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Original

Multiscale modelling techniques in life cycle assessment: Application to nanostructured polymer systems in the maritime industry / Mio, A., Bertagna, S., Cozzarini, L., Laurini, E., Bucci, V., Marino, A., Fermeglia, M.. - In: SUSTAINABLE MATERIALS AND TECHNOLOGIES. - ISSN 2214-9937. - 29:(2021), pp. e00327."-e00327."-". [10.1016/j.susmat.2021.e00327]

Availability:

This version is available at: 11368/2994292 since: 2024-10-18T17:54:22Z

Publisher:

Published

DOI:10.1016/j.susmat.2021.e00327

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Multiscale modelling techniques in life cycle assessment: Application to nanostructured polymer systems in the maritime industry

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ARTICLE INFO

Keywords:

Life cycle assessment
LCA
Multiscale molecular Modelling
Maritime
Nanostructured polymer
Material replacement

ABSTRACT

One of the major challenges of Life Cycle Assessment is in the generation of life cycle inventories for complex or novel materials. This paper aims at broadening the perspective in Life Cycle Assessment methodology, exploiting multiscale modelling towards the generation of inventory data during an early-stage product design. Our approach involves the usage of molecular modelling techniques, such as electronic, atomistic or mesoscale models, in combination with continuum models, such as process simulation or finite element methods, to provide data for the generation of life cycle inventories of nanostructured materials. In particular, each simulation is performed at a specific length and time scale through specific software, passing information from the lower to the upper scale. We applied our procedure to a comparative Life Cycle Assessment among suitable materials for the production of a set of cylinder head cover of a marine engine, *i.e.*, aluminium alloys and nano-engineered thermoplastic polymers. Engineering judgment, Ashby charts and maritime regulations led the initial identification of suitable materials. As a result, polyamide 6,6 reinforced with 30% wt. glass fibers and mixed with phosphate-based flame retardants have been identified as promising candidate for the replacement of aluminium traditional covers. Nonetheless, we introduced nanoclays, *i.e.*, exfoliated montmorillonite, as a replacement for a quota of conventional flame retardant, aiming at reducing the usage of pollutant chemicals. We then resorted to atomistic and finite-element techniques to investigate the compliance of nanocomposite materials with several Key Performance Indicators. The nanocomposite formulations obtained from simulations have been finally employed as input data for life cycle inventories of material alternatives. Using a Life Cycle Assessment approach, we could identify the most environmental-friendly nanocomposite formulation, which was then compared with traditional aluminium through an additional comparative cradle-to-grave study. Among the suitable nanocomposite formulations, the material with the minimum amount of traditional flame retardant exhibited the lowest scores among the majority of Environmental Footprint impact categories. To account for the entire lifetime of the marine engine, a set of four nanocomposite covers has been compared with a set of three aluminium covers made by two different metal alloys. Four recycling scenarios for aluminium covers have been examined, assuming an incremental number of end-of-use products reintroduced into a circular life cycle, while nanocomposite ones were disposed into landfill. In turn, if the aluminium products are insufficiently recycled, our results promote the usage of nano-engineered polymer products. As the amount of reused metal covers increases, indeed, polymer-based covers become unfavorable with respect to aluminium cast alloy products.

Abbreviations: CC-T, Climate Change Total; EF, Environmental Footprint; EQ-EF, Ecosystem Quality - Eutrophication Freshwater; EQ-EM, Ecosystem Quality - Eutrophication Marine; EQ-ET, Ecosystem Quality - Eutrophication Terrestrial; EQ-FE, Ecosystem Quality - Freshwater Ecotoxicity; EQ-FTA, Ecosystem Quality - Freshwater and Terrestrial Acidification; FE, Finite Element; FR, Flame Retardant; FTP, Fire Test Procedure; GF, Glass Fibers; GLO, Global; HH-CE, Human Health - Carcinogenic Effects; HH-IR, Human Health - Ionizing Radiation; HH-NCE, Human Health - Non-Carcinogenic Effects; HH-OD, Human Health - Ozone Layer Depletion; HH-PCOC, Human Health - Photochemical Ozone Creation; HH-RE, Human Health - Respiratory Effects; KPIs, Key Performance Indicators; LCA, Life Cycle Assessment; LCI, Life Cycle Inventory; LCIA, Life Cycle Impact Analysis; MCI, Material Circularity Indicator; MD, Molecular Dynamics; microFEM, Micro-Finite Element Modelling; MMT, Montmorillonite; NETP, Nano-engineered thermoplastic polymers; ODAM, 1-octadecylamine; PA66, Polyamide 6,6; PAM, 1-pentylamine; RER, European regionalization; RD-F, Resources Depletion - Fossil Fuels; RD-L, Resource Depletion - Land Use; RD-M, Resource Depletion - Minerals and Metals; RD-W, Resources Depletion - Dissipated Water; RVE, Representative Volume Element; TPP, Triphenyl phosphate.

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Accordingly, an increasing amount of post-consumer aluminium diminishes the need of primary metal, yielding considerable advantages in terms of environmental footprint. Consequently, stakeholders should commit in recycling metal components not only at ship dismantling, but also during ordinary maintenance. Our study showed how multiscale molecular modelling proved to be useful for providing necessary inventory data for complex nanostructured materials. This preliminary study paves the way for future development of the proposed framework, in which *in-silico* techniques based on distinct paradigms can mutually contribute towards an improvement of products ecodesign.

1. Introduction

Life Cycle Assessment (LCA) is a well-established methodology dedicated to the estimation of environmental impacts induced by manufacturing, usage and disposal of products, as well as by natural or artificial systems related to human activities. The LCA regulatory framework and its assessments requirements are described by the Standard Organization (ISO) 14,040 and 14,044 guidelines [62,63]. The methodology is based on material and energy balances of the overall life cycle of the product, including extraction of raw materials, manufacturing, distribution, use phase, recycling, final disposal and transportations between life cycle stages [18]. The outcomes of life cycle studies are expressed through several impact categories aiming at estimating the full range of ecological impacts associated with the product system to each environmental compartment. The LCA framework, as extensively discussed on a series of publications [52,57], involves the implementation of four phases. The first is the “Goal and Scope”, where practitioners shall specify the aim of their study, the intended readers, the functional unit, the system boundaries, the quality of data source, and the assumptions and limitations of their approach. This is followed by “Life Cycle Inventory” (LCI) analysis, where the practitioners collect the mass and energy balances of the product system under investigation. The inventory data are then employed within the “Life Cycle Impact Assessment” (LCIA) step, which relates them to specific environmental burdens through well-established emission factors. Finally, the “Interpretation” phase explains the results obtained by previous steps by discretionary using of sensitivity and uncertainty analyses.

The issues and challenges related to LCA procedure have been described by Reap et al. [55,56], shedding light on the unsettled methodology aspects which still require an acknowledged harmonization among the scientific community. Among the others, collecting data for life cycle inventory is usually a demanding task for practitioners. While the usage of accurate primary data is preferred, it is a common practice to rely on acknowledged databases, e.g., ecoinvent [73] or Gabi [51], when case-specific information is missing. It is widely known how data quality affects significantly LCA results, in terms of uncertainty and completeness of information [49,72]. Therefore, gaining accurate life cycle inventories of raw materials and manufacturing processes plays an essential role in LCA studies.

Despite the available databases embed a wide range of information, there is still a lack of data regarding novel materials or peculiar manufacturing processes. In case of missing information, ISO guidelines suggest the usage of proxy data, which is the inventory of a similar material or technology. The similarity between the two systems determines the accuracy of the data employed. Alternatively, molecular structure-based models [12,74] or artificial neural networks [14,35,75] have been employed to identify shortcuts and patterns between database information and impact assessment results. With the aim to limit the inaccuracy of the proxy data, numerous *in-silico* modelling techniques have been applied to estimate LCI of products. So far, innovative methodologies for generating raw materials inventories include process modelling [6,29,43,48,80], dedicated frameworks [40] and heuristics [34,79].

In combination with previous modelling techniques, the multiscale molecular modelling approach provides a complete set of material properties, comprising mechanical, thermal, electrical, magnetic and

toxicological properties [26]. By definition, multiscale molecular modelling involves the development of computational models at different length and time scales, which are often unrelated in their theoretical background. The set-up of the overall framework can be based on two distinct approaches. The former is defined as sequential approach, which involves the modelling of independent systems with some sort of parametric linking between them. The latter is based on a concurrent approach, in which several models run simultaneously, occupying different spatial regions of the simulation environment (also referred to as model coupling). Multiscale molecular modelling allows to capture all the phenomena at each scale, transferring the necessary information to the upper scale until the macroscopic system is reached [38].

The macroscopic scale is where methods and tools familiar to industrial engineers are used for the design of complex materials, such as process simulations or finite-element models. However, there is a broader perspective available for the investigation of novel materials, i.e., the life cycle perspective. Different models commonly used in the multiscale modelling hierarchy are shown in Fig. 1. The reader will notice the introduction of the Life Cycle Assessment technique on the top right corner of Fig. 1, where the characteristic time of the model scales to months/years and the characteristic length becomes kilometers.

The simulation models typical of the multiscale approach are now briefly described:

- *Electronic models* (10^{-10} - 10^{-9} m and 10^{-12} s): these models deal with quantum-mechanical interactions between nuclei and electrons. They provide information about, e.g., conductive/dielectric or optical properties using electronic band structure, activation energies and chemical reaction coefficients, properties of atomic defects and dopants through thermodynamic stability and kinetic elementary processes, magnetic anisotropy, diffusion coefficient, and more.
- *Atomistic models* (10^{-10} - 10^{-7} m and 10^{-12} - 10^{-6} s): the models belonging to atomistic category represent atoms explicitly or, sometimes, assembled into small groups referred to as beads or pseudo atoms. The interactions among them are calculated using potential energy estimation based on well-established force fields. Each force field is suitable for peculiar systems and is generally based on two classes of interactions: (i) bonded interactions including bond-length (stretching) potential, bond-angle (bending) potential, torsion (twisting) potential and cross-terms, and (ii) non-bonded interactions generally dealing with Coulomb interactions and dispersion forces. Results available from atomistic models include constitutive equation parameters, molecular trajectories, stiffness and mechanical properties, packing, surface and interface energies, and heat and mass transfer data.
- *Mesoscopic models* (10^{-9} - 10^{-1} m and 10^{-6} - 10^1 s): in these models, molecular details are implicitly acknowledged by a field-based description or a particle-based description. This allows to reproduce phenomena on length and time scales restricted to classical atomistic approaches, such as system morphology, domain formation and growth kinetics, thermal stability, rheological and magnetic behavior. In case of need, density distribution of beads at mesoscopic scale may be mapped in a 1:1 fashion towards a microFEM simulation. This allows to calculate physical and mechanical properties

using an approach commonly employed by continuum models. These properties can be finally transferred to the next scale up.

- **Engineering design models (10^{-3} – 10^1 m and 10^1 – 10^3 s):** these models assume a continuous distribution of material within the simulated volume, reason why they belong to the so-called continuum models. Since constitutive laws hold true at these time and length extents, the behavior of the physical system is no longer influenced by atomic and molecular structures. This allows to obtain information on materials with peculiar shape (using Finite Element Method – FEM), or to deal with substances considering their macroscopic thermodynamic properties (using Process Simulation). Examples of typical properties obtained from these models are heat and mass transport coefficients, chemical reaction kinetics and macroscopic structural and mechanical information.

The relationships among models at different scales are shown in Fig. 2. The information provided by each model can be either used as input for models at higher scales or stored as-is in a database, along with literature or experimental data. There are plenty of software packages available at each modelling scale. Among many others, notable examples include Gaussian, VASP, SIESTA and Quantum Espresso for electronic models; GROMOS, Amber and NAMD for atomistic models; Materials/Discovery Studio, GROMACS and LAMMPS for both atomistic and mesoscopic models; ABAQUS and Digimat for microFEM and FEM simulations; Aspen Plus, Aspen HYSYS, SuperPro Designer, PRO/II, gPROMS and CHEMCAD for Process Simulation; SimaPro, GaBi, openLCA and umberto for Life Cycle Assessment.

It is not strictly necessary to hierarchically follow every step from electronic models to LCA. The procedure may start at any scale, may stop before LCA and even neglect some steps if not required. The choice of the steps involved in the procedure is system-dependent.

The aim of this paper is showing how LCA perfectly fits within multiscale molecular modelling, providing the widest perspective on the material performances. Our investigation is based on the usage of various molecular modelling techniques for providing detailed inventory of a nanostructured material. The inventory data are then used to perform a comparative LCA for a material replacement in the maritime industry. It is necessary to resort to multiscale modelling techniques due to the complexity of the nanostructured materials to be designed in this project. Very few applications of the multiscale approach in support of LCA studies can be retrieved in scientific literature. Sengupta et al. [60] employed a multiscale approach to investigate

plant facilities in details, aiming at avoiding inaccurate allocations among multi-purpose production plants. The proposed framework focused on production processes and assigned inputs and outputs to specific product flows, increasing the depth of the analysis stepwise. Nevertheless, this multiscale approach provides an increasing accuracy of the production process details, not on the product itself, which is, in turn, the principal aim of our approach. The definition of system boundaries is another application where a multiscale approach supported LCA studies [28,31]. These publications deal with the integration of economy, value chain and production process within the modelling framework, using input-output models and optimization techniques for assessing the environmental impact of products. As previously mentioned, the novelty of our multiscale approach resides on the focus on the product itself, providing a detailed description of its characteristics and LCI through the usage of *in-silico* models at different scales. It is worth to mention here that in our approach a precise quantification of the uncertainty on the molecular simulation data is missing. The authors are aware that simulation uncertainty could affect the sensitivity of the LCA, although a favorable comparison with available experimental data has been performed. Given the objective complexity in quantifying uncertainty in molecular simulations, in particular for atomistic models, the authors reserve to refine this aspect in future works.

Our ecodesign study reveals useful for maritime industry, where LCA is still seldom employed. For a greener maritime sector, both navigation and shipbuilding activities need to be assessed, being the latter a well-known issue [39]. The key concepts of green shipbuilding are represented by the so-called triple R's: Reducing materials and energy consumption and pollutant emissions during ship construction; Recycling almost all parts in ship maintenance; and Reusing most of the materials at the ships end-of-life. In particular, the main purpose of green manufacturing is reducing material wastages and selecting innovative and more sustainable materials. In this circular perspective, the construction materials should be environmentally harmless, recyclable, easy to process, and require a low energy consumption [30,76]. Given these factors, metal replacement emerges as a promising practice towards green shipbuilding and the engine cylinder head cover reveals as a suitable candidate for preliminary studies. This cover is a non-structural component with the purpose of protecting mechanical tappets and injectors from external dust and containing any oil losses from the valve mechanisms. Even though the cylinder head cover is subjected to temperatures suitable for the use of plastic materials, ship classification societies require stricter heat resistance properties for materials in

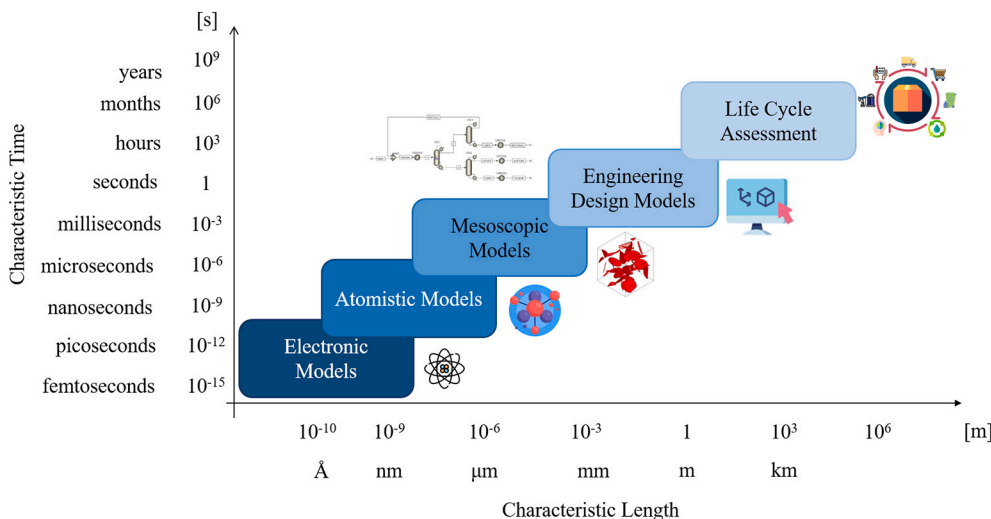


Fig. 1. Multiscale molecular modelling scheme. The axes report an approximate range of characteristic time and length scales covered by specific modelling techniques. Overlapping areas allow information exchange between models, which is usually needed for parameterization of higher scale simulations or for gaining a detailed resolution of selected portions of bigger systems.

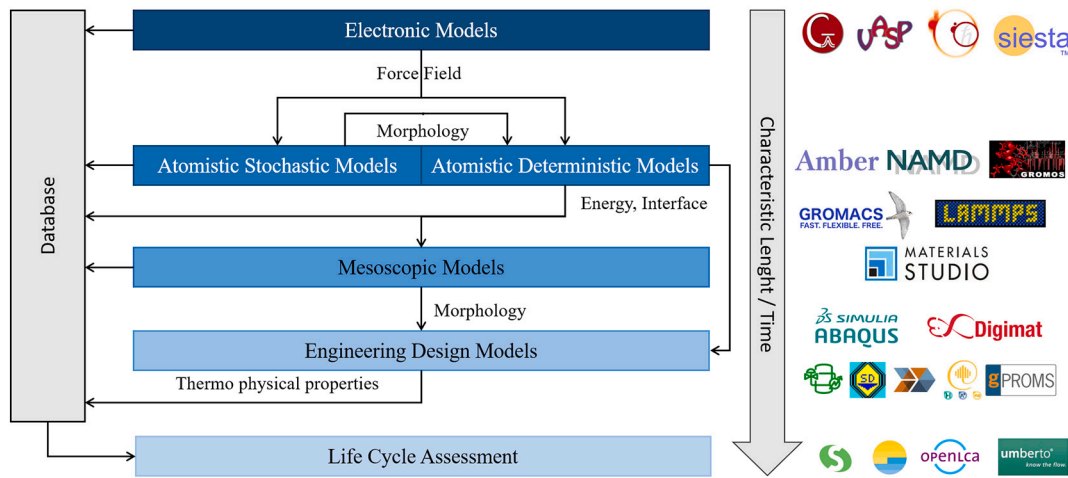


Fig. 2. Relationship among models suitable at different scales. Models can exchange information with each other or can feed data and structures to a database. On the right-hand side several available software for modelling at various scales are shown.

engine rooms. In particular, the UL 94 V-0 or V-1 classifications [65] is required in order to guarantee the fire resistance of the component and not to compromise normal and emergency operations.

The paper is organized as follows: Section 2 deals with the definition of materials under investigation and presents the techniques employed for estimation of LCI. Section 3 shows the results of Life Cycle Impact Assessment and carries on a critically discuss of the outcomes. Conclusive assertions on the study are reported in Section 4.

2. Materials and methods

2.1. Goal and scope

The aim of this study is to evaluate the replacement of a portion of an aluminium cover for a marine engine with a novel material, i.e. a nano-engineered thermoplastic polymer (NETP). The most used composites for structural marine applications are thermosetting-based materials [71], but their cost is still relatively high to justify an intensive use for non-structural components. In comparison with metal alloys, advanced NETPs benefit of lower specific weights (due to their lower volumetric mass density), easier and cheaper manufacturing technologies [66,71] and a wide variety of possible combination of materials with a broad range of mechanical and thermal properties [5,7,41].

A preliminary study has been performed aiming at defining the Key Performance Indicators (KPIs) of the novel material. The required performances can be summarized by the following specifications: “The cover must be light, fire-resistant, high-temperature resistant and it must support the weight of a standing person while the engine underneath is in operation. Furthermore, it should be economical and may provide good thermal insulation”. Although common polymers satisfy lightweight and affordability constraints, they do not guarantee enough mechanical and fire resistance performance. The former can be obtained through the inclusion of reinforcements, e.g., glass fibers (GF), which provide the required mechanical strength. The latter can be achieved through the blending with flame retardant and/or the dispersion of a sufficient amount of nanofiller within the matrix, e.g., exfoliated montmorillonite (MMT). These inclusions may increase the fire resistance above the regulation limit, which ought to be verified through specific tests according to the Fire Test Procedure (FTP) code [33] and to the provisions of the UL-94 flammability standard for plastic materials (Underwriters Laboratories [65]).

2.1.1. Material selection through Ashby model

A preliminary investigation of suitable thermoplastic polymers has

been performed via literature review [11,42,59] in combination with Ashby method [1] employed via Granta CES Selector software materials database [13]. Two aluminium alloys, with similar mechanical properties (yield strength $\sigma_Y \sim 260$ MPa, elastic modulus $E \sim 70$ GPa), have been chosen as reference materials: AA6082-T6 (wrought alloy) and AA354-T6 (cast alloy). Among the commercially available thermoplastic polymers, we excluded *a priori* all those with melting point < 200 °C and inadequate mechanical properties below 80 °C, thus narrowing the list only to polyamides (PA), polycarbonates (PC), polyethylene terephthalate (PET), polytetrafluoroethylene (PTFE), polyimide (PI), polyether ketone (PEK) and polyether ether ketone (PEEK). This shortlist of potential candidates is shown in Fig. 3, where the (density/ yield strength) vs (price) graph is shown. Ideally, the best materials are at the bottom left corner of the graph (low density, high yield strength and low price).

The materials below a straight line drawn parallel to the x-axis and passing through the reference (aluminium alloys) have an equal or better performance index than the traditional material. Only several of the unreinforced polymers (PI, PEK, PEEK) and 30% glass fibers reinforced polymers (PA, PC) are close or below this line. Nevertheless, PI, PEK and PEEK are very far right and thus they represent costly options. None of the materials shown in the graph are cheaper than the aluminium alloys. On the other hand, 30% glass fibers reinforced PA 6,6 represents a suitable candidate for metal replacement, as it shares an equivalent position with aluminium alloys on the performance axis and have a comparable price.

All these polymers exhibit lower densities with respect to that of aluminium alloys. The yield strength values are satisfactory only for PEK, PEEK and PI (40–50% of aluminium alloy σ_Y). The σ_Y of PTFE is very low (20 MPa), while those of PA, PET and PC are around 40–50 MPa (15–25% of the aluminium alloy σ_Y). Nevertheless, mechanical performances can be enhanced without rising significantly processing costs by the addition of short glass fibers. Concerning non-flammability, only PTFE, PI, PEK and PEEK fulfil the requirements without the need of flame-retardants. PA and PC are ranked as “slow horizontal burning”: they can withstand non-flammability properties with the addition of appropriate flame-retardants. PET is highly flammable and is not suitable for this application. As far as costs are concerned, PA, PET and PC lie in the same range of aluminium alloys (2–5 €/kg), while PTFE and PI (10–30 €/kg), PEK and PEEK (70–80 €/kg) are much more expensive.

As a result from previous analysis, polyamide 6,6 reinforced with 30% wt. short glass fibers (PA66 30% GF) has been selected as the best compromise between strength-to-density ratio and price. After adding appropriate flame-retardants, this compound is able to guarantee all the

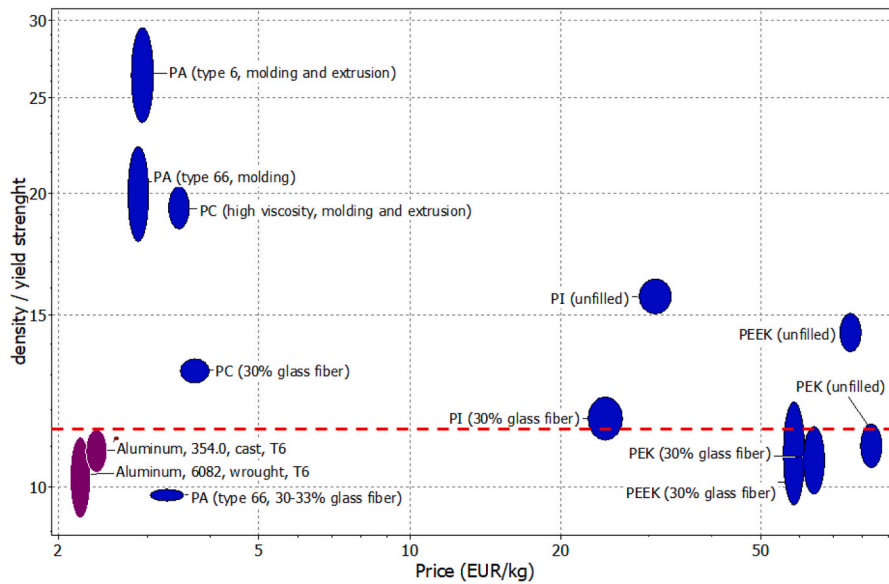


Fig. 3. Ashby chart of suitable polymer-based materials. The ones located under the red dashed line provide comparable performances with aluminium.

requirements with reasonable cost and suitable weight. PA are extensively used in injection moulded and extruded parts for engineering applications, thanks to their good mechanical properties [19,47] and can successfully be reinforced by short glass fibers and other inorganic additives [41,59].

To comply with non-flammability requirements, flame-retardants (FR) need to be blended with the matrix. Nano-sized montmorillonites (MMT) or “nanoclays” can be considered as a valid alternative to traditional FR. Nanoclays are defined as layered silicates with at least one dimension in the nanometer range intercalated by organic chains [8,50]. They are commonly used as fillers to improve many materials properties [27,46]. As the interfacial area between the polymer matrix and the nano-sized dispersed particles dramatically increase due to higher degree of exfoliation [15], these nanocomposites enhance both their mechanical and flame-retardant properties with respect to conventional composites [78].

2.1.2. Functional unit, impact categories and limitations

The lifetime of the marine engine is expected to be 30 years. However, the covers are not expected to guarantee the fulfilment of KPIs for the whole lifespan of the engine and they need to be replaced several times. Materials performances over the KPIs decay faster for NETP due to degradation and creeping of PA. Therefore, it is necessary to account for the production of a set of 4 NETP covers and a set of 3 aluminium covers in order to ensure the fulfilment of KPIs during the whole engine lifetime [10]. Accordingly, the functional unit has been defined as: “Production, use and disposal of a set of non-flammable or self-extinguishing covers, i.e. at least V-0 or V-1 according to UL-94 regulation, whose flexural elastic limit must be greater than 0.4 MPa at 110 °C. The covers need to provide satisfactory performances during the whole lifetime of the marine engine”. The cover elastic limit guarantees the support of a standing person with the engine in operation. The major limitation of our study is the lack of primary data on the mechanical and fire-resistance characteristics of each nanocomposite formulations. However, we developed a multiscale molecular modelling framework to compensate for the absence of experimental data. Moreover, due to the scarce information regarding the disposal of the covers, we assumed several end-of-life scenarios to account for different recycling ratios for aluminium, enforcing a cradle-to-grave perspective.

The LCIA phase is based on the Environmental Footprint (EF) LCIA midpoint methodology, formerly known as ILCD [25]. EF has been

chosen by the European Commission as the reference methodology for performing LCA studies within the initiative Single Market for Green Products [23]. This methodology embeds impact categories dealing with every environmental compartment and various harmful effects: (i) climate change with biogenic, fossil, land use/change and total (CC-T) perspectives; (ii) ecosystem quality which includes freshwater and terrestrial acidification (EQ-FTA), freshwater ecotoxicity (EQ-FE), eutrophication marine (EQ-EM), freshwater (EQ-EF) and terrestrial (EQ-ET); (iii) human health with regard to carcinogenic (HH-CE) or non-carcinogenic effects (HH-NCE), ionizing radiation (HH-IR), ozone layer depletion (HH-OD), photochemical ozone creation (HH-PCOC), respiratory effects (HH-RE); (iv) resources depletion in terms of dissipated water (RD-W), fossil fuels (RD-F), minerals and metals (RD-M) and land use (RD-L).

2.2. Life cycle inventory of aluminium cover

This life cycle inventory deals with the production of the covers in Europe based on ecoinvent v3.7 [73]. The calculations have been performed using of openLCA 1.10.1.

The description of aluminium life cycle is reported in detail in the Environmental Profile Report of Aluminium published by the European Aluminium Association [21].

The production processes, transports and end-of-life treatments are specific for the European scenario. Global contributions have been acknowledged for raw materials import and in case of lack of European-specific data.

A previous study reports a weight of 22.7 kg for the replaceable portion of the aluminium cover [10]. The aluminium cover under investigation is traditionally made of cast alloy and shaped through a die casting process. Raw aluminium is a blending of primary aluminium and recovered metal from re-melted scraps coming from manufacturing processes or post-consumer products. It represents the average aluminium market for cast alloy ingots in Europe. The die casting operation consists of the outpour of molten aluminium from the blending furnace to a ladle which then inject the material into the dedicated mould for final shaping of the product. The primary liquid aluminium, originally used as raw material, has been replaced by the market mix of aluminium. This required the introduction of a melting process for the post-consumer and the process scraps. Furthermore, aiming at providing an exhaustive panorama, an additional alloy

After the use and the collection phases, each recycled product is refined or remelted depending on the alloy employed (cast or wrought, respectively) enforcing the typical recycling practice of metal industry. In case recycling is not yet in place, covers are treated as they were disposed in landfill.

The life cycle inventories of the NETP constitutive materials have

Life cycle inventory for montmorillonite is based on the available raw material bentonite, which is a clay mostly constituted by three layers montmorillonite [37]. The ecoinvent reference process for bentonite production in Germany is used. Transports within European Union have been added following Eurostat transport statistics for railway, inland waterways and road freight transport of goods for the NST 2007 category “GT09 - Other non-metallic mineral products” (Eurostat). This process is followed by a milling operation aiming at reducing the

6

size of bentonite to nanometric scale: this process increases the ratio between particle surface and volume, enhancing fire resistance properties [4,53]. For its similarity with bentonite, milling operation is based on the ecoinvent process for the milling of lime in Switzerland. This process is followed by packing operation and transports, which have been calculated using the aforementioned Europe transport statistics.

Life cycle inventory of 1-pentylamine was not available in ecoinvent, therefore the process related to the production of propyl amine has been taken as a reference for similarity. The production of propyl amine follows the same path of the production of pentyl amine, both starting from an alcohol reacting with ammonia over a suitable catalyst, as reported in Ullmann’s Encyclopedia of Industrial Chemistry [58]. Therefore, in the ecoinvent reference process for the production of propyl amine in Europe, 1-propanol has been replaced with 1-pentanol coming from ecoinvent European market. Material balance has been modified according to stoichiometric ratios and reaction yields. End-of-life emissions from degradation have been calculated following the ecoinvent v3.0 guidelines recommendation [44]. Final transport has been included following Eurostat transport statistics for railway, inland waterways and road freight transport of goods for the NST 2007 category “GT08 - Chemicals, chemical products, and man-made fibers; rubber and plastic products; nuclear fuel” in the year 2016 for all countries for which data was available [24].

Since life cycle inventory of 1-octadecylamine was missing from ecoinvent database, the production process had to be modelled using proxy data. The starting raw material is a fatty carboxylic acid, i.e. stearic acid, which comes from the ecoinvent process located in Europe.

The carboxylic acid is converted to the related fatty alcohol through a catalytic hydrogenation process [2]. A similar process for the conversion of fatty acid to dodecanol via catalytic hydrogenation is available within ecoinvent database and it has been adopted as a proxy for stearyl alcohol production. Material balance have been adjusted in order to take into account stoichiometric ratios and yields. Emissions have been predicted following ecoinvent 3.0 recommendations [44] and transports have been included using European transport statistics [24].

Octadecylamine is finally produced via amination of the stearyl alcohol obtained following the pathway just mentioned. The mass balances of the ecoinvent reference process for production of propyl amine have been adjusted considering stoichiometric ratios and reaction yield for octadecylamine. Emissions and transports have been subsequently included using the same criteria as before.

The life cycle inventories of the mixing process for the production of the modified exfoliated montmorillonite (with both PAM and ODAM) have been optimized in a real production plant in collaboration with the nanoparticles manufacturer [36], obtaining primary mass and energy balances for the final production of nanoparticles. The inclusion of transports followed the procedure described above for MMT. The emission related to the disposal into unsanitary landfill of exfoliated MMT contemplate the release of clay and the total oxidation of aliphatic amines.

The final product is compounded through the extrusion of the materials followed by an injection moulding process, which have been based on the available ecoinvent processes for plastics. We assumed an adequate similarity between the available operations and the real production processes. After the use phase, a landfill disposal scenario of NETP covers has been modelled in a cradle-to-grave perspective. The cover has been conceived to be fire resistant, hence its disposal into a waste-to-energy plant is not convenient. The unsanitary dry infiltration class landfill has been chosen as it appears as a fair compromise between an open dump and a sanitary landfill. The landfill supposed scenario guarantees a more conservative approach, if compared to a waste-to-energy alternative treatment. In fact, our assumptions neglected any emission credit from an energetic recovery of the nanocomposite material.

Our investigation embodied 3 different NETP formulations, each one characterized by a specific combination of flame retardant and MMT

dispersant (Table 2). Cover 1 and 2 have been included as reference-based materials, as the former do not provide the required fire resistance, while the latter does not include MMT nanoparticles.

The schemes of the cradle-to-grave life cycle of the NETP covers are reported in Fig. 5.

2.3.1. Mechanical properties verification

We used multiscale molecular modelling techniques for estimating critical properties of the polymer-nanoclay-GF nanocomposite. Our procedure started at the atomistic scale, where we created a system composed by multiple layers of exfoliated MMT platelets surrounded by compatibilizer and polymer. Our purpose was to estimate the effects of the interface on the mechanical properties of the overall material (Fig. 6a). We used molecular dynamics (MD) to estimate the elastic modulus of the polymer-clay nanocomposite by applying external tensile stresses along the axis orthogonal with respect to the platelet surface. We then averaged the results for different degrees of platelet exfoliations, following the procedure described by Xu et al. [77]. The function describing elastic modulus of PA66 with temperature has been taken from Vlasved’s work [69]. The modelling results, which are confirmed by experiments on similar systems [3], display an enhancement factor ($E_{matrix}/E_{polymer}$) of about 50% of the elastic modulus for an inclusion of 4% wt. of MMT, i.e., from 3.1 GPa to 4.7 GPa. The material’s formulation with the lowest amount of MMT complies with the mechanical resistance KPI. Consequently, since the material’s elastic modulus increases proportionally with the amount of MMT, the conformity of nanocomposites with higher MMT contents is guaranteed. Accordingly, the following simulation steps have been performed for the material with minimum MMT inclusion only (i.e., 4% MMT wt.). The results of the atomistic simulations have been transferred to a higher simulation scale, namely the microFEM, where we used Digimat-FE (Fig. 6b). It is a finite element-based homogenization module of Digimat [17] able to generate a realistic Representative Volume Element (RVE) of a large variety of material microstructures. The useful information obtained from MD for the matrix with 4% wt. MMT are the material characteristics in terms of density, Poisson’s ratio and elastic modulus. We employed this data to investigate the influence of the GF aspect ratio, which have been added as short fibers. Simulations were executed at 110 °C, which is the compulsory working temperature of the material. Our results exhibit a realistic elastic modulus of 3.2 GPa for a GF aspect ratio of 10, which is in good agreement with experimental values [16]. Finally, we used our previous results to execute further analysis on the finite element (FE) model developed by Bertagna et al. [10] as shown in Fig. 6c. Our aim was to verify the mechanical resistance of the shaped material under the specific stress scenario of an average person standing on the cover. Therefore, the model was tested under the application of a static load consisting in a vertical load equal to 2000 N (representing the load of a person applied on the cover lid) and two vertical loads, each equal to 6000 N (representing the tightening loads applied on the two bushings of the cover lid). The model mesh was based

Table 2
Overall composite material formulations developed in this study. PA66: nylon 66, GF: Glass Fibers; TPP: Triphenyl phosphate MMT: exfoliated montmorillonite; PAM: 1-pentylamine; ODAM: 1-octadecylamine. The values reported are % wt.

#	1	2	3	4	5
ID	PA66GF	PA66GF-FR1	PA66GF-FR2	PA66GF-FR3	PA66GF-FR4
PA66	70	56	58.8	57.4	59.5
GF	30	30	30	30	30
TPP		14	8.4	8.4	7
MMT + PAM			2.8	4.2	
MMT + ODAM					3.5

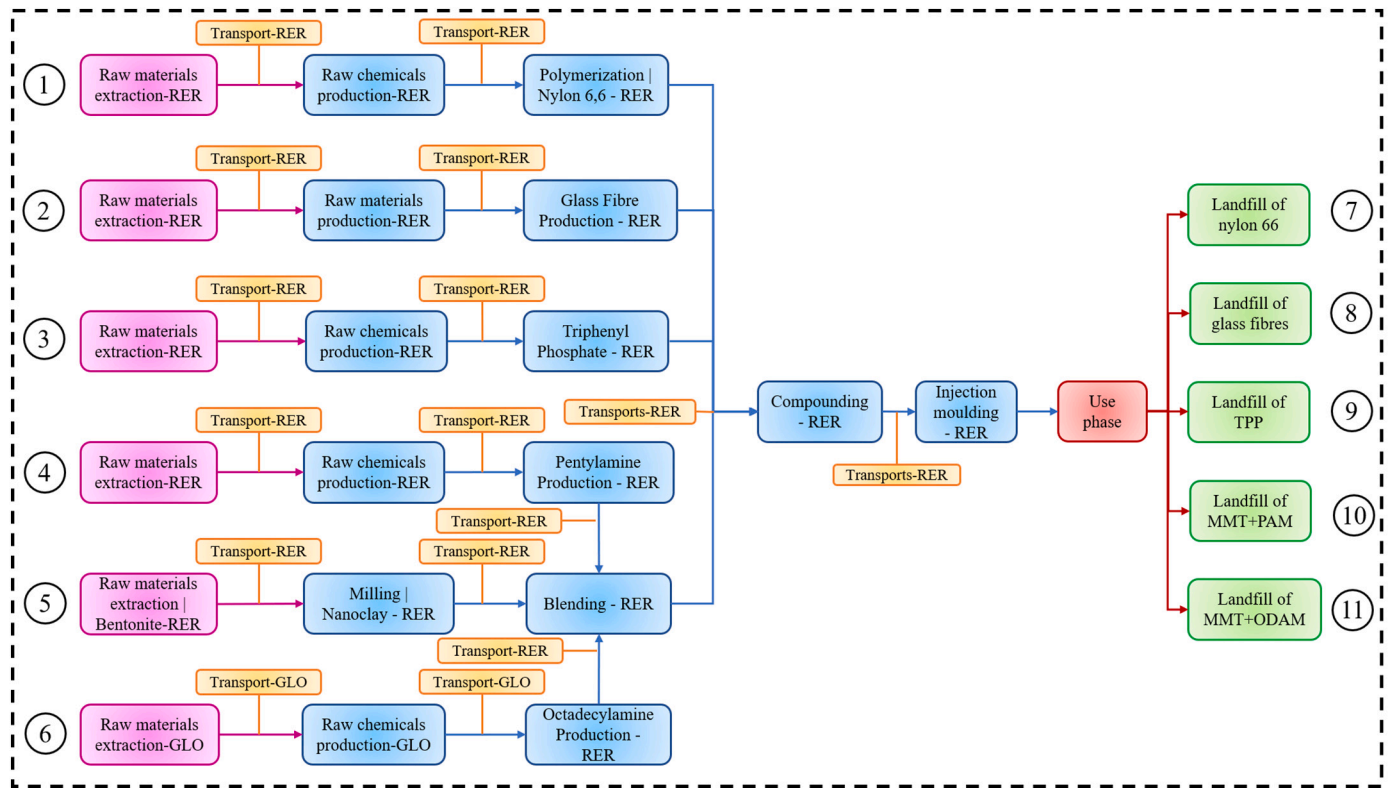


Fig. 5. Comprehensive flowsheet for the description of life cycle stages of the various formulations under investigation. Each material follows dedicated branches related to constitutive raw materials: PA66GF: 1,2,7,8; PA66GF-FR1: 1,2,3,7,8,9; PA66GF-FR2: 1,2,3,4,5,7,8,9,10; PA66GF-FR3: 1,2,3,4,5,7,8,9,10; PA66GF-FR4: 1,2,3,5,6,7,8,9,11.

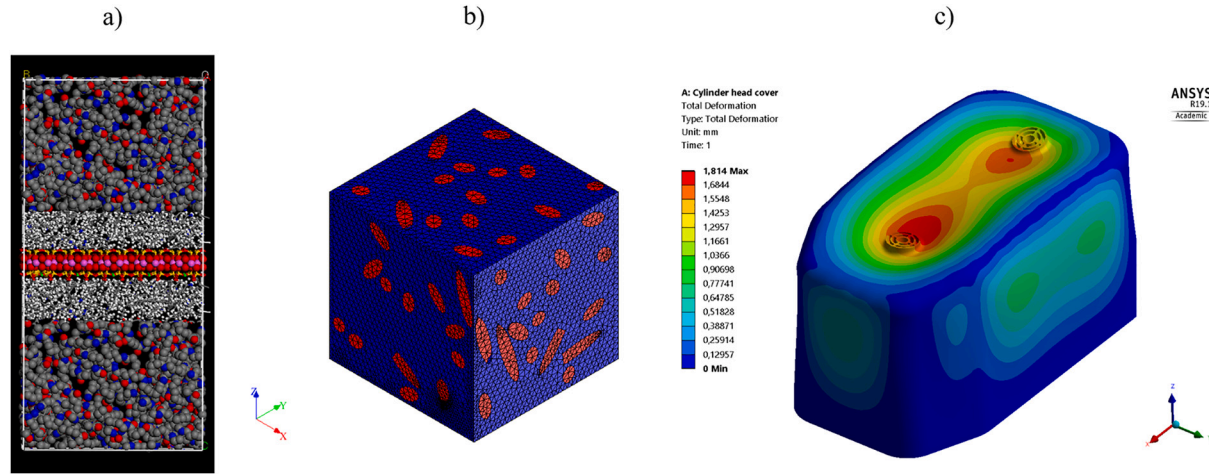


Fig. 6. Material appearance at the various scales from atomistic model (a), to microFEM (b) to the finite element (FEM) representation (c).

on an unstructured grid involving tetrahedral solid elements and was refined in nearness of geometry and curvature changes. The maximum local thickness of the model was set as the maximum size of the mesh elements. The entire cover model was fully fixed at the base by constraining all the degrees of freedom. Furthermore, contact bonds were applied to all the surfaces in order to avoid sliding and separation between faces. The results of the FE simulation were evaluated in terms of total deformation, maximum stress and strain, and the values resulted to be far lower than the threshold limits. Thanks to our *in-silico* outcomes, we defined the weight of 11.7 kg for the NETP replacing cover. Input file of Digimat SW used in this work is included in Appendix A.

2.3.2. Thermal properties verification

The flame resistance properties have been tested experimentally, using a sample of PA66GF-FR4 obtained by melt compounding 85% of Denyl-66 (a Vamptech product composed by 70% PA 66 with 30% GFs, % wt.) with exfoliated MMT (5%) and phosphate-based FR (10%) [16]. This formulation embeds the minimum amount of traditional FR among the available materials and represents the most critical NETP from a flame resistance viewpoint. Exfoliated MMT were obtained from high-grade bentonite (98% purity) functionalized with 1-octadecylamine to enhance the degree of exfoliation and favor the proper dispersion of the platelets inside the hosting polymeric matrix. The experimental tests revealed the material compliance to UL94-V1 class, *i.e.* a self-

extinguishing material without dropping flammable material, which provided the necessary evidence for flammability resistance KPI.

3. Results and discussion

Our first task was identifying the most sustainable formulation among the available NETP. The chosen material was then used for the manufacturing of 4 head covers, which were involved in a comparative study with 3 aluminium head cover produced by different manufacturing processes, *i.e.* casting and rolling. It is worth underlining that, albeit the number of NETP covers is greater than aluminium ones (4 *versus* 3, respectively), the weight of total material involved is higher for aluminium (68.1 kg) than NETP (35.1 kg): this contributes to worsen the aluminium impact assessment performance. Another drawback related to heavier aluminium products is the need for cranes to lift and handle the covers, which causes an additional life cycle impact that has not been accounted in this study. Several end-of-life scenarios for the aluminium covers have been evaluated, focusing on the sensitivity of the results in relation with the amount of aluminium covers reintroduced in a circular recycling loop.

3.1. Identification of the optimal NETP

The comparison among NETP has been performed considering a single cylinder head cover made of 11.7 kg of nanocomposite material. The results are reported in Table B.1 of Appendix B, while Fig. 7 shows the relative performance normalized to the maximum value for each impact category *via* a radar plot.

Worst performances are gained by the formulations with greater values for each impact category. Since none of the formulations performed best in every impact category, a compromise has to be identified in order to choose the most sustainable alternative. The material without flame retardants (PA66GF) has been included as a reference, since it is not compliant with maritime usage regulations. It is evident how the introduction of traditional phosphate-based flame retardant (PA66GF-FR1) worsens the material performance in terms of freshwater eutrophication (EQ-EF), human health (HH-CE, HH-NCE, HH-IR, HH-OD) and resource depletion (RD-L, RD-M). On the other hand, it improves the results with regard to marine eutrophication EQ-EM (due to the lower usage of nitrogen-based polyamide) and water consumption (RD-W). Aiming at reducing the impacts induced by traditional flame retardants, a quota of TPP has been replaced with exfoliated MMT as previously reported in Table 1, looking for a trade-off between benefits and drawbacks. The three NETP covers impacts are generally in between the ones related to the maximum (PA66GF-FR1) and minimum (PA66GF)

amount of phosphate-based flame retardants. Their values are comparable in most categories, meaning that the compatibilizer used for exfoliation (PAM or ODAM) does not affect substantially the final impact assessment, as the mass involved appears negligible. Indeed, it is the amount of traditional FR that mostly influences the performance of each formulation, particularly regarding freshwater eutrophication (which is minimum for the material with lowest amount of FR). Since the differences among NETP on the other impact categories look negligible, PA66GF-FR4 has been elected as the most environmental-friendly formulation and it has been compared with traditional aluminium alloys in order to highlight the advantages and drawbacks of material substitution.

3.2. Comparison between NETP and aluminium covers

The comparison among 4 covers made of PA66GF-FR4 and 3 covers made of cast or wrought alloys (as specified in the functional unit description) is presented in this section.

Since the amount of recovered aluminium is based on secondary data, we performed a sensitivity analysis considering different amount of metal recovered, while the conservative scenario of NETP landfilling is kept fixed. Four different scenarios have been implemented, each one representing different recycling practice for aluminium covers. The LCIA results are reported in Tables B.2–5 of Appendix B and are strongly influenced by the amount of aluminium recovered. The end-of-life impacts allocation for metal products follows the substitution method [22]. It means that if the inherent metallic properties are maintained, the emission related to the incoming portion of recycled aluminium can be neglected, since only the metal loss during the complete life cycle of the product must be taken into account. Furthermore, the incoming recycled aluminium have to be handled with the same methods used for treating recycled metal leaving the system.

In order to implement this approach, while accounting for ecoinvent market mix for each alloy, raw database processes have been used for a non-recycling scenario only. In this first scenario, primary metal share of raw materials (which is around 26% and 70% for cast and wrought alloys, respectively) is kept fixed and considered landfilled at the end-of-life of the covers. This scenario is represented by Fig. 8,a) where the contribution of primary metal content to impact categories reveals crucial. In fact, the set of covers made of wrought alloy scores the highest values for the majority of impacts, due to the massive usage of primary metal. As predictable, NETP covers set appears as the more environmental-friendly solution overall, despite it reveals detrimental for water consumption (RD-W) and for eutrophication (EQ-EF,EM) due to the nitrogen and phosphorous emissions related to decomposition of

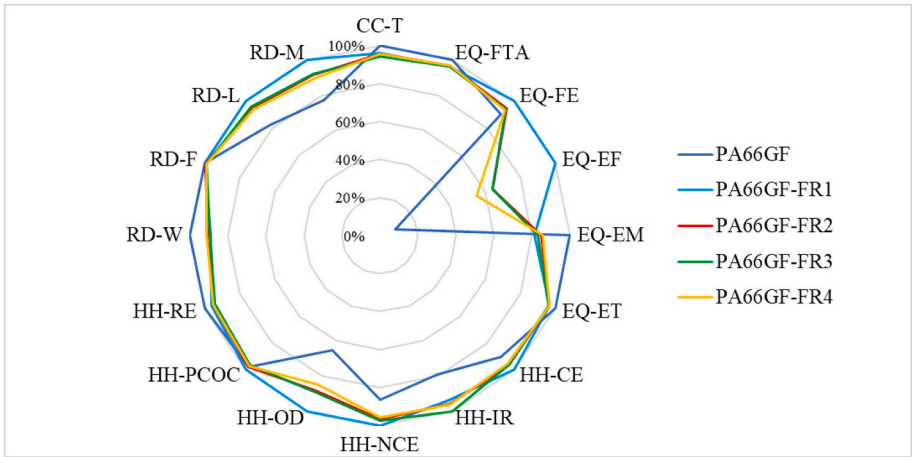


Fig. 7. Comparison among different NETP products. Each category has been normalized to 100, meaning that the formulation with highest impact scores 100 and resides on the border of the polygon. Other formulations scale their values in relation to the maximum on each category.

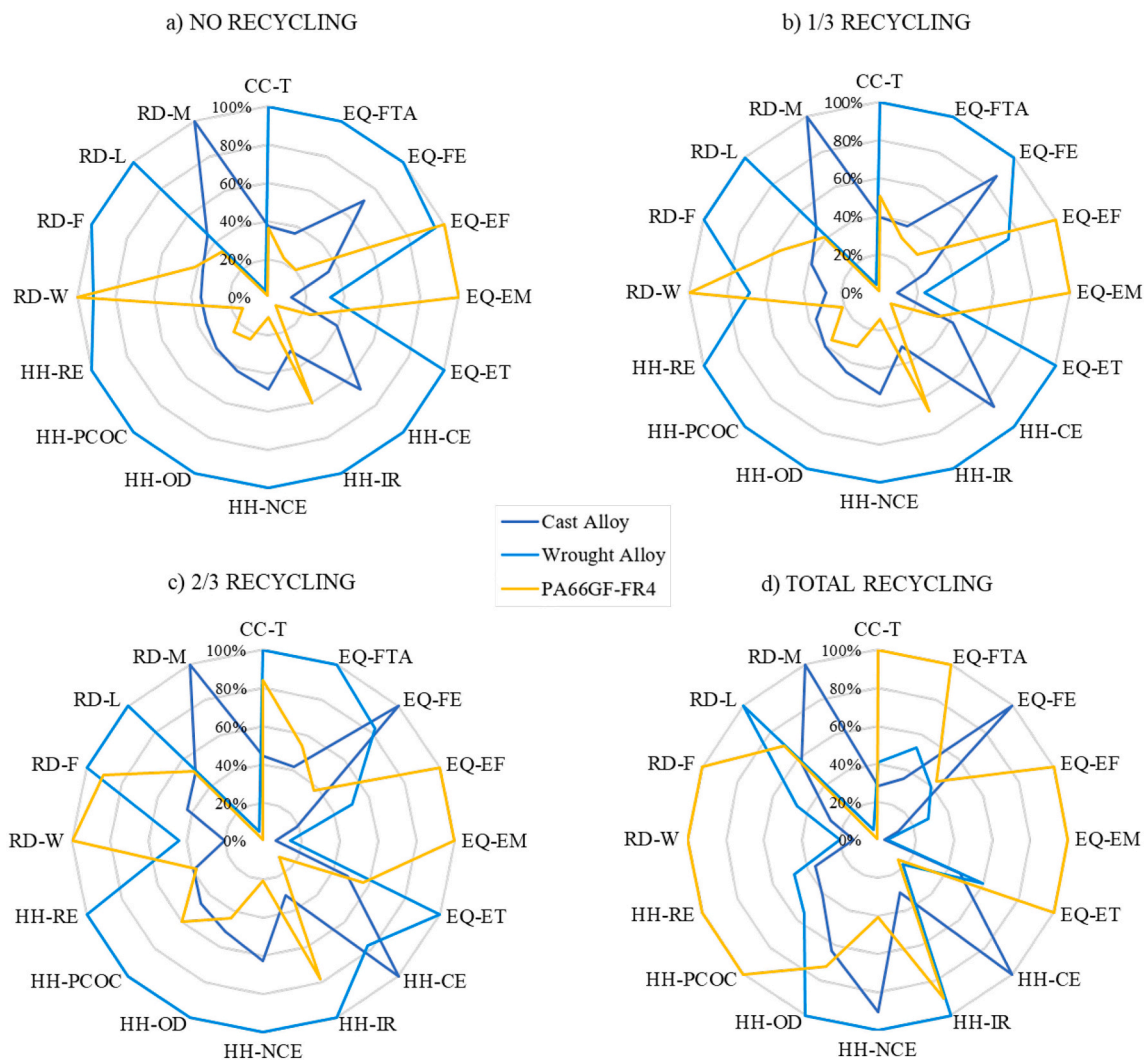


Fig. 8. Comparison among PA66GF-FR4, cast alloy and wrought alloy products. Each category has been normalized to 100, meaning that the material with highest impact scores 100 and resides on the border of the polygon. Other materials scale their values in relation to the maximum on each category. a) none of the aluminium cover is reintroduced into the life cycle of aluminium (MCI: Cast = 0.739; Wrought = 0.304) b) one out of the three aluminium covers is reintroduced into the life cycle of aluminium (MCI: Cast = 0.800; Wrought = 0.496) c) two out of the three aluminium covers are reintroduced into the life cycle of aluminium (MCI: Cast = 0.886; Wrought = 0.716) d) The aluminium covers are completely reintroduced into the metal supply chain (MCI: Cast = 0.97; Wrought = 0.929).

polyamide and traditional flame retardants. Quite unexpectedly, the depletion of metals and minerals (RD-M) category is far higher for cast aluminium than for wrought one, even if the recycled content of the former is much greater. A further investigation revealed that the treatment of aluminium scraps includes a zinc usage, whose extraction provided the major contribution to this impact category.

So far, the end-of-life of aluminium covers did not foresee a reintroduction into the circular economy of metal. However, decreasing the usage of primary aluminium is fundamental for the reduction of impacts related to shipbuilding and manufacturing. In this perspective, we developed a series of scenarios where aluminium covers recycling process has been implemented. As prescribed by the substitution method, we reduced the amount of primary aluminium related to the manufacturing of products, introducing a higher amount of recycled aluminium.

We employed an established circularity indicator to account for the increasing amount of recycled aluminium for both cast and wrought aluminium alloys in the different end-of-life scenarios considered. The Material Circularity Indicator (MCI) [20] accounts for the input of virgin/recycled raw materials, the utility during use phase, the destination after use and the efficiency for recycling. The MCI takes values between

0 and 1 where higher values indicate a higher circularity. The MCI values calculated for each end-of-life scenario are reported in Table 3. The MCI value for no recycled covers equals the secondary aluminium value for ecointent market mix for the specific alloy. The MCI values calculated for completely recovered covers scenarios are different than 1 due to metal losses during recovery treatment or manufacturing of the products.

Environmental burdens have been allocated according to the polluter-pays-principle, which assigns the manufacturing emissions to

Table 3
Calculated MCI values for different end-of-life scenarios for aluminium covers.

Material	Recycled Covers	MCI
Al - Cast Alloy	0/3	0.739
	1/3	0.800
	2/3	0.886
	3/3	0.970
Al - Wrought Alloy	0/3	0.304
	1/3	0.496
	2/3	0.716
	3/3	0.929

the process that generate them at first instance [45]. The decrease of primary aluminium has been performed stepwise, implementing the recovery of each of the three covers incrementally. The primary aluminium savings have been converted into post-consumer scraps contributions, aiming at including the same amount of material for each scenario. This procedure should provide an indication of the minimum quota of recycled covers that promotes the substitution of traditional covers, as well as the minimum value of MCI that guarantees an advantage in terms of environmental performance.

The results of each scenario are reported in the radar plots of Fig. 8, b),c),d).

The recovery of a single cover impacts poorly (Fig. 8,b)) if compared to the no-recycling scenario, as the different materials hold roughly the same positions among the majority of impact categories.

With a further increase of the recycled amount, several impact categories turn favorable for aluminium, as shown in Fig. 8,c). Eutrophication (both freshwater and marine, i.e. EQ-EF, EM) decreases decisively for aluminium covers and while wrought alloy covers still score higher impact in most of the impact categories, cast alloy covers become the best choice for several impact categories, e.g., climate change (CC-T), acidification (EQ-FTA), depletion of fossil sources (RD-F) and photochemical ozone creation (HH-PCOC).

The last scenario foresees a complete recovery of covers material. In this case, the introduction of primary metal is not required for manufacturing a novel product, since the available metal in the market satisfies the manufacturing needs. The related radar plot is reported in Fig. 8,d) which exhibits impressive differences when compared to the other scenarios. The covers made of NETP appear as the worst solution for the majority of ecosystem quality impact categories (EQ-FTA, EF, EM, ET), human health impact categories (HH-PCOC, RE), resource depletion categories (RD-W,F) and climate change (CC-T). Besides that, cast alloy covers set appears as the best choice thanks to the rather satisfactory results in comparison with wrought alloy one. Indeed, the latter gains better results regarding freshwater ecotoxicity (EQ-FE), human health carcinogenic effects (HH-CE) and metal resource depletion (RD-M), while the former provides lower impacts among all the other environmental categories.

It clearly appears how the number of aluminium covers reintroduced into the circular life cycle of the metal reveals as the main criterion for assessing whether a substitution with NETP covers generates lower environmental impacts. Sure enough, in the event that one or less out of the three aluminium products are recovered (e.g., during dismantling of the ship), the best performances in terms of environmental impact assessment are exhibited by the NETP covers among the majority of impact categories. As the number of recovered aluminium covers increases to two, the metal cylinder head covers become progressively the greener choice, providing a lower effect on each natural compartment. This evidence is confirmed when primary aluminium is completely neglected in favor of post-consumer scraps, meaning that the aluminium already distributed in the global market is able to fulfil the metal needs for novel products. In this virtuous scenario, promoted by the green shipbuilding approach, the cast aluminium alloy reveals as the most environmental-friendly material among the greater number of impact categories. This result is mainly driven by the availableecoinvent data regarding the addition of different alloying metals to the aluminium scrap during recycling treatment, such as zinc for cast alloy and copper for wrought aluminium products. Since the lack of primary data is the major limitation of this study, stakeholders should apply caution and take into account primary data availability and specific alloy compositions. Taking the ecoinvent market mix for granted, eutrophication impact categories suffer the presence of a considerable amount of nitrogen and phosphorus within the polymer matrix and the flame retardant, exhibiting a higher value for NETP product system. However, as a result from this investigation, NETP covers set achieves higher

performances in terms of diminishing environmental impact in comparison with aluminium covers set, when an efficient recycling scenario for aluminium is not yet in place.

4. Conclusions

The aim of our study is showing the potential application of *in-silico* techniques for generating life cycle inventories. The integration of life cycle assessment within the multiscale molecular modelling framework provided a novelty with a twofold contribution: i) we broaden the horizons of multiscale molecular modelling including the widest possible perspective, and ii) we employed an innovative methodology for future life cycle assessment applications. The presented methodology reveals extremely valuable for advanced and innovative materials requiring an evaluation in terms of environmental footprint. This peculiar application has been validated through the development of a case study, focusing on a material replacement in the maritime sector. We first generated a polymer (nylon 66) filled with nanoparticles (exfoliated montmorillonite) using atomistic simulations. We then transferred the results to micro-FEM, where we created the composite material under investigation (NETP). Specifically, we assigned the material properties obtained from the atomistic simulations to the composite matrix, while as fillers we used short glass fibers randomly dispersed in the matrix. After calculating the mechanical properties of the desired formulation, we performed a FEM analysis to ensure the fulfilment of a mechanical resistance KPI. The amount of the substances (nylon 66, glass fibers, montmorillonite, exfoliating agents, traditional flame retardant) used for NETP manufacturing and gained through the aforementioned *in-silico* techniques have been implemented within life cycle assessment procedure for generating the inventories of materials under investigation. We then performed a life cycle assessment of several nanostructured materials, identifying the most environmental-friendly NETP. Finally, we compared the selected NETP with traditional materials (aluminium alloys) under various disposal scenarios. The procedure applied in this work is rather general and can be applied to complex nanostructured polymer systems, enabling the practitioner to estimate out-of-market formulations in case of particular needs. Future development will deal with the generation of interconnected models typical of each simulation scale, starting from the smallest one up to the Life Cycle Assessment perspective.

CRedit authorship contribution statement

Andrea Mio: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Visualization, Writing – original draft. **Serena Bertagna:** Data curation, Software, Writing – original draft. **Luca Cozzarini:** Investigation, Data curation, Writing – original draft. **Erik Laurini:** Data curation, Methodology, Software, Validation. **Vittorio Bucci:** Writing – review & editing. **Alberto Marinò:** Writing – review & editing. **Maurizio Fermeglia:** Conceptualization, Project administration, Resources, Supervision, Validation, Writing – review & editing.

Declaration of Competing Interest

None.

Acknowledgment

The authors have no conflicts of interest to declare that are relevant to the content of this article.

Part of the work was supported by “PLASTICO – Plastic Cover for Marine Engine” research program, funded by the Regione Autonoma Friuli Venezia Giulia with POR-FESR 2014–2020, Asse 1 Azione 1.3.b.

Appendix A

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Table B.1

LCIA results using EF methodology for the comparison of the suitable NETP formulations.

Indicator	PA66GF	PA66GF-FR1	PA66GF-FR2	PA66GF-FR3	PA66GF-FR4	Unit
CC-T	112.94	108.39	107.91	106.76	107.83	kg CO2-Eq
EQ-FTA	0.4241	0.4085	0.4100	0.4076	0.4104	mol H + -Eq
EQ-FE	56.07	62.07	58.84	58.42	58.04	CTU
EQ-EF	0.02	0.19	0.12	0.13	0.11	kg P-Eq
EQ-EM	1.13	0.92	0.96	0.94	0.97	kg N-Eq
EQ-ET	0.8036	0.7786	0.7774	0.7717	0.7771	mol N-Eq
HH-CE	1.04E-06	1.15E-06	1.10E-06	1.10E-06	1.09E-06	CTUh
HH-IR	7.03	8.38	8.55	8.90	8.59	kg U235-Eq
HH-NCE	4.95E-06	5.74E-06	5.54E-06	5.60E-06	5.49E-06	CTUh
HH-OD	2.29E-06	3.51E-06	3.09E-06	3.12E-06	2.98E-06	kg CFC-11-Eq
HH-PCOC	0.242	0.247	0.241	0.239	0.240	kg NMVOC-Eq
HH-RE	3.21E-06	3.08E-06	3.05E-06	3.01E-06	3.05E-06	disease incidence
RD-W	95.09	84.67	86.29	85.01	86.69	m3 water-Eq
RD-F	1554.72	1554.99	1541.68	1535.08	1538.19	MJ
RD-L	334.03	405.25	385.46	389.80	380.48	points
RD-M	8.57E-04	1.11E-03	1.02E-03	1.02E-03	9.95E-04	kg Sb-Eq

Table B.2

LCIA results using EF methodology for the comparison of alternative materials covers with a recycled quota of aluminium covers of 0%.

Indicator	Cast	Wrought	PA66GF-FR4	Unit
CC-T	441.94	1185.13	431.31	kg CO2-Eq
EQ-FTA	2.7071	7.4695	1.6414	mol H + -Eq
EQ-FE	808.12	1129.47	232.16	CTU
EQ-EF	0.15	0.41	0.43	kg P-Eq
EQ-EM	0.48	1.27	3.88	kg N-Eq
EQ-ET	5.0144	12.8886	3.1083	mol N-Eq
HH-CE	5.06E-05	7.39E-05	4.37E-06	CTUh
HH-IR	17.50	57.35	34.36	kg U235-Eq
HH-NCE	1.00E-04	2.06E-04	2.20E-05	CTUh
HH-OD	2.10E-05	5.00E-05	1.19E-05	kg CFC-11-Eq
HH-PCOC	1.435	3.756	0.959	kg NMVOC-Eq
HH-RE	2.95E-05	8.41E-05	1.22E-05	disease incidence
RD-W	122.48	317.63	346.77	m3 water-Eq
RD-F	5478.40	14,803.80	6152.76	MJ
RD-L	2016.68	4471.29	1521.92	points
RD-M	3.97E-01	1.45E-02	3.98E-03	kg Sb-Eq

Table B.3

LCIA results using EF methodology for the comparison of alternative materials covers with a recycled quota of aluminium covers of 33%.

Indicator	Cast	Wrought	PA66GF-FR4	Unit
CC-T	336.29	854.01	431.31	kg CO2-Eq
EQ-FTA	2.0036	5.2980	1.6414	mol H + -Eq
EQ-FE	717.87	828.35	232.16	CTU
EQ-EF	0.11	0.31	0.43	kg P-Eq
EQ-EM	0.37	0.91	3.88	kg N-Eq
EQ-ET	3.8378	9.2589	3.1083	mol N-Eq
HH-CE	4.36E-05	5.13E-05	4.37E-06	CTUh
HH-IR	15.53	50.75	34.36	kg U235-Eq
HH-NCE	8.32E-05	1.56E-04	2.20E-05	CTUh
HH-OD	1.76E-05	3.88E-05	1.19E-05	kg CFC-11-Eq
HH-PCOC	1.091	2.693	0.959	kg NMVOC-Eq
HH-RE	2.12E-05	5.84E-05	1.22E-05	disease incidence
RD-W	96.82	236.10	346.77	m3 water-Eq
RD-F	4219.81	10,861.80	6152.76	MJ
RD-L	1760.39	3730.75	1521.92	points
RD-M	4.16E-01	1.89E-02	3.98E-03	kg Sb-Eq

Table B.4

LCIA results using EF methodology for the comparison of alternative materials covers with a recycled quota of aluminium covers of 67%.

Indicator	Cast	Wrought	PA66GF-FR4	Unit
CC-T	227.44	512.85	431.31	kg CO2-Eq
EQ-FTA	1.2787	3.0607	1.6414	mol H + -Eq
EQ-FE	624.89	518.12	232.16	CTU
EQ-EF	0.08	0.22	0.43	kg P-Eq
EQ-EM	0.25	0.55	3.88	kg N-Eq
EQ-ET	2.6256	5.5193	3.1083	mol N-Eq
HH-CE	3.63E-05	2.80E-05	4.37E-06	CTUh
HH-IR	13.51	43.96	34.36	kg U235-Eq
HH-NCE	6.58E-05	1.05E-04	2.20E-05	CTUh
HH-OD	1.40E-05	2.73E-05	1.19E-05	kg CFC-11-Eq
HH-PCOC	0.737	1.598	0.959	kg NMVOC-Eq
HH-RE	1.27E-05	3.20E-05	1.22E-05	disease incidence
RD-W	70.39	152.10	346.77	m3 water-Eq
RD-F	2923.09	6800.38	6152.76	MJ
RD-L	1496.34	2967.77	1521.92	points
RD-M	4.36E-01	2.33E-02	3.98E-03	kg Sb-Eq

Table B.5

LCIA results using EF methodology for the comparison of alternative materials covers with a recycled quota of aluminium covers of 100%.

Indicator	Cast	Wrought	PA66GF-FR4	Unit
CC-T	121.79	176.57	431.31	kg CO2-Eq
EQ-FTA	0.5752	0.8661	1.6414	mol H + -Eq
EQ-FE	534.65	211.41	232.16	CTU
EQ-EF	0.05	0.12	0.43	kg P-Eq
EQ-EM	0.14	0.20	3.88	kg N-Eq
EQ-ET	1.4490	1.8496	3.1083	mol N-Eq
HH-CE	2.93E-05	5.31E-06	4.37E-06	CTUh
HH-IR	11.54	38.13	34.36	kg U235-Eq
HH-NCE	4.90E-05	5.41E-05	2.20E-05	CTUh
HH-OD	1.05E-05	1.66E-05	1.19E-05	kg CFC-11-Eq
HH-PCOC	0.394	0.524	0.959	kg NMVOC-Eq
HH-RE	4.35E-06	5.81E-06	1.22E-05	disease incidence
RD-W	44.74	70.02	346.77	m3 water-Eq
RD-F	1664.50	2850.38	6152.76	MJ
RD-L	1240.06	2171.55	1521.92	points
RD-M	4.55E-01	2.73E-02	3.98E-03	kg Sb-Eq

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