# (325b) Novel Approach to Material Selection: A Joint Venture of Multiscale Simulations and LCA

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Since the sustainability related to materials and processes has become a relevant criterion within the products design procedures, a novel approach to materials choice has been adopted in order to minimize the impacts related to the products life cycle. The selection of innovative materials for specific applications has been adopted by numerous manufacturers belonging to different areas, including marine engine constructors sector which was formerly dominated by metallic alloys. Indeed, the introduction of nano-engineered thermoplastic polymers (NETPs) as the main constituent of marine engine non-structural components, provided an enhancement towards the reduction of cost and weights as well as simplified maintenance and inspection operations. However, the substitution of former material doesnâ€™t come without any drawbacks, since an in-depth investigation on compelling alternatives is mandatory. In this regard, computer multiscale simulations established as a valuable support to identify the influence of several molecular structures on the parameters that most affect the performances required by specific product purposes.

In this work, we present a case study for the material substitution of a four-stroke marine engine plastic cylinder head cover, commonly made of aluminium alloys. Accordingly, different NETPs have been computationally evaluated and ranked in order to find the best compromise between mechanical properties and material costs. To reach this goal, a multiscale molecular modelling approach has been adopted in which the results from the atomistic scale have been used as inputs for the simulation of the final product performed with Finite Elements Method (FEM).

Finally, in order to have a complete scenario of the replacement of aluminium with the selected NETP, a detailed Life Cycle Assessment related to the different material products has been performed in order to identify the most sustainable product design using a cradle to grave life cycle perspective on openLCA v1.8.0. While performing Life Cycle Inventory, we were able to embed data provided by the actual suppliers and manufacturers, including geographical specific contributions, waste production, energy consumption and processing details. Well-established impact categories have been adopted for Life Cycle Impact Analysis in order to abide by the state-of-the-art of LCA practice. Finally, the main contributions to the whole product life cycle have been identified, highlighting the critical phases with the aim of applying the essential improvement for reducing the product-related impacts.