pisaroni [21], as well as considering uncertainty at the level of the material's energy properties. The latter step would lead to a reformulation of the optimisation problem introduced in Equations 3, 4, 5 and 6 to involve statistics of $E_L(X)$ in the objective function to minimise. It is worth noting here that this reformulation significantly increases the computational complexity of the problem as it would involve solving a nested optimisation problem (that may itself involve a sampling-based approach similar to that presented in this paper) at every sample needed for the computation of the LCE's statistics.

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