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Multiscale modelling techniques in Life Cycle Assessment: application to product design

Andrea Mio[a]*, Maurizio Fermeglia[a]

[a]*Molecular Biology and Nanotechnology Laboratory (MolBNL@UniTS), Department of Engineering and Architecture, University of Trieste, Italy*

* Corresponding author. Tel.: +390405583440. E-mail address: amio@units.it

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Abstract

This paper aims at broadening the perspective in life cycle assessment methodology, exploiting multiscale modelling towards the generation of life cycle 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 complex materials and production processes. In particular, each simulation is performed at a specific length and time scale through dedicated software, passing information from the lower to the upper scale.

A practical application of the proposed approach will be illustrated for property predictions of nanostructured polymer systems used for manufacturing a marine engine cover. The material formulations capable of fulfilling the marine thermomechanical constraints were defined using *in-silico* techniques, allowing for the generation of materials life cycle inventories, which have been compared to identify the most environmentally friendly option.

Keywords: Life Cycle Assessment; LCA; Multiscale Molecular Modelling; Product Design; Life Cycle Inventory

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Nomenclature

CC-T: Climate Change - Total
CF: Carbon Fibers
EQ-A: Ecosystem Quality - Acidification
EQ-EF: Ecosystem Quality - Eutrophication Freshwater
EQ-EM: Ecosystem Quality - Eutrophication Marine
EQ-ET: Ecosystem Quality - Eutrophication Terrestrial
EQ-FE: Ecosystem Quality - Freshwater Ecotoxicity
FEM: Finite Element Method
FR: Flame Retardant
GF: Glass Fibers
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-PCOF: Human Health-Photochemical Ozone Formation
HH-PM: Human Health – Particulate Matter
KPI: Key Performance Indicator
MD: Molecular Dynamics
MMT: Montmorillonite
NETP: Nano-Engineered Thermoplastic Polymer
ODAM: Octadecyl amine
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
TPP: Triphenyl phosphate

1. Introduction

One of the major challenges of life cycle assessment (LCA) is in the generation of life cycle inventories for complex or novel processes and products, such as nano-bio materials. Existing databases supporting LCA studies rarely include reliable data for

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such systems and consequently it is necessary to predict the properties of new materials and perform material and energy balance for the production processes. Despite the tremendous advances in the modelling of structural, thermal, mechanical and transport properties of materials at the macroscopic level, there remains a high level of uncertainty about how to predict many critical properties related to advanced materials, which strongly depend on nanostructure.

On the other hand, process simulators emerged as powerful tools for solving the material and energy balances for any production process. Specifically, they can deal with innovative processes for the production of nano-bio materials involving batch operations, complex separations and reactions. These *in-silico* techniques may be useful to LCA practitioners, particularly when real specific data is missing.

The life cycle assessment technique is a widespread methodology for estimating the environmental consequences caused by organizations, human activities and products manufacture, use, and disposal. The LCA regulatory framework and standards are internationally recognized and outlined by The International Organization for Standardization (ISO) 14040 and 14044 guidelines[1,2]. Material and energy balances of the product's full life cycle, which includes raw material extraction, manufacture, distribution, use phase, recycling, final disposal, and transit between life cycle phases, are used in the manufacturing industry. The findings of life cycle assessments are reported using a variety of impact categories, with the goal of assessing the complete range of ecological consequences associated with a product system to each environmental compartment. The description of LCA framework, along with its advantages and drawbacks, is extensively discussed on a series of publications [3,4].

Reap et al. [5,6] addressed the difficulties and obstacles associated with the LCA technique, bringing light on the unresolved methodological elements that still require accepted agreement within the scientific community. Collecting data for life cycle inventory (LCI), for instance, is generally a difficult task for practitioners. While reliable primary data is desirable, when case-specific information is lacking, it is standard practice to rely on recognized databases, such as ecoinvent [7] or Gabi[8]. However, even though current databases include a wide range of information, data on innovative materials or unusual production methods is still lacking. In the event of insufficient data, ISO recommends using proxy inventories, i.e., the mass and energy balances of equivalent products/processes. Surely, the accuracy of the final outcomes is determined by the resemblance between the two systems. Therefore, several *in-silico* modelling approaches have been used to estimate LCI of products in order to reduce the inaccuracy of proxy data. Process modelling [9–12], dedicated frameworks [13,14], molecular structure-based models [15] or artificial neural networks [16] are some examples of computational approaches for generating raw materials inventories thus far.

The multiscale molecular modelling paradigm, which includes some of the aforementioned *in-silico* techniques as well as others, provides a full collection of material properties, such as mechanical, thermal, electrical, magnetic, and toxicological properties [17]. Multiscale molecular modelling, by definition, involves the generation of computational models at several length and temporal scales, which are frequently unconnected theoretically. Multiscale molecular modelling permits all phenomena to be captured at each scale, with the essential information being transferred to the upper scale until the macroscopic system is achieved [18].

Traditionally, the macroscopic model used to be the largest model to be developed, using methods and tools familiar to industrial engineers for the design of complex materials, such as process simulations or finite-element technique. For the investigation of novel and well-known materials, however, there is a broader outlook accessible, namely the life cycle perspective. The variety of methods and models commonly employed in the multiscale modelling hierarchy are shown in Fig. 1, where the life cycle assessment technique has been introduced on the top right corner.

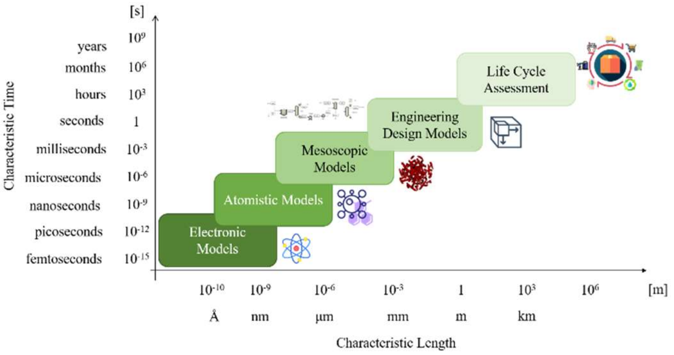

Fig. 1: Multiscale molecular modelling scheme

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

- *Electronic models* (10^{-10}-10^{-9} m and 10^{-12} s): quantum-mechanical interactions between nuclei and electrons are simulated at this scale, giving information such as conductive/dielectric or optical properties, activation energies and chemical reaction coefficients, properties of atomic defects and dopants, magnetic anisotropy, diffusion coefficient, and more.
- *Atomistic models* (10^{-10}-10^{-7} m and 10^{-12}-10^{-6} s): atomistic models explicitly depict atoms or, in certain cases, small ensembles of atoms referred to as beads. Potential energy calculation based on well-established force fields is used to determine their interactions. Each force field is suitable for peculiar systems and is generally based on bonded and non-bonded interactions. The general outcomes from atomistic models comprise 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 features are implicitly implemented by a field-based or particle-based description. This enables the simulation of phenomena on length and time scales that were previously restricted to traditional atomistic methods, such as system morphology, domain creation and growth kinetics, thermal stability, rheological and magnetic behaviour. MicroFEM simulations allows to calculate physical and mechanical properties using an approach commonly employed by continuum models, after the density distribution of beads at mesoscopic scale is mapped.

- *Engineering design models* (10^{-3}-10^{1} m and 10^{1}-10^{3} s): these models are classified as continuum models because they assume a continuous distribution of material inside the simulated volume. The behaviour of the physical system is no longer impacted by atomic and molecular structures since constitutive principles hold true at these time and length scales. This enables for the analysis of materials with unusual shapes (using the Finite Element Method – FEM) or the processing of substances based on their macroscopic thermodynamic properties (using process simulation). Heat and mass transfer coefficients, chemical reaction kinetics, and macroscopic structural and mechanical information are some of the typical properties obtained by these models.

Each model's output can be utilized as input to larger-scale models or stored in a database along with literature or experimental data. The relationships among models at different scales are shown in Fig. 2, where several software packages available at each modelling scale are reported.

It is not mandatory to follow every step from electronic models to LCA in a hierarchical order. The procedure may initiate at any scale, end before LCA, and even skip certain steps if they aren't necessary. The choice of the steps involved in the procedure is system-dependent and can be adapted to the purpose of the study. In this context, LCA perfectly fits within multiscale modelling, providing the widest possible perspective.

To demonstrate the benefit of this approach, we evaluated the environmental performances of numerous nanostructured materials for maritime applications, applying several modelling techniques to generate detailed inventories. The inventory data have then been used in combination with well-known database to perform comparative LCA, aiming at identifying the best possible alternative. Due to the complexity of the nanostructured materials to be developed, a multiscale modeling approach was required, which comprised the development of atomistic, mesoscale and finite element models.

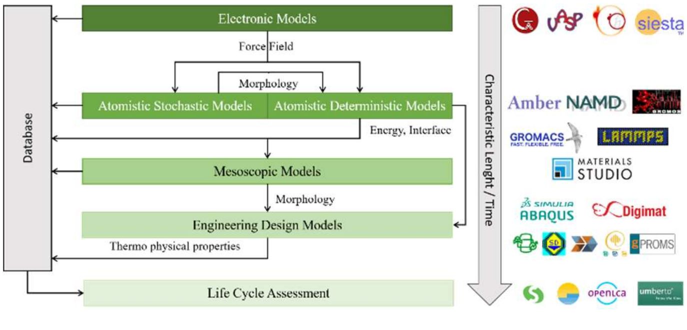

Fig. 2: Relationship among models suitable at different scales.

2. Materials and methods

This section provides a brief description of the procedures, the models and the materials employed within the assessment.

The purpose of this study was to assess the environmental implications of using nano-engineered thermoplastic polymers (NETPs) as part of a marine engine cover, following the metal replacement trend of green shipbuilding [19]. Preliminary research was conducted with the goal of determining the material's Key Performance Indicators (KPIs) in terms of weight, high temperature resistance, and mechanical strength. The material elastic module must be greater than 3.2 GPa to support a standing person with the engine in operation at 120°C, as shown in a similar work [20]. Following a thorough analysis of the available materials, several options among composite materials revealed to be acceptable for this purpose. Suitable matrices comprehended polyamide 6,6 (PA66), polyamide 6 (PA6) and polyether ether ketone (PEEK), using inclusions such as short glass fibers (GF) or carbon fibers (CF). To comply with non-flammability requirements and temperature resistance KPIs (at least 120 °C) a sufficient amount of flame retardants (FRs) must be added to the material formulation of polyamide-based composites. Nano-sized montmorillonites (MMT), often known as nanoclays, are a viable alternative to replace part of traditional phosphate-based FR (triphenyl phosphate – TPP), which is not an environmentally friendly compound, particularly concerning eutrophication. We generally refer to "nanoclays" as layered silicates with at least one dimension in the nanoscale range intercalated by organic chains. In comparison to traditional composites, the nanocomposite improves both mechanical and flame-retardant properties as the degree of nanoclays exfoliation rises [21]. The absence of primary data on the mechanical and fire-resistance properties of each nanocomposite formulation is the study's fundamental shortcoming. For determining key performance characteristics of the polymer-nanoclay-fibers nanocomposites, we employed multiscale molecular modeling methods. At the atomistic level, we built a system consisting of several layers of exfoliated MMT platelets surrounded by a compatibilizer (*i.e.,* octadecyl amine - ODAM) and the polymer. Our purpose was to estimate the effects of the interface on the mechanical properties of the matrix (Fig. 3a). By applying external tensile loads along an axis orthogonal to the platelet surface, we utilized molecular dynamics (MD) to determine the elastic modulus of the polymer-clay nanocomposite. The modeling findings, which are supported by studies on comparable systems [22,23], show an elastic modulus enhancement factor ($E_{matrix}/E_{polymer}$) of approx. 1.5 for a 4% wt. of MMT inclusion, i.e., from 3.1 GPa to 4.7 GPa for PA66 and from 2.85 to 4.3 GPa for PA6. Based on material on the market, the elastic modulus of PEEK at ambient temperature has been taken as 3.6 GPa, as it satisfies the heat resistance requirements on its own. The results of the atomistic simulations such as density, Poisson's ratio and matrix elastic modulus have been transferred to a higher simulation scale, namely the microFEM, where we used Digimat-FE (Fig. 3b). It is a finite element-based homogenization module able to generate a realistic Representative Volume Element (RVE) of a large variety of material microstructures. We estimate the elastic modulus at 120 °C for six material formulations, progressively increasing the amount of inclusions (GF or CF) to meet the required mechanical KPI of 3.2 GPa at 120 °C. (Table 1). We defined the aspect ratios of inclusions as 10 and 300 for GF and CF, respectively. Finally, as shown in Fig. 3c, we used our prior findings to perform additional analysis using Bertagna et al. [24] finite element (FE) model on the shaped material. 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. We designed a single cylinder head cover, built using the same volume of nanocomposite material due to geometry restrictions. Depending on the in-silico estimated density, we defined the weight for the each NETP replacing cover (Table 1).

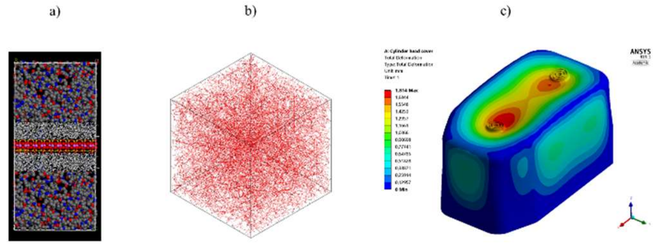

Fig. 3: Material appearance at the various scales from atomistic model (a), to microFEM (b) to the finite element (FEM) representation (c)

Table 1: Formulations (% wt.) of the materials assessed

NETP	Matrix			Inclusion	Weight [kg]
	Polymer	Flame Retard.	Filler		
1-PA66GF	PA66 0.5762	TPP 0.067	MMT 0.0268	GF 0.33	11.87
2-PA66CF	PA66 0.7095	TPP 0.0825	MMT 0.033	CF 0.175	10.97
3-PA6GF	PA6 0.5504	TPP 0.064	MMT 0.0256	GF 0.36	12.13
4-PA6CF	PA6 0.70176	TPP 0.0816	MMT 0.03264	CF 0.184	10.75
5-PEEKGF		PEEK 0.89		GF 0.11	11.87
6-PEEKCF		PEEK 0.93		CF 0.07	11.44

Following the ISO standards [1,2] we first defined the functional unit as "the production, use and disposal of a non-flammable or self-extinguishing cover, i.e., at least V-0 or V-1 according to UL-94 regulation [25], whose elastic modulus must be greater than 3.2 GPa at 120 °C", as it is supposed to support a standing person with the engine in operation. The Environmental Footprint (EF) v3.0 LCIA midpoint method, formerly known as ILCD, has been used in the LCIA phase [26]. This model incorporates impact categories for each environmental compartment as well as different adverse effects:(i) climate change includes biogenic, fossil, land use/change and total (CC-T) perspectives; (ii) ecosystem quality comprehends acidification (EQ-A), freshwater ecotoxicity (EQ-FE), eutrophication marine (EQ-EM), freshwater (EQ-EF) and terrestrial (EQ-ET); (iii) human health deals with carcinogenic (HH-CE) or non-carcinogenic effects (HH-NCE), ionizing radiation (HH-IR), ozone depletion (HH-OD), photochemical ozone formation (HH-PCOF), particulate matter (HH-PM); (iv) resources depletion takes into account dissipated water (RD-W), fossil fuels (RD-F), minerals and metals (RD-M) and land use (RD-L).

Secondary data of the NETP constitutive materials have been retrieved within well-established database (ecoinvent v3.7, Idemat) considering a European production, usage and landfill. Life cycle inventories of polyamide-based materials are based on the ecoinvent processes specific for nylon 66 and nylon 6 market in Europe, while Idemat, a database based on ecoinvent background data, is the source of PEEK life cycle inventory.

Emissions of polymers at landfill are based on the total degradation of the materials modelled using the excel template "Calculation Tool for waste disposal in Municipal Solid Waste Incinerators" available at ecoinvent website [27]. Common market moisture contents are 2.5% for polyamide and 0.5% for PEEK. The metal trace content for polyamide-based matrices is based on the work of Sungur and Gülmez [28], who analyzed the metal content of common polymeric fibers. In order to keep a conservative approach, the maximum content detected for each metal in polyamide has been chosen as the reference value in our study.

Life cycle inventory of glass fibers (GF) is based on a dedicated ecoinvent process. Transports have been included based on eurostat transport statistics for railway, inland waterways and road freight transport of goods for the NST 2007 category "GT09 - Other non-metallic mineral products" in the year 2016 for all countries for which data was available [29]. End-of-life treatment takes place in an unsanitary dry infiltration landfill using an ecoinvent representative process.

Life cycle inventory of carbon fibers (CF) has been retrieved in the publication of Cox *et al.*[30], which is also used by ecoinvent. The transport and disposal of carbon fibers followed the same principles as glass fibers.

The ecoinvent database, which details the manufacturing and distribution of triphenyl phosphate (TPP) in the European market, is used to create its life cycle inventory. End-of-life emissions are based on the total oxidation of the substance during landfilling.

The available ecoinvent raw material for montmorillonite is bentonite extracted in Germany, which is a clay that is generally made up of a three layers montmorillonite [31]. 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" [29]. The ecoinvent processes for milling and packing of lime in Europe is then used as a proxy for bentonite, aiming at reducing its size to nanometric scale to increase the nanoparticle surface/volume ratio. Transports have been calculated using the aforementioned Europe transport statistics.

The life cycle inventory of the compatibilizer, *i.e.,* octadecyl amine (ODAM) has been retrieved in a previous work by Mio et al. [20], as well as the mixing process for the production of the modified exfoliated montmorillonite, the compounding of the various components and the injection moulding of the final product.

A cradle-to-grave landfill disposal scenario of NETP covers has been developed. Since the cover was designed to be fire resistant, it is not conveniently disposed at a waste-to-energy facility. The unsanitary dry infiltration class landfill was chosen because it is a reasonable compromise between an open dump and a sanitary landfill. When compared to a waste-to-energy alternative treatment, the landfill scenario ensures a more cautious approach, neglecting any emission credit from an energetic recovery of the nanocomposite material. The system boundary of the cradle-to-grave life cycle of the NETP covers are reported in Fig.4.

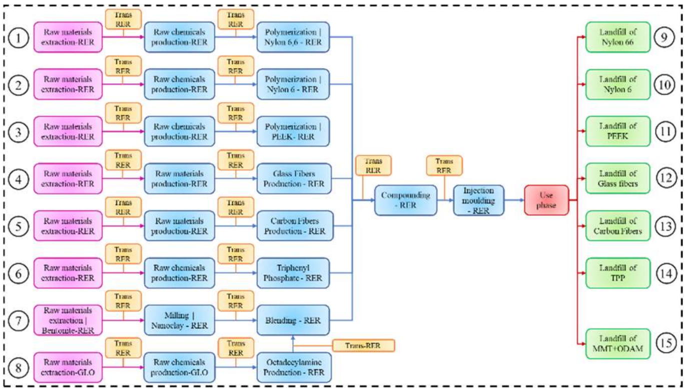

Fig. 4: System boundary of life cycle stages of the various formulations under investigation. Each material follows dedicated branches related to specific raw materials: 1-PA66GF:1,4,6,7,8,9,12,14,15; 2-PA66CF:1,5,6,7,8,9,13,14,15; 3-PA6GF: 2,4,6,7,8,10,12,14,15; 4-PA6CF: 2,5,6,7,8,10,13,14,15; 5-PEEKGF: 3,4,11,12; 6-PEEKCF: 3,5,11,13

3. Results and discussion

The normalized impact categories scores for each NETP are reported in Fig. 5.

None of the formulations outperformed the others in every impact category, hence a compromise must be found in order to identify the most sustainable option.

Given the acknowledged inconsistencies across databases, it is recommended to take the following findings with care [32].

Concerning the impact category related to climate change (CC-T), polyamide-based formulations gained better results than PEEK-based NETP. This is mostly due to the significant greenhouse gas emissions associated with PEEK manufacturing, which, since it must be created at the labscale, currently consumes a lot of electricity [33].

On the other hand, 5-PEEKGF gained the best performances for impact categories related to ecosystem quality, ranking in the top three formulations for all impact categories (EQ-A,FE,EF,EM,ET). In particular, eutrophication in freshwater and marine environments (EQ-EF,EM) is linked to phosphorus- and nitrogen-based chemical emissions, respectively. As a consequence, polyamide-based NETPs, which are a nitrogen source, added with conventional FR (TPP), which is a phosphorous source, have the worst outcomes.

Within the human health-related impact categories, a clear pattern can be identified: formulations containing GF outperformed those including CF. This is owing to the high energy consumption associated with CF manufacture, which degrades the overall NETP performance, whereas emissions for GF formulations are mostly driven by manufacturing methods and raw materials. Among the investigated formulations, 5-PEEKGF gained the best results, followed by 1-PA66GF and 3-PA6GF. Even though the specific emissions for PEEK are higher than polyamides for several impact categories (HH-CE,IR,OD), the introduction of nanoclays, FRs and a considerable amount of glass fibers resulted in an increment of the overall emissions for polyamide-based formulations.

Except for the use of fossil fuel (RD-F), which is associated to the higher energy consumption during the manufacturing process, resource depletion (RD-L,M,W) appears to be lower for PEEK-based nanocomposites. For instance, the depletion of minerals and metals (RD-M) is mainly affected by inclusions, therefore the formulations including less fibers gained better performances. Also, the specific impact of CF among the resource depletion impact categories is more significant than GF, resulting in bigger contribution to the overall NETP environmental performance.

4. Conclusion

The goal of this study is to demonstrate how *in-silico* techniques may be used to generate life cycle inventories. The integration of life cycle assessment into a multiscale molecular modeling framework produces a double benefit: i) an expansion of the scope of multiscale molecular modelling by taking the most comprehensive approach feasible, and ii) future life cycle applications may benefit of this cutting-edge approach. The proposed approach is particularly useful for sophisticated and novel materials that need to be evaluated in terms of their environmental impact, as shown for a product design case study. The results of this comparative LCA show that a material formulation including PEEK packed with glass fibers outperforms polyamide-based materials and carbon fibers inclusions in terms of overall environmental performance. Further improvements will need the employment of all simulation techniques within the multiscale modelling approach for the assessment of a single product.

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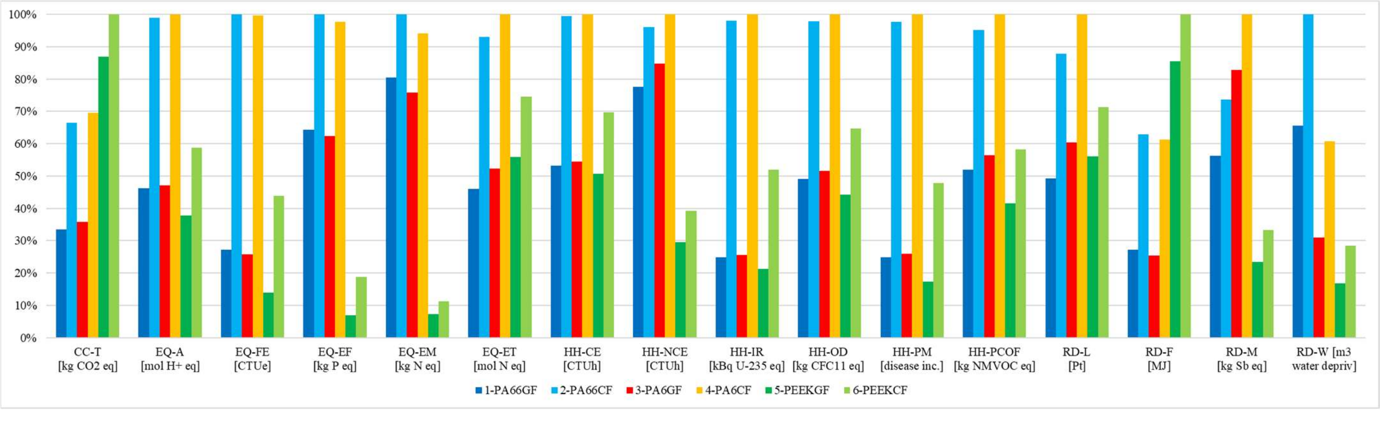

Fig.5: Normalized impact categories scores for each NETP formulation considered in this study

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