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# D5.3 Sustainability assessment of single phase HX material

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| **Main authors/contributors:** | M A Hye Chowdhury, Tausif Ahmed, Ashadul Hoque, M A Rahman, F Chowdhury | |
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# Executive Summary

This document provides the sustainability assessment of GeoHex heat exchanger (HX) materials by combining the cost analysis and environmental impacts of these materials developed for single phase heat exchangers. Four types of GeoHex materials, which include metal oxide nanoporous, multi-wall carbon nanotubes, amorphous metal and Ni-P/Ni-P-PTFE duplex, for deposition onto carbon steel and stainless steel substrates have been developed for single phase heat exchangers as alternatives to the state of the art materials (SOA) 316L and 254SMO. Cost impacts have been estimated using a developed parametric cost modelling and environmental impacts have been assessed using ISO standard Life Cycle Assessment (LCA) model for GeoHex HX materials. Parametric cost modelling has been used to evaluate the total costs of production of four types of synthesised coatings accounting for the substrate, substrate surface preparation, coating deposition and overhead costs. The cradle to gate LCA analyses of the synthesised coatings have been carried out using SimaPro 9.1.1.1 LCA tool, considering the impact assessment methodology IMPACT 2002+ v2.15. The functional unit of the environmental and cost performances is 1 $m^2$ flat GeoHex engineered surfaces developed with four types of synthesised coatings. The results of the sustainability assessment give partners a bird's-eye view of the HX materials development and allow them to further optimise materials and processes. The cradle to grave LCA and cost models developed will be used for evaluating the cost and environmental impacts in terms of 1 $m^2$ heat transfer surface area for respective types of GeoHex enabled HXs are being developed through the proposed manufacturing route and design considerations.

# Objectives Met

The deliverable contributed towards the work package objectives:

- To model environmental and cost performance of the HX material developed in WP2
- To model environmental and cost performance of the HXs developed through the proposed route.

# CONTENTS

# 1. INTRODUCTION

One of the GeoHex goals is to develop heat exchanger materials that protect the single-phase heat exchangers (e.g., recuperator, superheater and preheater) from degradation due to corrosion and scaling damage and another goal is to enhance heat transfer performance. These developments will lead to smaller, more efficient, cost effective heat exchanger systems for geothermal sectors and beyond with lower environmental footprints. In work package 2 (WP2) of the project, Ni-P/Ni-P-PTFE duplex and amorphous metal glass coating materials providing anti-scaling and anti-corrosion properties to a low-cost carbon steel substrate and metal oxide nanoporous and Multi-wall carbon nanotube (MWCNT) coating materials providing heat transfer enhancement are being developed.

We have investigated both environmental and economic performances of the materials developed for single phase heat transfer heat exchangers. To promote eco-design in GeoHex materials and value chain, life cycle assessment (LCA) can be used as a useful tool to assess the environmental impacts of products and processes. We have used LCA tool SimaPro 9.1.1.1 (commercial LCA software which includes ecoinvent database version 3.6) software; the following relevant standards followed are:

- LCA framework of ISO 14040[2] and 14044[3] standards,
- International Reference Life Cycle Data System (ILCD)[4].

The LCA tool assessed the energy and resources consumed for a functional unit of synthesised coatings (i.e., 1µm thick over 1 $m^2$ substrate area) for a specific surface material developed for heat exchangers. Based on the energy and resources consumption, the LCA tool evaluates the emissions (to air, water and soil) associated to the materials development, which will be used to evaluate the environmental impacts over four endpoint damage categories:

- human health,
- climate change,
- ecosystem quality and
- resources.

Hence, the evaluation of LCA results will enable:

- Selection of the best GeoHex technology option(s), which have a minimum environmental impact, for a specific application.
- Support of R&D activities to develop GeoHex technology and consumables with minimum environmental impacts.

In addition to the evaluation of environmental performances, parametrised cost modelling has been used to evaluate the cost performance of various materials developed for single phase heat transfer heat exchangers. The parametric cost model accounts for the substrate material, substrate surface preparation, coating

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[2] ISO 14040: 2006 – Environmental management – Life cycle assessment – Principles and framework; Geneva. (2006a).

[3] ISO 14044: 2006 – Environmental management – Life cycle assessment – Requirements and guidelines; Geneva. (2006b).

[4] European Commission - Joint Research Centre - Institute for Environment and Sustainability: International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment – Detailed guidance. First edition March 2010. EUR 24708 EN.

deposition and overhead costs and quantifies the total costs of the synthesised coatings each of 1 µm thick layer of coating on a 1 m$^2$ substrate area.

This study provides the sustainability assessment by combining the economic and environmental impacts of GeoHex materials developed in WP2. The LCA and cost results will promote the sustainability assessment of the materials developed for single phase heat transfer heat exchangers. Therefore, the environmental and economic impacts will contribute to assessing initiatives taken to develop sustainable materials for heat exchangers. The sustainability concerns associated with the developed GeoHex materials are linked with the various input and output streams such as electrical energy requirement, input material consumptions, hazardous chemical substances associated with the human health, climate change and others. The results of the sustainability assessment give partners a bird's-eye view of the project development and allow them to further optimise materials and processes.

For assessing the sustainability of HX materials, the total costing for different types of coatings synthesised onto carbon steel and stainless steel substrates through different deposition processes and the respective environmental impacts have been quantified and analysed. In this study, we are dealing with 4 types of coating materials, 4 deposition processes, and 2 different substrates (S275JR, 316L). A total of 18 synthesised coating combinations have been considered and evaluated, which accounts for the total costs (parametric cost modelling) and environmental impacts (LCA modelling) for deposition of a functional unit of 1 µm thick over 1 m$^2$ substrate area.

The parametric cost model that accounts for four cost components:

- substrate,
- substrate surface preparation,
- coating material deposition and
- overhead.

The LCA modelling includes mass, energy and transportation flows of these synthesised coatings considering cradle to gate approach. Table 1.1 lists the total number of synthesised coatings using the S-HVOF process with metal oxide nanoporous coatings, CVD process with MWCNT, PVD process with amorphous metal coatings and ENP process with Ni-P/Ni-P-PTFE coating materials deposited onto carbon and stainless steel substrates. The naming of the 18 synthesised coatings follows the sequence as [substrate type]_[Surface preparation method]_[Deposition method]_[coating types]. The abbreviations for carbon steel and stainless steel substrate types are CS and SS, respectively. Before applying deposition of coating materials one of three surface preparation methods was adopted, grit blasting (GB), grinding linishing (GL) or surface treatment (ST). Within the costing and LCA evaluation, each of the coatings is deposited at one specific set of deposition parameters even on two different substrates. In addition, the costing and environmental impacts of SOA materials (316L and 254SMO) each of 1 m$^2$ area of 6 mm thick have been evaluated.

**Table 1.1 -** List of coatings-substrate combinations ID evaluated in this study.

| Sample ID | Substrates | Surface Preparation methods | Deposition processes | Coating types |
|---|---|---|---|---|
| CS_GB_S-HVOF_TiO2-10 | Carbon steel (CS) | Grit blasting (GB) | S-HVOF | TiO2 |
| CS_GB_S-HVOF_TiO2-20 | Carbon steel (CS) | Grit blasting (GB) | S-HVOF | TiO2 |
| SS_GB_S-HVOF_TiO2-10 | 316L (SS) | Grit blasting (GB) | S-HVOF | TiO2 |
| SS_GB_S-HVOF_TiO2-20 | 316L (SS) | Grit blasting (GB) | S-HVOF | TiO2 |
| CS_GB_CVD_MWCNT | Carbon steel (CS) | Grit blasting (GB) | CVD | MWCNT |
| SS_GB_CVD_MWCNT | 316L (SS) | Grit blasting (GB) | CVD | MWCNT |

| Sample ID | Substrates | Surface Preparation methods | Deposition processes | Coating types |
|---|---|---|---|---|
| CS_ST_PVD_Si:Ta:Al | Carbon steel (CS) | Surface treatment (ST) | PVD | Si:Ta:Al |
| CS_ST_PVD_Si:Ta:Cr | Carbon steel (CS) | Surface treatment (ST) | PVD | Si:Ta:Cr |
| CS_ST_PVD_Si:Ta:Fe | Carbon steel (CS) | Surface treatment (ST) | PVD | Si:Ta:Fe |
| CS_ST_PVD_Si:Ta:Ti | Carbon steel (CS) | Surface treatment (ST) | PVD | Si:Ta:Ti |
| SS_ST_PVD_Si:Ta:Al | 316L (SS) | Surface treatment (ST) | PVD | Si:Ta:Al |
| SS_ST_PVD_Si:Ta:Cr | 316L (SS) | Surface treatment (ST) | PVD | Si:Ta:Cr |
| SS_ST_PVD_Si:Ta:Fe | 316L (SS) | Surface treatment (ST) | PVD | Si:Ta:Fe |
| SS_ST_PVD_Si:Ta:Ti | 316L (SS) | Surface treatment (ST) | PVD | Si:Ta:Ti |
| CS_GL_ENP_HPLP | Carbon steel (CS) | Grinding linishing (GL) | ENP | Ni-P/Ni-P-PTFE |
| CS_GL_ENP_HPHP | Carbon steel (CS) | Grinding linishing (GL) | ENP | Ni-P/Ni-P-PTFE |
| SS_GL_ENP_HPLP | 316L (SS) | Grinding linishing (GL) | ENP | Ni-P/Ni-P-PTFE |
| SS_GL_ENP_HPHP | 316L (SS) | Grinding linishing (GL) | ENP | Ni-P/Ni-P-PTFE |

Section 2 describes four types of coating materials developed for single phase heat exchangers. Cost modelling using parametric costing equations and LCA modelling using ISO LCA standards developed for assessing the sustainability of GeoHex HX materials are described in Section 3. Cost and LCA modelling results of GeoHex engineered materials are described and discussed in Section 4. Finally, we conclude the results and findings in Section 5.

# 2. SINGLE-PHASE HEAT EXCHANGER MATERIALS

## 2.1 Metal Oxide Nano-porous Coatings

Thermal spraying process offers the deposition of fine particles (submicron and nano-sized) with enhanced functional performance in terms of wear, erosion, corrosion, thermal barrier properties, etc. compared to corresponding conventional coarse-structured coatings[5]. Plasma Spray, high velocity oxy-fuel (HVOF), flame spray, arc deposition are commonly used thermal spray methods. Plasma spray and HVOF methods are preferred over other thermal spray methods due to the better coating quality. In both processes, coating material could be fed in powder or liquid form. Coating material suspended or dissolved into a solvent is preferred over powder feedstock. Liquid feedstock uses submicron or nanosized particles suspended in a liquid medium, which introduces a multiscale feature in coatings after deposition[6]. When liquid feedstock encounters the plasma/flame, after atomization, its droplets follow different zones of plasma/flame, which is determined by their size and velocity. The heavier and bigger droplets end-up traveling in the core region of plasma/flame, where temperature and velocity are highest and vice-versa. Besides, particles in the central area hit the substrate perpendicularly. While, outer region particles, under the influence of gas trajectory move parallel to the substrate and deposit at the shallow angle on its asperities, developing columnar or cauliflower-like surface morphology[7]. These thermo-chemical (in the case of solution precursor feedstock) and thermo-physical interactions between feedstock and plasma are common in both plasma and HVOF spray processes. Apart from the deposition methods, coating quality varies with other spray parameters such as heat source, feedstock flowrate, standoff distance (SOD), suspension medium, fuel type (for HVOF), injection mode (radial or axial) etc.[8,9].

In D2.2, CuO, $TiO_2$ and $Fe_3O_4$ coatings using suspension-based plasma spray (SPS) and HVOF (S-HVOF) spray methods were deposited onto the carbon steel substrates. The aqueous suspensions of 5 wt.% $TiO_2$, CuO and $Fe_3O_4$ nanoparticles (<50 nm particles size), commercially obtained from Promethean Particles Ltd., UK, were prepared and used as feedstock material for SPS and S-HVOF methods. Prior to deposition of homogeneous coatings, suspensions were pre-treated in a high-shear mixer (~2400 rpm; for 15 min) followed by an ultrasonic probe (for 10 mins at 40kHz frequency) to minimize sedimentation and disperse agglomeration of suspended nanoparticles and to avoid clogging the nozzle and injection pump. For better adhesion between coating materials and substrate surface, the substrate was grit blasted with #100 mesh white alumina followed by degreasing with acetone. The main deposition parameters of SPS and S-HVOF methods were standoff distance (SOD), fuel type and feedstock flowrate.

TWI has previously developed suspension spray methods using modified thermal-spray guns to achieve nano-structured coatings. This expertise and the optimised process parameters have been used to achieve desired nano-porous coatings of CuO and $TiO_2$. Coated samples were characterised using scanning electron microscopy (SEM), crosshatch adhesion testing, and wettability via contact angle measurements. It was obtained that $TiO_2$

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[5] Toma, F.-L., et al., Comparison of the microstructural characteristics and electrical properties of thermally sprayed Al2O3 coatings from aqueous suspensions and feedstock powders. J. Therm. Spray Technol. **2012**, 21, 480–488.

[6] S. Joshi, P. Nylen, "Advanced Coatings by Thermal Spray Processes," *Technologies*, Vol. 7, No. 4 (2019), p 79. doi: 10.3390/technologies7040079.

[7] L. Pawlowski, "Suspension and solution thermal spray coatings," *Surface and coating technology*, Vol. 203, No. 19 (2009), p 2807-2829. doi: 10.1016/j.surfcoat.2009.03.005.

[8] P. Fauchais, et al.,, "What Do We Know, What are the Current Limitations of Suspension Plasma Spraying?," *Journal of Thermal Spray Technology*, Vol. 24, No. 7 (2015), p 1120–1129. doi: 10.1007/s11666-015-0286-3

[9] A. Killinger, et al., "What Do We Know, What are the Current Limitations of Suspension HVOF Spraying?," *Journal of Thermal Spray Technology,* Vol. 24, No. 7 (2015), p 1130–1142. doi: 10.1007/s11666-015-0264-9

coatings deposited using S-HVOF at lower (150 mm) SOD showed better deposition, in relation to the KPIs. While for CuO, longer (200 mm) SOD produced better coatings. $Fe_3O_4$ coatings could not be deposited due to the high instability of $Fe_3O_4$ particles in the aqueous medium. Among all these coatings, $TiO_2$ coatings deposited through S-HVOF at 150 mm SOD were the most promising in terms of thickness, porosity and lack of cracking and defects. The parameters used for S-HVOF are listed in Table 2.1.

**Table 2.1 -** S-HVOF spray parameters used for $TiO_2$ coating deposition.

| Parameters | Unit | $TiO_2$-10 | $TiO_2$-20 |
|---|---|---|---|
| $H_2$ Fuel flow rate | liters/min | 788 | 788 |
| $O_2$ fuel rate | liters/min | 280 | 280 |
| Feedstock flow rate | ml/min | 10 | 20 |
| Standoff distances | mm | 150 | 150 |
| Hardware power | kW | 80 | 80 |
| Number of passes | - | 30 | 30 |

Two candidates of $TiO_2$ coatings ($TiO_2$-10 and $TiO_2$-20) were down-selected for further testing of the heat transfer and durability performances.

## 2.2 Multi-Wall Carbon Nano-tube Coating materials

Carbon nanotubes (CNTs) are cylindrical molecules that consist of rolled-up sheets of single-layer carbon atoms (graphene). They can be single-walled (SWCNT) with a diameter of less than 1 nanometer (nm) or multi-walled (MWCNT), consisting of several concentrically interlinked nanotubes, with diameters reaching more than 100 nm. Their length can reach several micrometers or even millimeters. Three main methods are currently available to produce CNTs: arc discharge, laser ablation of graphite, and chemical vapor deposition (CVD). In this study, MWCNT coating is being developed using CVD method. The decomposition of the gas phase carbon source such as methane, ethylene, acetylene & CNT formation take place on the surface of catalyst particles of Fe, Co and Ni. There is a two-step process to synthesise CNT: i) catalyst preparation by physical vapour deposition (PVD) and ii) CNT synthesisation through CVD method which involves many parameters such as carbon precursor (hydrocarbon), catalyst, temperature, pressure, gas-flow rate, deposition time, reactor geometry. Only the three key parameters: hydrocarbon, catalyst, temperature have been considered for developing single wall CNT (SWCNT) or multi-wall CNT (MWCNT). The formation of SWCNT and MWCNT are dependent on the size of the catalyst particle and growth temperature. The crystallinity and diameters of MWCNTs are being investigated by an X-ray diffractometer and scanning electron microscope (SEM) images, respectively. The number of graphitic walled layers and the inner diameter of MWCNTs are being determined using a transmission electron microscope (TEM). Raman spectroscopy technique is also being used to confirm the growth and quality of MWCNTs. The MWCNT coated (on one side of carbon steel substrate) samples are being developed using optimised process parameters and will be sent for further testing the single phase heat transfer performances and durability assessment.

## 2.3 Amorphous Metal coatings

The ternary thin film metallic glasses are promising materials with wide-ranging applications due to their unique mechanical and excellent anti-corrosion properties. In this study, six elements such as Aluminium (Al), Chromium (Cr), Iron (Fe), Silicon (Si), Tantalum (Ta) and Titanium (Ti) were used. For these six elements there were four ternary compositions of interest, Si:Ta:Al, Si:Ta:Cr, Si:Ta:Fe and Si:Ta:Ti. The thin film ternary compositions were mapped out using a computational model. The combinatorial approach allows a large range of compositions to be screened in terms of amorphicity, temperature stability and anti-scaling properties etc, with high efficiency. After mapping out the distribution for six different samples for each ternary composition the compositions were deposited onto the substrates using DC magnetron sputtering. Each recipe is built up around the ratio of the composite elements in the centre of the substrate. To synthesise the metal amorphous coating, physical vapor deposition (sputtering) technique has been used along with combinational methodology, whereby co-depositing from two or more sources at the same time under an angle, keeping a relatively large substrate stationary during deposition, a compositional gradient is achieved across the sample. This gradient comes about simply due to the varying distance between the target and different parts of the sample, the highest composition of a given material is seen closest to that source. Six samples were prepared for each of the four coatings, making a total of 24 samples, each with a specific ratio value in the centre, the compositions and ratios are listed in Table 2.2.

**Table 2.2 -** The ternary composition at the centre of each of the 24 samples in wt%

| **Sample no.** | **Ternary composition of the samples in wt%** | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **Si:Ta:Al** | | | **Si:Ta:Cr** | | | **Si:Ta:Fe** | | | **Si:Ta:Ti** | | |
| | **Si** | **Ta** | **Al** | **Si** | **Ta** | **Cr** | **Si** | **Ta** | **Fe** | **Si** | **Ta** | **Ti** |
| 1 | 15 | 35 | 50 | 15 | 35 | 50 | 15 | 35 | 50 | 15 | 35 | 50 |
| 2 | 15 | 70 | 15 | 15 | 70 | 15 | 15 | 70 | 15 | 15 | 70 | 15 |
| 3 | 22 | 18 | 60 | 22 | 18 | 60 | 22 | 18 | 60 | 22 | 18 | 60 |
| 4 | 25 | 55 | 20 | 25 | 55 | 20 | 25 | 55 | 20 | 25 | 55 | 20 |
| 5 | 34 | 33 | 33 | 34 | 33 | 33 | 34 | 33 | 33 | 34 | 33 | 33 |
| 6 | 50 | 30 | 20 | 50 | 30 | 20 | 50 | 30 | 20 | 50 | 30 | 20 |

All of the samples went through pre-testing; after going through the pre-testing process, they were examined via XRD. All samples that were examined were found to have a thin film of $SiO_2$ across the whole surface. Furthermore, no signs of crystal formation or any other form of corrosion could be found. The details of the pre-screening test are described in D2.4. Four candidate coatings have been down-selected for further testing, from the 24 compositions investigated.

- Si:Ta:Al - 34:33:33 - GHX054
- Si:Ta:Cr - 15:35:50 - GHX028
- Si:Ta:Fe - 25:55:20 - GHX036
- Si:Ta:Ti - 34:33:33 - GHX042

Out of all the samples tested GHX028 had the least amount of $SiO_2$ deposited on its surface after the pre-test period. All six of the samples in the Si:Ta:Al group performed similarly; the 34:33:33 ratio in GHX054, was selected for further development due to its ease of use. The GHX042 was similarly selected for ease of use and the ratio 25:55:20 in sample GHX036 was selected due to its better performance. The selected coatings will be applied to steel plates for further testing of the heat transfer and durability properties.

## 2.4 Ni-P/Ni-P-PTFE Duplex Coatings

The main motivation for using nickel-based PTFE composite coating in this project is for improving the corrosion and scaling performance of the heat exchanger tubes. To improve performance, electroless nickel plating has been used to develop Ni-P/Ni-P-PTFE duplex coating on a carbon steel substrate, where in the topcoat layer, PTFE particles were added in the Ni-P matrix to form the Ni-P-PTFE composite coating. To develop duplex coating, the undercoat layer Ni-P has been developed first in one bath and the topcoat layer Ni-P-PTFE has been developed in the second bath. The optimised process parameters for the synthesis of Ni-P/Ni-P-PTFE duplex coating have been considered to achieve the desired tribological as well as corrosion, scaling and fouling resistant properties. After the completion of the undercoat layer deposition, the coated substrate has been immersed in the second bath to deposit Ni-P-PTFE composite coating. The main compositions of undercoat (Ni-P) and topcoat (Ni-P-PTFE) electroless nickel plating baths are given in Table 2.3.

**Table 2.3 -** Chemical reagents and their role for Ni-P and Ni-P-PTFE baths

| Role | Chemical reagents | Units | Ni-P | Ni-P-PTFE |
|---|---|---|---|---|
| Nickel source | Nickel Sulphate (NiSO4.6H2O) | g/l | 30 | 30 |
| Reducing agent to supply electrons for the reduction of nickel | Sodium hypophosphite (NaH2PO2.H2O) | g/l | 30 | 23/30 |
| Complexing agent (chelator) to control the free nickel available to the reaction | Sodium citrate dihydrate (C6H5Na3O7.2H2O) | g/l | 10.5 | 10.5 |
| Accelerator (exultant) to help increase the speed of the reaction | Ammonium acetate (NH4CH3COO) | g/l | 25 | 20/25 |
| Stabiliser (inhibitor) to help control reduction | Thiourea (CH4N2S) | ppm | - | 1 |
| Lubricious antifouling agent | Polytetrafluoroethylene or PTFE (C2F4)n ≤1.0µm | g/l | - | 10 |
| Immersion time | - | min | 90 | 90 |
| Targeted layer | Thickness | µm | 25 | 25 |
| Agitation | - | rpm | 100 | 150/100 |
| pH regulators | 50% ammonium hydroxide NH4OH, 10% sulfuric acid H2SO4 | ml | 500 | 500 |
| Energy | Temperature | °C | 85 | 85 |

In addition to excellent resistance to corrosion and scaling, the heat transfer performance of carbon steel coated with nickel-based PTFE composite coatings will be much better than the heat transfer performance of, for example, stainless steel or titanium. This is because carbon steel has much higher thermal conductivity, ~54 W/mK, than stainless steel (~16 W/mK) or titanium (22 W/mK). The Ni-P and Ni-P-PTFE layers are thin, as well as have thermal conductivities like carbon steel, giving Ni-P/Ni-P-PTFE coated carbon steel an effective thermal conductivity of ~54 W/mK. Using this in a geothermal heat exchanger would thus lead to:

- ✓ Improved heat transfer
- ✓ Reduced corrosion
- ✓ Reduced scaling
- ✓ Reduce cost of materials for geothermal applications

The two candidates of Ni-P/Ni-P-PTFE duplex coatings (HPLP and HPHP) have been selected for investigating the heat transfer and durability performances.

# 3. SUSTAINABILITY ASSESSMENT METHODS

The sustainability assessment of heat exchanger materials developed for single phase heat transfer heat exchangers have been studied by combining the economic and environmental impacts. Cost impacts have been analysed using a parametric cost model developed for GeoHex HX materials and environmental impacts have been assessed using an ISO standard LCA model.

# 3.1 Cost Modelling

## 3.1.1 Introduction

In this study, we quantify the total costing for different types of coatings synthesised onto carbon steel or other substrates through different deposition processes. Specifically, parametric cost modelling is used to evaluate the cost of production of all synthesised coatings and analyse the cost of synthesised coatings. A parametric cost model that accounts for the substrate material, substrate surface preparation, coating deposition and overhead costs has been used in this study. The overhead cost usually includes items such as services, insurance, taxes, facilities maintenance, and the depreciation of the equipment. This analysis is a part of a laboratory-scale and modelling effort to identify and develop coating materials and methods that can be scaled up. For this analysis, we aim to develop a parametric cost modelling of synthesised coatings in terms of the total costs of the synthesised coatings per µm of thickness of 1 $m^2$ area [€ $µm^{-1}$ $m^{-2}$]. The parametric cost model quantifies the cost of the 1 µm thick layer of coating on a 1 $m^2$ substrate area with different deposition techniques for different coating materials.

## 3.1.2 Parametrised Costing Equations

A general equation for the total costing (${}_{a}^{x}C_T$) in € for 1 µm thick of coating material (say, $x$) deposited over 1 $m^2$ area of substrate (say, $y$) using a deposition process (say, $a$) is given by:

$$ {}_{a}^{x}C_T = SM^y + SP_z + CD_a + OH \tag{3.1}$$

Here, $SM^y =$ cost of 6mm thickness substrate material, per 1 $m^2$ area in €;

$SP_z$ = substrate surface preparation cost, per 1 $m^2$ area in € using a given preparation method (say, $z$);

$CD_a =$ coating deposition cost, per 1µm coating thickness, for 1 $m^2$ area in €;

$OH$ = overhead cost per $m^2$ area of coating of 1 µm thick.

Each cost component in equation (3.1) has been considered and equations deduced for the costs of substrate material, substrate preparation, coating deposition and overhead for metal oxide, MWCNT, amorphous metal and Ni-P/Ni-P-PTFE Duplex synthesised coatings and expressed in €.

**a) Metal oxide coating materials deposition through S-HVOF process**

The substrate material cost component is given by:

$$\begin{aligned} SM^y(\text{€}) = {} & Mass\ of\ the\ substrate\ (kg) \times unit\ cost\ of\ the\ substrate\ \left(\frac{\text{€}}{kg}\right) + \\ & power\ of\ hardware\ machine\ for\ cutting\ (kW) \times time\ (\mathrm{h}) \times unit\ energy\ cost\ \left(\frac{\text{€}}{kWh}\right) + \\ & Labour\ time\ (h) \times unit\ labour\ cost\ \left(\frac{\text{€}}{h}\right) \end{aligned} \tag{3.2}$$

The expression for this cost component is the same for all the substrates used in this study.

The substrate surface preparation cost component is given by:

$$\begin{aligned} SP_z(\text{€}) = {} & \left[\frac{grit\ flow\ rate\ \left(\frac{g}{min}\right) \times grit\ blasting\ time\ (\mathrm{min})}{1000 \times reuse\ factor}\right] \times unit\ cost\ of\ grit\ \left(\frac{\text{€}}{kg}\right) + \\ & amount\ of\ cleaning\ materials\ (l) \times unit\ cost\ of\ respective\ cleaning\ materials\left(\frac{\text{€}}{l}\right) + \\ & Labour\ time\ (h) \times unit\ labour\ cost\ \left(\frac{\text{€}}{h}\right) \end{aligned} \tag{3.3}$$

The coating deposition cost component is given by

$$CD_a(€) = [Fuel\ and/or\ shielding\ gas\ flow\ rate\ (\frac{l}{\mathrm{min}}) \times deposition\ time\ (\mathrm{min}) \times \frac{unit\ cost\ of\ fuel\ (\frac{€}{m3})}{1000} + power\ of\ deposition\ machine\ (kW) \times time\ (\mathrm{h}) \times unit\ energy\ cost\ (\frac{€}{kWh}) + suspension\ flow\ rate\ \left(\frac{ml}{\mathrm{min}}\right) \times deposition\ time\ \times \frac{unit\ cost\ of\ suspension\ (\frac{€}{l})}{1000} + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h})]/[thickness\ of\ coating\ (\mu m)] \tag{3.4}$$

and the overhead cost component is given by

$$OH(€) = overhead\ cost\ factor\ \times total\ labour\ cost\ (€) \tag{3.5}$$

Where, overhead cost factor is assumed to be 0.5 and the same for all coating deposition. However, this factor will be tuned to match with the large-scale applications.

### b) MWCNT coating materials deposition through CVD process

The substrate surface preparation cost component is given by

$$SP_z(€) = \left[\frac{grit\ flow\ rate\ \left(\frac{g}{min}\right) \times grit\ blasting\ time\ (\mathrm{min})}{1000 \times reuse\ factor}\right] \times unit\ cost\ of\ grit\ \left(\frac{€}{kg}\right) + amount\ of\ cleaning\ materials\ (l)\ \times\ unit\ cost\ of\ respective\ cleaning\ materials(\frac{€}{l}) + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h}). \tag{3.6}$$

It is assumed that the substrate surface preparation cost component for MWCNT is the same as that of metal oxide nanoporous coating deposition since data was the unavailable from either primary or secondary sources.

The coating deposition cost component is given by:

$$CD_a = [Amount\ of\ active\ gas\ (cm^3) \times unit\ cost\ of\ active\ gas\ (\frac{€}{cm^3}) + Hardware\ power\ of\ CVD\ reactor\ (kW) \times time\ (\mathrm{h}) \times unit\ energy\ cost\ (\frac{€}{kWh}) + Amount\ of\ Nitrogen\ gas\ (cm^3) \times unit\ cost\ of\ nitrogen\ gas\ \left(\frac{€}{cm^3}\right) + Amount\ of\ Argon\ gas\ (cm^3) \times unit\ cost\ of\ argon\ gas\ \left(\frac{€}{cm^3}\right) + Amount\ of\ Hydrogen\ gas\ (cm^3) \times unit\ cost\ of\ hydrogen\ gas\ \left(\frac{€}{cm^3}\right) + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h})] + \text{Amount of catalyst (kg)} \times \text{unit cost of catalyst} (\frac{€}{kg}) \tag{3.7}$$

### c) Amorphous metal coating materials deposition through PVD (DC magnetron sputtering) process

The substrate surface preparation cost component is given by:

$$SP_z(€) = [Amount\ of\ acetone\ (l) \times unit\ cost\ of\ acetone\ (\frac{€}{l}) + amount\ of\ isopropanol\ (l) \times unit\ cost\ of\ isopropanol\ (\frac{€}{l}) + amount\ of\ polishing\ materials\ (pcs) \times unit\ cost\ of\ polishing\ materials(\frac{€}{pcs}) + amount\ of\ deionised\ water\ (l) \times unit\ cost\ of\ deionised\ water\ (\frac{€}{l}) + labour\ time\ (h) \times unit\ of\ labour\ cost\ (\frac{€}{h}) + amount\ of\ inert\ gas\ used\ for\ Cr\ layer\ (l) \times unit\ cost\ of\ inert\ gas\ (\frac{€}{l})] \tag{3.8}$$

The coating deposition cost component is given by:

$$CD_a = [Amount\ of\ inert\ gas\ (l) \times unit\ cost\ of\ inert\ gas\ (\frac{€}{l}) + Hardware\ power\ of\ vacuum\ system\ (kW) \times time\ (\mathrm{h}) \times unit\ energy\ cost\ (\frac{€}{kWh}) + mass\ of\ coating\ composition\ (kg) \times unit\ cost\ of\ coating\ composition\ (\frac{€}{l}) + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h})] \tag{3.9}$$

**d) Ni-P/Ni-P-PTFE Duplex coating deposition through ENP process**

The substrate surface preparation cost component is given by:

$$SP_z(€) = [Amount\ of\ grit\ material\ (kg)] \times unit\ cost\ of\ grit\ \left(\frac{€}{kg}\right) + power\ of\ grinding\ machine\ (kW) \times\ Grinding\ time\ (h) \times unit\ cost\ of\ energy (\frac{€}{kWh}) + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h}) \tag{3.10}$$

The coating deposition cost component is given by:

$$CD_a = [\ Amount\ of\ nickel\ sulphate\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ sodium\ hypophosphate\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ sodium\ citrate\ dyhydrate\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ ammonium\ acetate\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ PTFE\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ fluorocarbon\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Amount\ of\ pH\ regulators\ (kg) \times unit\ cost\ \left(\frac{€}{\mathrm{kg}}\right) + Labour\ time\ (h) \times unit\ labour\ cost\ (\frac{€}{h})]/[thickness\ of\ coating\ (\mu m)]. \tag{3.11}$$

## 3.2 LCA Modelling

### 3.2.1 Formal components of LCA

In this study, Life cycle assessment (LCA) has been used as a tool to evaluate the environmental footprints of four different coating materials deposited on carbon steel and stainless steel substrates through S-HVOF, PVD, CVD and ENP deposition processes. The LCA methodology applied in this study follows the methodology defined by the ISO 14040 and 14044 standards. LCA involves compilation of relevant inputs and outputs, subsequent evaluation of their associated environmental impacts and finally interpretation of the results with respect to the goals of the analysis. Environmental impacts of these synthesised coatings have been studied throughout the cradle-to-gate life cycle approach.

The LCA methodology comprises four stages (shown in Figure 3.1):

- goal and scope,
- inventory analysis,
- impact assessment and
- interpretation,

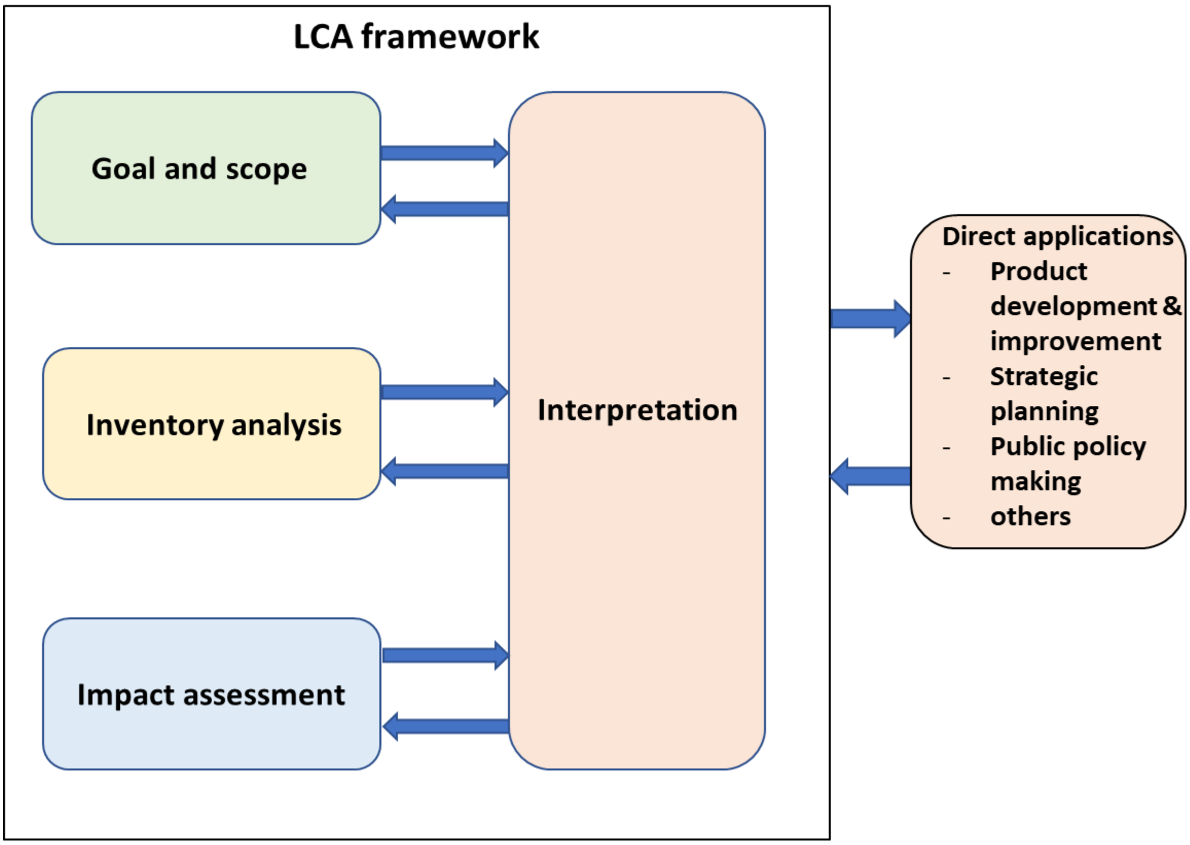

**Figure 3.1 -** A framework for the LCA from ISO:2006, modified[10].

In the goal and scope definition, the intention of the study with reference to the study design parameters need to be defined. The system boundaries and functional unit should also be defined.

In inventory analysis, a detailed description of the system is provided, including flow diagrams. Relevant input and output data are then collected and estimated related to the functional unit. This typically includes raw materials and energy inputs, waste streams and emissions. Data limitations and assumptions are also discussed.

In the impact assessment stage, the results of the inventory analysis are assigned to environmental categories such as global warming, non-renewable energy, mineral extraction, carcinogens, non-carcinogens, respiratory inorganics, ionising radiation, ozone layer depletion, respiratory organics, aquatic ecotoxicity, terrestrial ecotoxicity, aquatic acidification, aquatic eutrophication, terrestrial acid/nutri, and land occupation; this is known as classification. Subsequently, characterisation is carried out to estimate the environmental impacts for each category based on the inventory data. There are different methods to estimate the impact, but they are generally classified as midpoint and endpoint approaches[11]. The former estimate potential impacts at an intermediate position between the point of environmental intervention and the ultimate damage caused by

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[10] European Commission-JRC-Institute for Environment and Sustainability: ILCD Handbook: General guide for Life Cycle Assessment -Detailed guidance; 2010; EUR 24708 EN.

[11] Azapagic, A. (2006). Life Cycle Assessment as an Environmental Sustainability Tool. Chapter 6, p87-110. In: Renewables-based Technology: Sustainability Assessment (J. Dewulf and H. van Langenhove, eds.). John Wiley & Sons, London.

that intervention. 'Endpoint' approaches consider damage caused by the interventions to 'areas of protection', which include human health, ecosystem quality, climate change and resources. Several impact assessment methods are contained in the SimaPro 9.1.1.1 LCA tool [12] . The impact assessment method IMPACT2002+V2.15/IMPACT2002+ method[13], which uses a midpoint approach for calculating the impacts, has been selected for use in this analysis. Following characterisation, normalisation and weighting of environmental impacts can also be performed, however, they are not compulsory parts of an LCA, and were therefore excluded for this study.

The final stage, interpretation, involves a discussion of the results in the context of the methodology, scope and study goals. As a result, recommendations or decisions are made based on the findings of the study.

To perform the intended LCA study, we have used SimaPro 9.1.1.1 LCA tool, which is a well-known, internationally accepted and validated tool. Since its development in 1990 SimaPro has been used in many LCA studies by consultants, research institutes, and universities. The Simapro 9.1.1.1 software allows us to model and analyse complex life cycles in a systematic and transparent way, following the recommendations of the ISO 14040:2006 series of standards. In the SimaPro 9.1.1.1 tool, there are several inventory databases such as ecoinvent 3.6, a Swiss input output database, and Industry data 2.0 USLCI with a range of data on most used materials and processes, such as electricity production, transport and materials such as plastics, alloys or metals, which can be used for background data in the studies.

## 3.2.2 Goal and scope of the study

### Goal of the study

The goal of the LCA study is to assess the environmental impacts for a defined functional unit of each of the synthesised coatings. The following goals should be achieved:

- Quantify and evaluate the environmental footprints of the synthesised coatings
- Use the study results for synthesised coating developers and other stakeholders.

The intended audiences for this study are listed below:

1. Geothermal power plant industries
2. Heat exchanger materials manufacturers
3. Policy makers in Geothermal industries
4. Stakeholders in Geothermal industries
5. Environmental agencies
6. Consortium members
7. European Commission

### Scope the study

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[12] SimaPro 9.1.1.1 Pre Consultants, 2020, Netherlands

[13] Jolliet, O. et al., IMPACT 2002+: A new life cycle impact assessment methodology, The International Journal of Life Cycle Assessment 6 (2003) 324.

The scope of the study is to establish the baseline information to produce synthesised coatings and then examine the relative environmental impacts. The baseline data consists of resources and energy requirements and the environmental loading of each surface preparation and coating deposition processes includes:

- Substrate and its preparation processes: grit blasting, grinding linishing and surface treatment (excluding the manufacturing of the infrastructure materials of grit basting and grinding machines);
- Coating elements and/or compounds and processes used to manufacture four different types of coating materials: metal oxide nanoporous, MWCNT, amorphous metal and Ni-P/Ni-P-PTFE (excluding the manufacturing of the infrastructure materials and others);
- Coating deposition processes used for different coating materials: Suspension High Velocity Oxy-Fuel (S-HVOF) Thermal spraying, Chemical Vapour Deposition (CVD), Physical Vapour Deposition (PVD) and Electroless Nickel Plating (ENP). We exclude the manufacturing of the infrastructure materials (e.g., spray gun, powder feeder, robotics, electroplating tanks, etc.)

Specifically, the scope of the study of synthesised coatings (Figure 3.2) will be focused to:

- Cradle to gate analysis which will quantify the environmental burdens of the required materials needed to produce the synthesised coatings.
- Gate to gate analysis which will cover the environmental impacts of different processes involved in substrate preparation and coating material deposition.

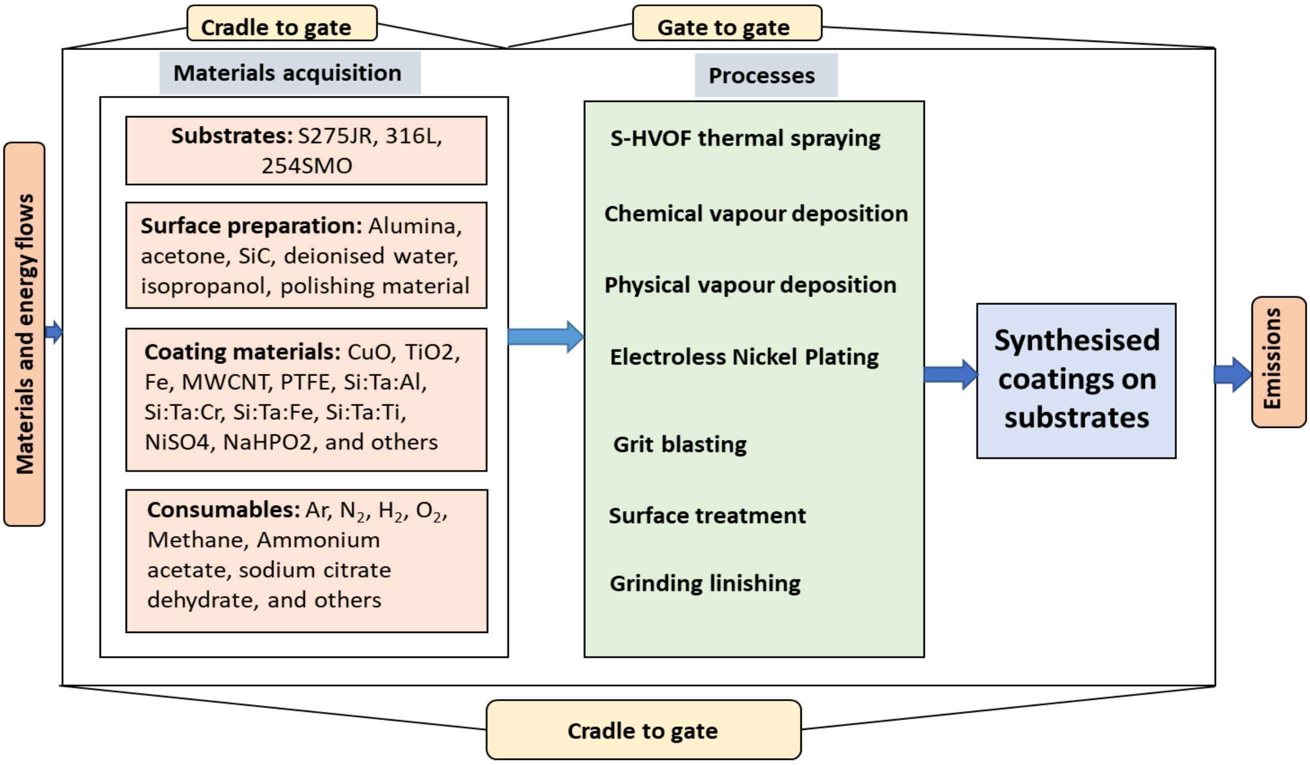

**Figure 3.2 -** A scope of study for the LCA studies of synthesised coatings

## Functional unit

The functional unit of the cradle to gate LCA study is 1 μm thick coating material deposited on a 1 m$^2$ substrate area for all synthesised coatings developed.

**Limitations of the study**

Due to unavailability of some primary processing data and the specifications of ancillary equipment, we have calculated and estimated the data based on some assumptions and secondary sources.

### 3.2.3 LCA modelling of synthesised coatings

A Life Cycle Inventory (LCI) is the identification and quantification of the material, resource, emission, waste, and product flows from different unit processes (substrates and its preparation and coating deposition) in the cradle to gate analyses of the synthesised coatings on substrates. For a 1 µm thick coating over $1m^2$ area, LCI inputs include coating materials and other consumables used in processing and manufacturing of the synthesised coatings, and energy and other resources consumed in the manufacturing. LCI process output flows include products, as well as releases to air, water, and land. The components of LCA modelling of synthesised coatings are substrate and its surface preparation and coating deposition and shown in Figure 3.3.

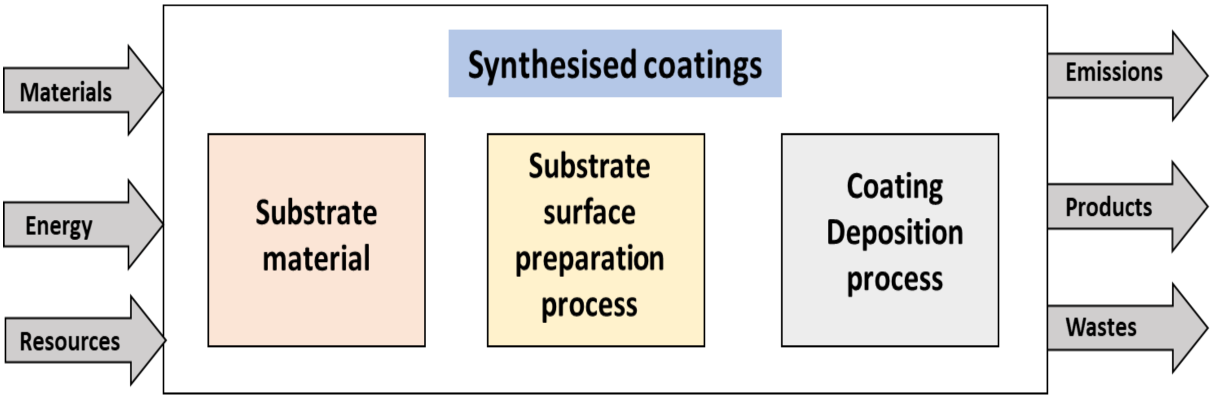

**Figure 3.3 –** Components of LCA modelling of synthesised coatings

**Data collection and Data sources**

The product synthesised coatings' LCI data was mainly collected from primary sources. Some data is estimated and calculated from the secondary sources. The secondary data comes from literature sources, being specific to either a product, material or process in question. For those processes where secondary data were lacking, modelled data or assumptions served as defaults. All the collected data was normalised to the study functional unit of 1 µm thick coating over 1 $m^2$ substrate area and then imported into SimaPro 9.1.1.1 LCA tool. This tool stores and organises life-cycle inventory and calculates life cycle impacts for a product profile. It is designed to allow flexibility in conducting life-cycle design and cradle to gate LCA functions, and to provide the means to organize inventory data, investigate alternative scenarios, evaluate impacts, and assess data quality.

**Life cycle Inventory Database**

Environmental institutions have taken the initiative to develop LCI background databases, to provide standard data for LCA assessments. The databases are continuously updated and maintained to ensure that the LCI data are up-to-date, consistent, and reliable. Some databases provide regional data, while others only contain national data. The available LCI databases usually also provide the facility for life cycle impact assessment (LCIA) based on the common assessment methodologies, such as Eco-indicator 99 and IMPACT2002+.

The Ecoinvent database covers more than 15,000 processes, including energy, transportation, waste disposal, construction, chemicals, detergents, paper and board, agriculture and waste management. It is the most widely used LCI database in Europe, and the data are valid for Swiss and Western European conditions. Each process is available in two versions, i.e., unit processes and system processes. A unit process contains only emission and resource inputs from one process step, and references to input from other unit processes. In a system process, the emissions from all the phases are included in a black-box format. In this study, we used the Ecoinvent database which is linked to the LCA tool SimaPro 9.1.1.1.

## 3.3 Cost and LCA models for Monophasic Heat Exchangers

For the application of GeoHex materials, shell & tube (tubular) and plate type heat exchangers are considered. Shell and tube heat exchangers consist of a number of tubes mounted inside a cylindrical shell. The function of this type of HX can exchange heat between two fluids, one fluid flows through the tubes while the other fluid flows outside the tubes. There are four major parts in a shell and tube heat exchanger: front end, rear end, tube bundle and shell. Plate type heat exchangers consist of two rectangular end members which hold together several pressed rectangular plates with holes in the corners for the fluid to pass through, thereby separating the fluids exchanging heat through the plates. The tube bundle comprises the tubes and the plates where the developing GeoHex materials can be adopted for enhancing the performance of the HXs.

Based on the outcomes of the scalability and manufacturability issues (D5.1) and the design of heat exchangers (D7.1), the cost and LCA models for 1 m$^2$ heat transfer area for monophasic tubular and plate type HXs with and without the adoption of GeoHex materials will be as follows:

**Cost model**

For a typical ORC geothermal binary plant (say, 10 MW installed capacity), the structural design and specifications of monophasic heat exchangers (superheater, preheater and recuperator) are defined. Based on these design and specification details, total cost of the respective HXs made with GeoHex enabled and SOA materials will be estimated, considering the flowing cost components in €:

- Manufacturing and installation
- Operation & maintenance
- End of life

Using the dimensions (length, thickness, diameters and areas) of the tubes and plates of HXs, the total surface area of the tubes and plates in m$^2$ will be calculated for the respective HXs. Therefore, the costs of the respective HXs made with GeoHex enabled and SOA materials in units of € m$^{-2}$ will be evaluated and compared.

**LCA model**

The functional unit of the LCA studies for monophasic heat exchangers made with GeoHex enabled and SOA materials is 1 m$^2$ heat transfer surface area. The cradle to grave LCA approach considered in this LCA model includes:

- Manufacturing & installation phase,
- Use phase and
- End of life phase.

The ISO 14040 and 14044 LCA standards and guidelines of the ILCD handbook were considered for analysing the environmental impacts of the respective HXs in terms of functional unit. The data inventories of 1 m$^2$ surface area of the tubes and plates of HXs made with GeoHex enabled and SOA materials have been carried out. Using these data inventories of GeoHex enabled HXs and SOA materials, SimaPro 9.1.1.1 LCA tool has been used to evaluate the respective environmental impacts in terms of functional unit, considering the life cycle impact assessment methodology IMPACT 2002+ version 2.15 and the results compared.

In GeoHex tasks 7.4 and 7.5, these LCA and cost models will be used to estimate the environmental and economic performances for GeoHex enabled HXs and compared these results with representative HXs using SOA materials for 1 m$^2$ heat transfer surface area.

# 4. RESULTS AND DISCUSSIONS

## 4.1 Cost Modelling Results

### 4.1.1 Data Inventories

Data inventories of coating materials, substrate and its preparation, coating deposition using S-HVOF thermal spraying, Physical vapour deposition, Chemical vapour deposition, and Electroless Nickel plating deposition techniques for a certain area and thickness of coating, and others were obtained from discussions with experts from consortium partners TWI, Grein Research, UoB and are given in Appendix A. Estimated unit rates of labour and electricity and other factors were obtained from secondary sources. Electricity pricing was based on average UK rates.

The following unit rates of electricity and labour, coating materials and reagents costs, reuse and consumable factors are considered in the costing calculations of synthesised coatings:

**Reuse factor:** In grit blasting process, grit materials are reused 20 times. A factor of 20 is considered as a reuse factor for the grit materials required for the surface preparation.

**Unit Labour rate:** In 2020, average hourly labour costs were estimated at € 28.5 in the EU, ranging from €6.5 in Bulgaria to €45.8 in Denmark[14].

**Electricity unit rate:** According to the Department for Business, Energy & Industrial Strategy (BEIS) the average cost for standard electricity in the UK in 2020 was 17.2p/kWh[15]. We convert it into € using a conversion factor of 1 GBP = 1.15 €. We estimated the average unit rate of electricity as € 0.20 per kWh.

**Consumable factor:** It is assumed that the amount of coating materials and reagents used in undercoat and topcoat bath solutions are enough to produce two times coating deposition. The total consumables costs for these bath solutions are divided by a factor 2 to get the cost of consumables for one deposition of a certain thickness. So, the consumable factor is considered to be 2 as provided by the partner TWI.

**Coating materials and chemical reagents unit costs:** Aqueous suspensions of 5 wt.% $TiO_2$ and CuO nanoparticles (<50 nm particles size), commercially obtained from Promethean Particles Ltd., UK, used as feedstock material for metal oxide nanoporous coatings. The unit costs of the suspensions of $TiO_2$ and CuO suspensions are €245 and €680 per litre, provided by the partner TWI. For MWCNT coatings, the unit costs of methane active gas and nitrogen, argon and hydrogen carrier gas are €35, €3.5, €4.5, and €10 per $cm^3$, respectively, provided by the partner UoB. The unit cost of Fe catalyst is about €57 per kg[16].

The total unit cost of composite powders has been calculated based on the unit price of high purity elemental powders provided by the consortium partner Grein Research. It is assumed that the processing cost of coating powders is 50% of the respective composite powder cost and listed in Table 4.1.

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[14] https://ec.europa.eu/eurostat/statistics-explained/index.php/Wages_and_labour_costs; accessed on 02 April 2021.

[15] https://www.ukpower.co.uk/home_energy/tariffs-per-unit-kwh; accessed on 02 April 2021.

[16] https://www.sigmaaldrich.com/chemistry/chemistry-products.html?TablePage=16246002; accessed on 02 April 2021.

**Table 4.1 –** Total unit cost of composite powders used for amorphous metal coatings

| Coating name | Coating composition | Elemental ratios | Unit cost of composite powders | Processing cost of coating powders | Total unit cost of composite powders |
|---|---|---|---|---|---|
| | | (wt%) | (€/kg) | (€/kg) | (€/kg) |
| GHX054 | Si:Ta:Al | 34:33:33 | 333.80 | 166.90 | 500.70 |
| GHX028 | Si:Ta:Cr | 15:35:50 | 339.20 | 169.60 | 508.80 |
| GHX036 | Si:Ta:Fe | 25:55:20 | 534.00 | 267.00 | 801.00 |
| GHX042 | Si:Ta:Ti | 34:33:33 | 374.80 | 187.40 | 562.20 |

Table 4.2 lists the chemical reagents costs used for Ni-P/Ni-P-PTFE duplex coatings deposited through ENP process provided by TWI.

**Table 4.2 –** Unit costs of chemical reagents used for Ni-P/Ni-P-PTFE coatings

| Role | Chemical/Compounds | Unit | Unit cost |
|---|---|---|---|
| | | | (€/unit) |
| Nickel source | Nickel Sulphate ($NiSO_4.6H_2O$) | 1kg | 136 |
| Reducing agent to supply electrons for the reduction of nickel | Sodium hypophosphite ($NaH_2PO_2.H_2O$) | 1kg | 91 |
| Complexing agent (chelator) to control the free nickel available to the reaction | Sodium citrate dihydrate ($C_6H_5Na_3O_7.2H_2O$) | 1kg | 54 |
| Accelerator (exultant) to help increase the speed of the reaction | Ammonium acetate ($NH_4CH_3COO$) | 1kg | 116 |
| Stabiliser (inhibitor) to help control reduction | Thiourea ($CH_4N_2S$) | 0.1kg | 31 |
| Lubricious antifouling agent | Polytetrafluoroethylene or PTFE ($(C_2F_4)_n$) | 0.1kg | 185 |
| Surfactant | Fluorocarbon or FC4 ($C_{20}H_{20}F_{23}N_2O_4I$) | 0.1kg | 41 |
| pH regulators/<br>Buffer solution | 50% ammonium hydroxide $NH_4OH$,<br>10% sulfuric acid $H_2SO_4$ | 1L | 45 |

## 4.1.2 Costing Results of GeoHex Engineered Materials

Using the costing equations (Section 3.1.2), the data provided by the partners (Appendix A) and the unit costs of electricity, labour, and coating materials and others described in Section 4.1.1, the costing of substrate and SOA materials, substrate surface preparation, coating deposition and overhead cost components in € have been calculated and estimated for metal oxide nanoporous, MWCNT, amorphous metal, Ni-P/Ni-P-PTFE duplex synthesised coatings each of 1 µm thick deposited onto carbon steel and stainless steel substrates of 1 $m^2$ area and listed in Tables 4.3-4.6.

The S-HVOF thermal spray method with different combinations of spray parameters has been used to deposit metal oxide nanoporous $TiO_2$, CuO and $Fe_3O_4$ coating materials onto the substrates. Among all coatings, $TiO_2$ coatings with suspension flow rates of 10 ml $min^{-1}$ and 20 ml $min^{-1}$ deposited at 150 mm SOD showed the most promising in terms of thickness, porosity and lack of cracking and defects. The cost components of substrate, surface preparation, coating deposition and overhead for the $TiO_2$-10 and $TiO_2$-20 synthesised coatings each of 1 µm thick deposited onto carbon steel and stainless steel substrates of 1 $m^2$ area have been evaluated using the data given in Table A5 of Appendix A and listed in Table 4.3.

**Table 4.3 –** Costs of cost components for metal oxide nanoporous coatings ($TiO_2$) each of 1µm thick over 1 $m^2$ area deposition onto carbon and stainless steel substrates using S-HVOF method

| Sample ID | Substrate cost | Surface preparation cost | Coating deposition cost | Overhead cost | Total cost |
|---|---|---|---|---|---|
| | (€) | (€) | (€) | (€) | (€) |
| CS_GB_S-HVOF_TiO2-10 | 89 | 10 | 17 | 34 | 150 |
| CS_GB_S-HVOF_TiO2-20 | 89 | 10 | 21 | 34 | 154 |
| SS_GB_S-HVOF_TiO2-10 | 350 | 10 | 17 | 34 | 411 |
| SS_GB_S-HVOF_TiO2-20 | 350 | 10 | 21 | 34 | 415 |

The percentage contributions of the cost components for $TiO_2$-10 synthesised coatings onto carbon steel and stainless steel are shown in Figures 4.1 and 4.2, respectively.

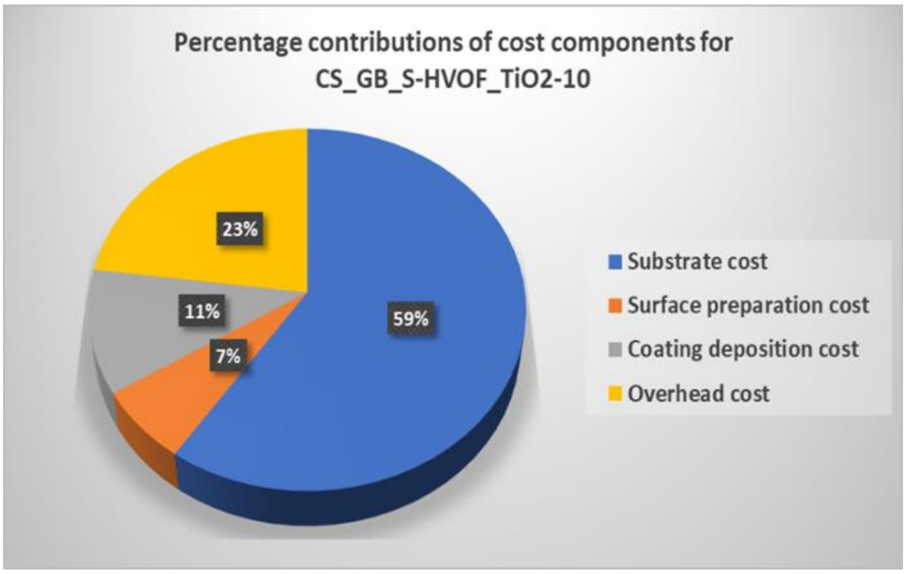


**Figure 4.1 –** Cost component contributions for $TiO_2$-10 synthesised coatings onto carbon steel.

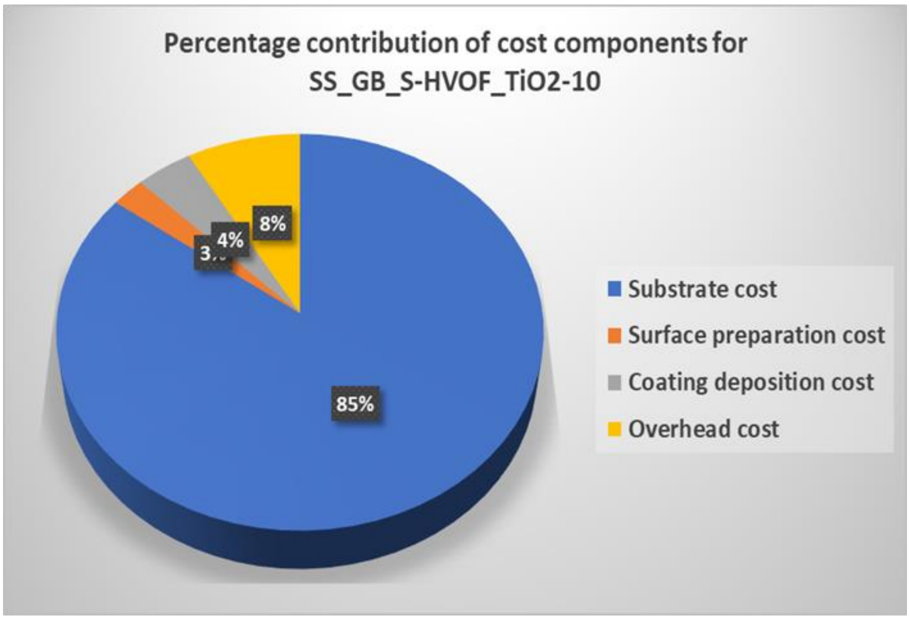


**Figure 4.2 –** Cost component contributions for $TiO_2$-10 synthesised coatings onto stainless steel.

Figure 4.3 shows the percentage contributions of cost components for both $TiO_2$ coatings deposited onto carbon and stainless steel substrates.

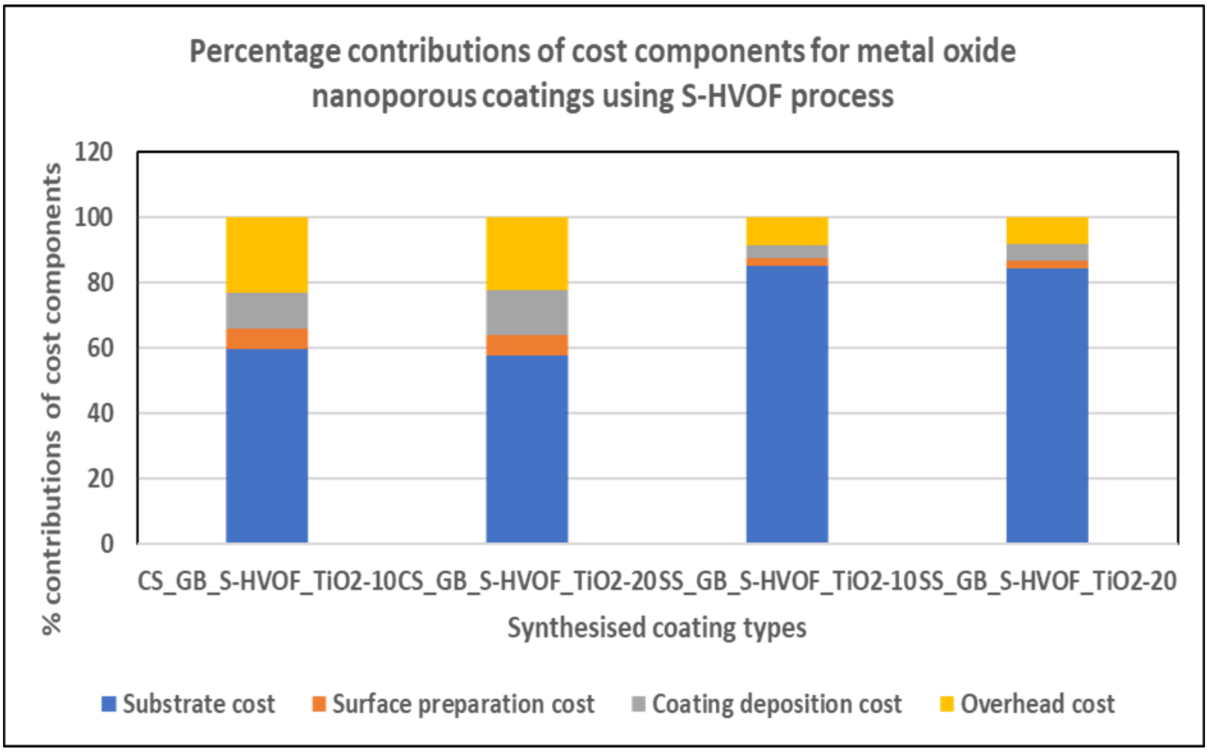


**Figure 4.3 -** Cost component contributions for $TiO_2$-10 and $TiO_2$-20 synthesised coatings onto carbon steel and stainless steel substrates.

The coating deposition and overhead costs of MWCNT coating materials deposited onto carbon and stainless steel substrates through CVD method have been estimated based on the data given in Table A6 of Appendix A and assumptions and estimation made and presented in Table 4.4.

**Table 4.4 –** Costs of cost components for MWCNT coatings each of 1µm thick over 1 $m^2$ area deposition onto carbon and stainless steel substrates using CVD method

| Sample ID | Substrate cost | Surface preparation cost | Coating deposition cost | Overhead cost | Total cost |
|---|---|---|---|---|---|
| | (€) | (€) | (€) | (€) | (€) |
| CS_GB_CVD_MWCNT | 89 | 10 | 1478 | 501 | 2078 |
| SS_GB_CVD_MWCNT | 350 | 10 | 1478 | 501 | 2339 |

The percentage contributions of the cost components for MWCNT synthesised coatings onto carbon steel and stainless steel are shown in Figures 4.4 and 4.5, respectively.

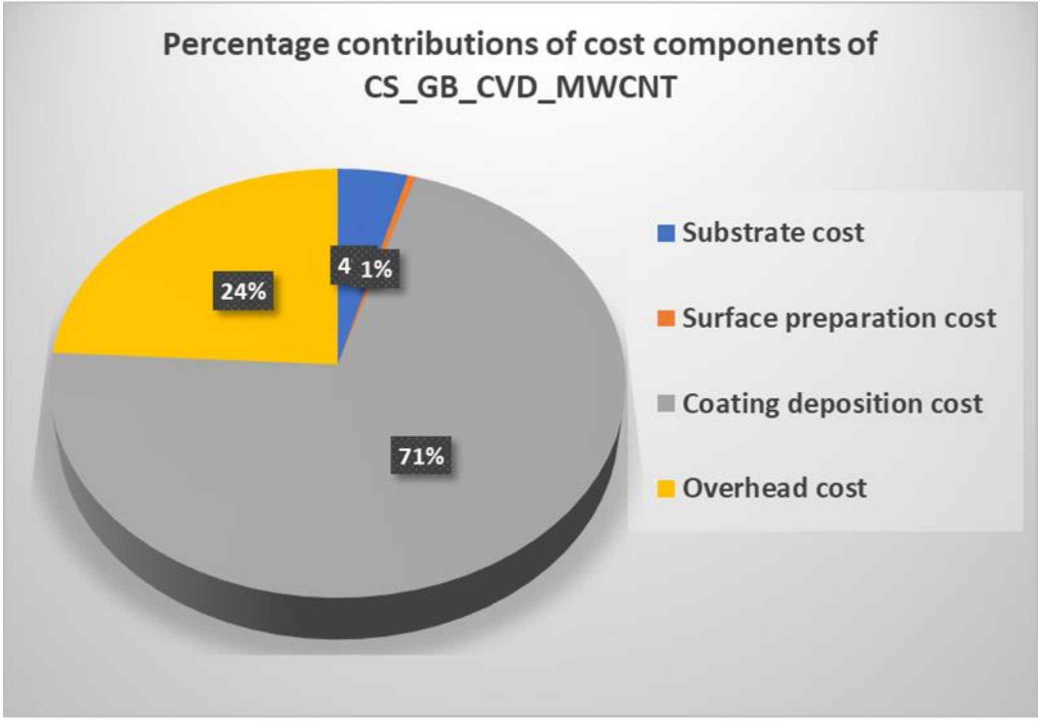


**Figure 4.4 -** Cost component contributions for MWCNT synthesised coating onto carbon steel

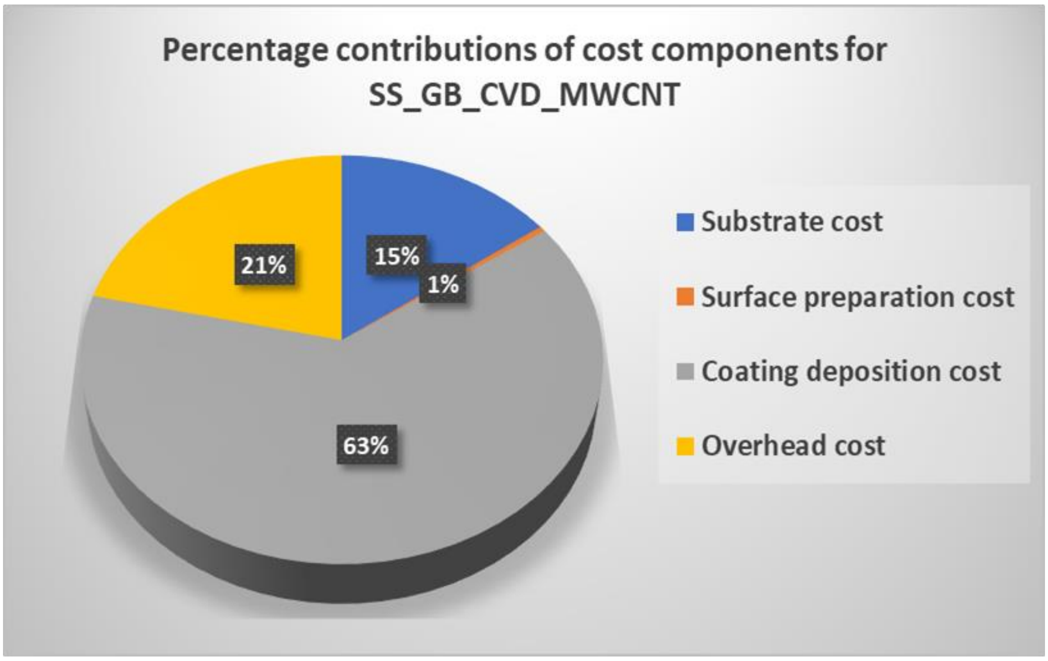


**Figure 4.5 -** Cost component contributions for MWCNT synthesised coating onto stainless steel.

Physical vapour deposition (PVD) using DC magnetron sputtering technique has been used to synthesise four amorphous metal coatings - Si:Ta:Al (GHX054), Si:Ta:Cr (GHX028), Si:Ta:Fe (GHX036) and Si:Ta:Ti (GHX042). The costs of the cost components for these amorphous metal coatings each of 1µm thick over 1 $m^2$ area deposition onto carbon and stainless steel substrates have been evaluated using the data given in Table A7 of Appendix A and listed in Table 4.5.

**Table 4.5 –** Costs of cost components for amorphous metal coatings each of 1µm thick over 1 m$^2$ area deposition onto carbon and stainless steel substrates using PVD method.

| Sample ID | Substrate cost | Surface preparation cost | Coating deposition cost | Overhead cost | Total cost |
|---|---|---|---|---|---|
| | (€) | (€) | (€) | (€) | (€) |
| CS_ST_PVD_Si:Ta:Al | 89 | 78 | 292 | 81 | 540 |
| CS_ST_PVD_Si:Ta:Cr | 89 | 78 | 310 | 81 | 558 |
| CS_ST_PVD_Si:Ta:Fe | 89 | 78 | 333 | 81 | 581 |
| CS_ST_PVD_Si:Ta:Ti | 89 | 78 | 318 | 81 | 566 |
| SS_ST_PVD_Si:Ta:Al | 350 | 64 | 292 | 81 | 787 |
| SS_ST_PVD_Si:Ta:Cr | 350 | 64 | 310 | 81 | 805 |
| SS_ST_PVD_Si:Ta:Fe | 350 | 64 | 333 | 81 | 828 |
| SS_ST_PVD_Si:Ta:Ti | 350 | 64 | 318 | 81 | 813 |

The percentage contributions of the cost components for Si:Ta:Al synthesised coatings onto carbon steel and stainless steel are shown in Figures 4.6 and 4.7, respectively.

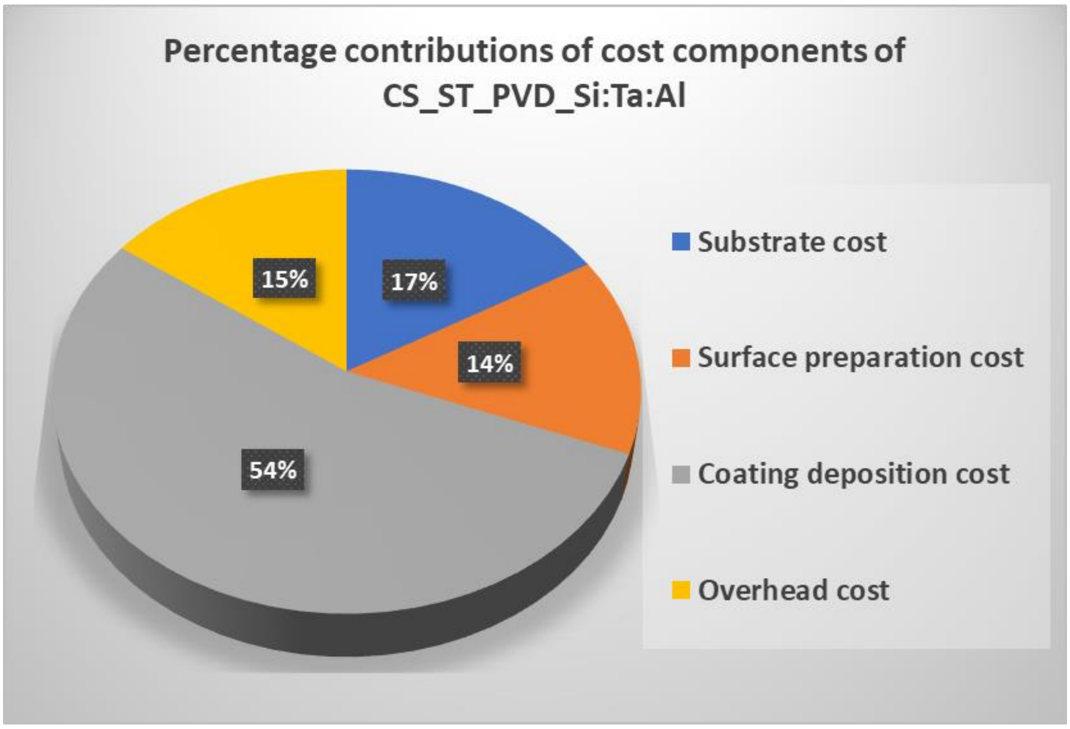


**Figure 4.6 -** Cost component contributions for Si:Ta:Al synthesised coating onto carbon steel.

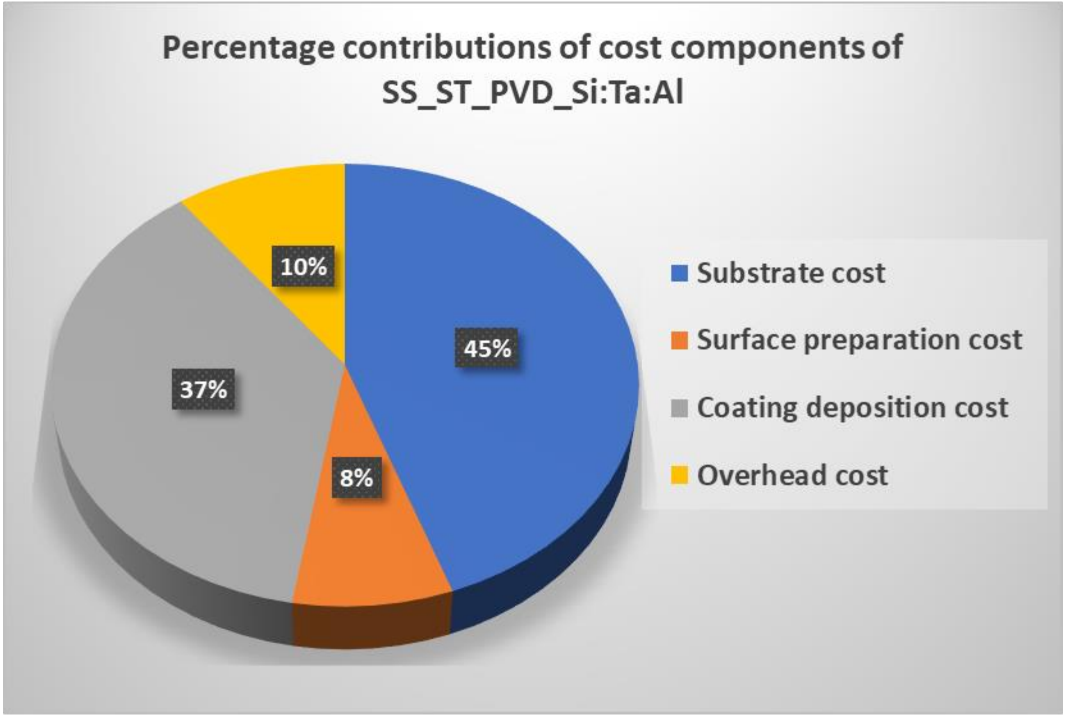


**Figure 4.7 -** Cost component contributions for Si:Ta:Al synthesised coating onto stainless steel.

Figure 4.8 shows the costs of cost components for four amorphous metal coatings deposited onto carbon and stainless steel substrates.

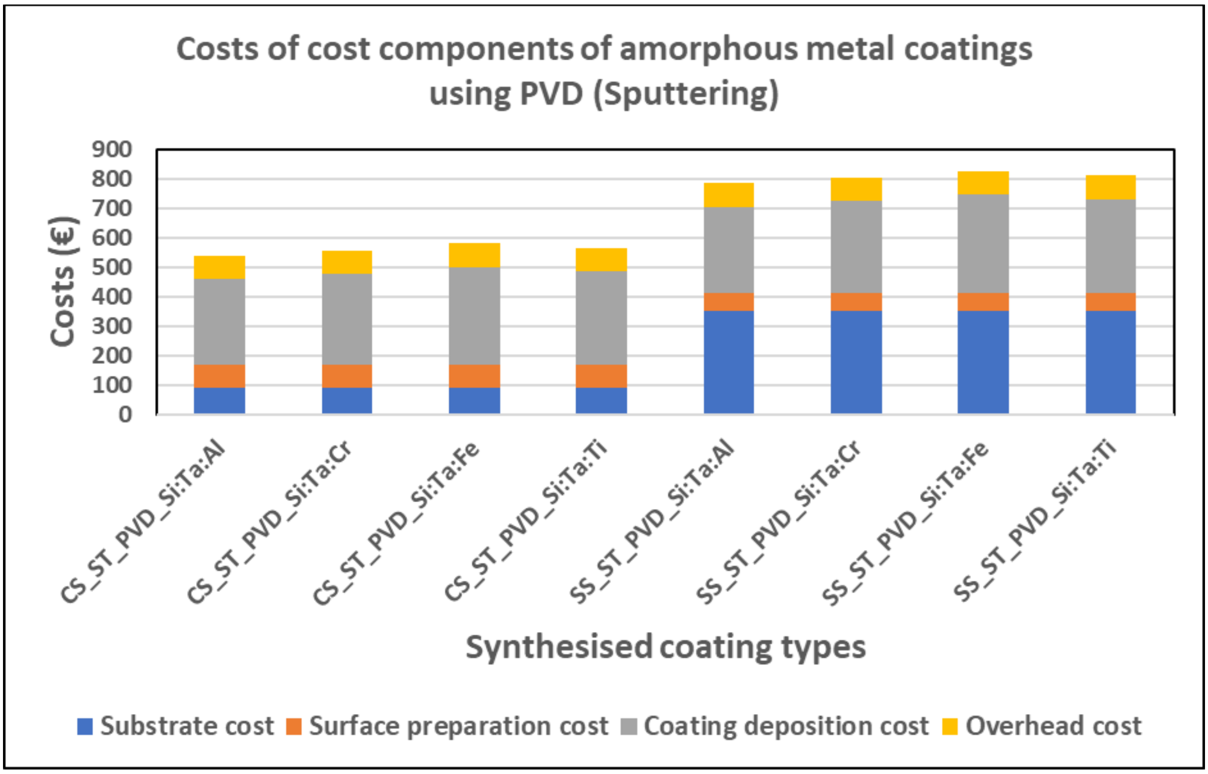


**Figure 4.8 –** Costs of four cost components for four amorphous metal coatings deposited onto carbon and stainless steel substrates.

Electroless nickel plating (ENP) method has been used to develop Ni-P/Ni-P-PTFE duplex coatings (HPLP and HPHP) on a carbon steel and stainless steel substrates. The costs of the cost components for these duplex coatings each of 1µm thick over 1 $m^2$ area deposition onto carbon and stainless steel substrates have been evaluated using the data given in Table A8 of Appendix A and listed in Table 4.6.

**Table 4.6 –** Costs of cost components for Ni-P/Ni-P-PTFE coatings each of 1µm thick over 1 $m^2$ area deposition onto carbon and stainless steel substrates using ENP method.

| Sample ID | Substrate cost | Surface preparation cost | Coating deposition cost | Overhead cost | Total cost |
|---|---|---|---|---|---|
| | (€) | (€) | (€) | (€) | (€) |
| CS_GL_ENP_HPLP | 89 | 62 | 546 | 59 | 756 |
| CS_GL_ENP_HPHP | 89 | 62 | 577 | 59 | 787 |
| SS_GL_ENP_HPLP | 350 | 62 | 546 | 59 | 1017 |
| SS_GL_ENP_HPHP | 350 | 62 | 577 | 59 | 1048 |

The percentage contributions of the cost components for HPLP duplex coating onto carbon steel and stainless steel are shown in Figures 4.9 and 4.10, respectively.

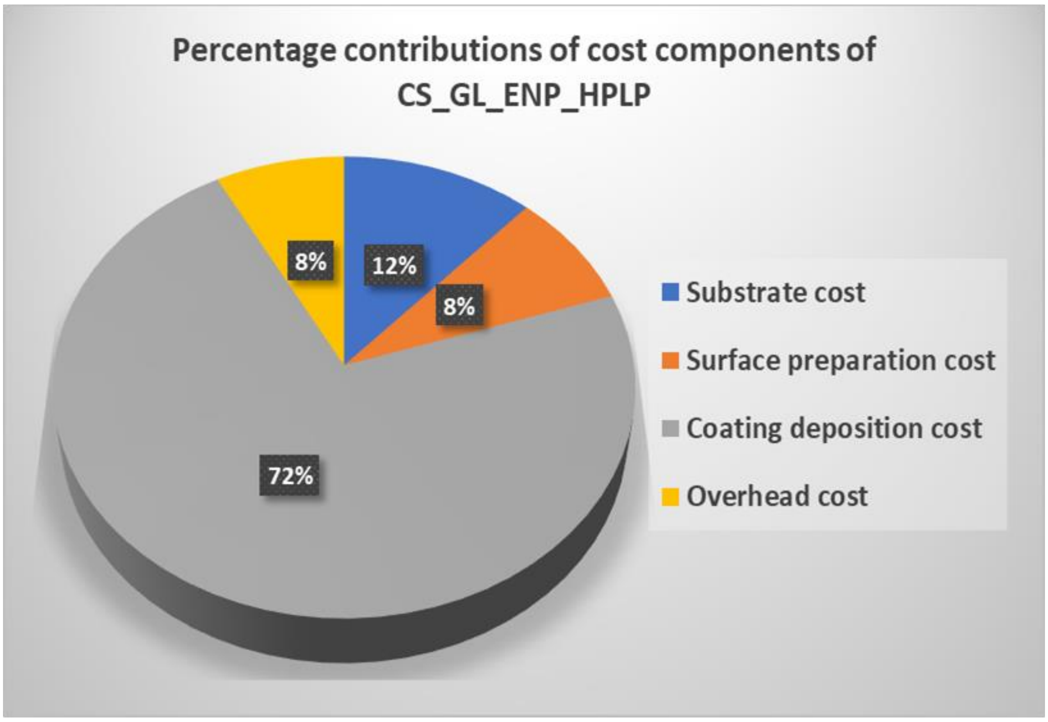


**Figure 4.9 -** Cost component contributions for HPLP duplex coating onto carbon steel

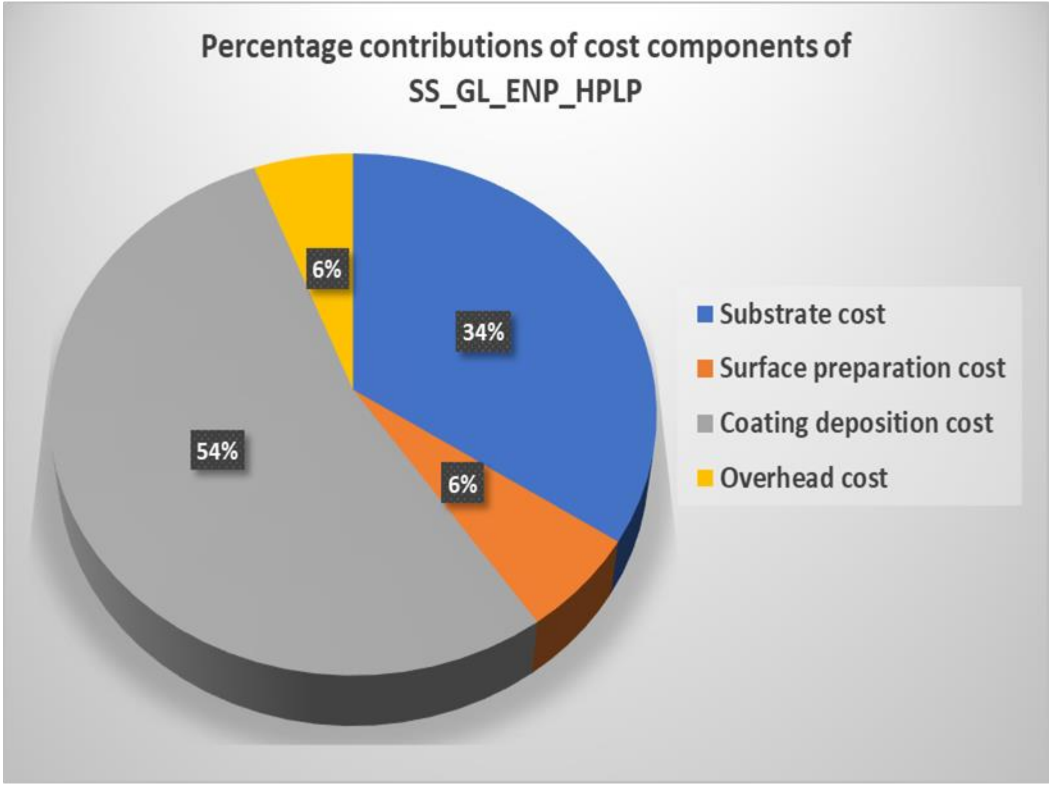


**Figure 4.10 –** Cost component contributions for HPLP duplex coating onto stainless steel.

Figure 4.11 shows the costs of cost components for HPLP and HPHP duplex coatings deposited onto carbon and stainless steel substrates.

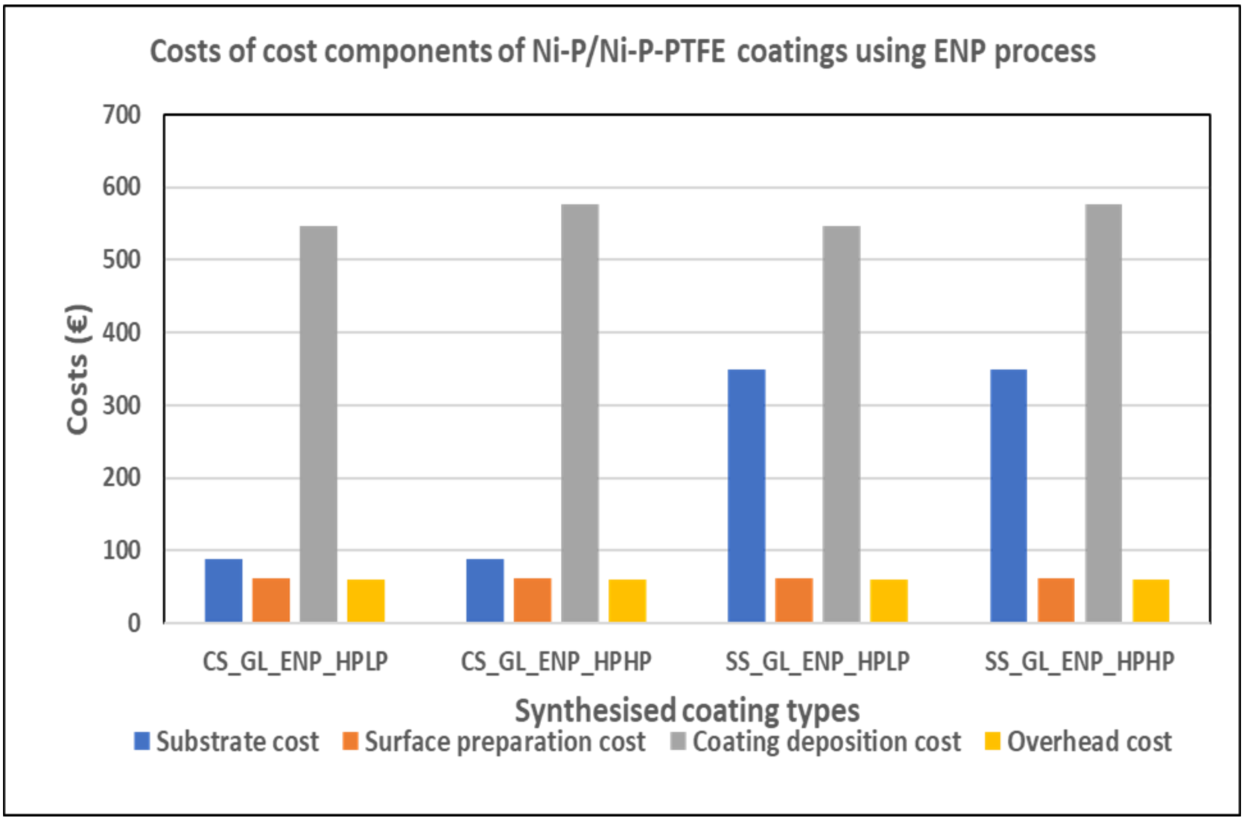


**Figure 4.11 -** Costs of cost components for HPLP and HPHP duplex coatings deposited onto carbon and stainless steel substrates.

# 4.2 LCA MODELLING RESULTS

## 4.2.1 Data Inventories

It is a really challenging task to develop data inventories for heat exchanger materials developed for monophasic heat exchangers. In this regard, to capture relevant domain knowledge, we have used following sources:

- Inputs from the partners developing GeoHex materials,
- Relevant submitted deliverables from Geo-Hex projects (D2.2 and D2.4) and
- Literature studies.

The Life Cycle Inventory (LCI) building is a fundamental activity necessary to carry out a LCA study of a product system. The LCI is a holistic view of the inputs and outputs for a given system such as a heat exchanger (HX) made with either state of art (SOA) or GeoHex materials. The cradle to gate LCA study of SOA and GeoHex materials used for tubes and plates of HXs has been performed in terms of a functional unit of 1 m$^2$ surface area of tubes and plates of HXs. The inventories of all other production processes for making different HX tubes and plates using SOA and GeoHex substrate (GHS) materials are not considered in this LCA study as they both follow similar production processes. The elemental composition (in wt%) of different SOA and GHS materials used for HX tubes and plates are given in Table 4.7.

**Table 4.7 -** Elemental composition of relevant SOA and GHS materials in wt%.

| **Element name** | **Elemental composition (wt%)** | | |
|---|---|---|---|
| | **S275JR (GHS)** | **316L (GHX/SOA)** | **254SMO (SOA)** |
| C | 0.25 | 0.08 | 0.01 |
| Mn | 1.6 | 2 | - |
| Si | 0.05 | 0.75 | - |
| P | 0.04 | 0.045 | - |
| S | 0.05 | 0.03 | - |
| N | - | 0.1 | 0.2 |
| Cr | - | 17 | 20 |
| Ni | - | 12 | 18 |
| Fe | 98.01 | 65.495 | 55.69 |
| Nb | - | 2.5 | 6.1 |

The mass, energy and transportation flows for S275JR, 316L and 254SMO materials each of 1 m$^2$ area of 6 mm thick have been estimated and calculated based on the primary data given in Table A1 of Appendix A and the assumption made for transportation distance. The average transportation distance for the materials is assumed to be 200 km. The LCA data for these materials each of 1 m$^2$ area of 6 mm thick have been evaluated and given in Table 4.8.

**Table 4.8 –** Mass, energy and transportation flows for S275JR, 316L and 254SMO materials.

| **Material grade** | **Dimension (mm)** | **Mass (kg)** | **Energy (kWh)** | **Transportation (tkm)** |
|---|---|---|---|---|
| S275JR | 1000x1000x6 | 47.1 | 0.67 | 9.42 |
| 316L | 1000x1000x6 | 47.4 | 0.67 | 9.48 |
| 254SMO | 1000x1000x6 | 48.3 | 0.67 | 9.66 |

Before applying nanoporous coating materials onto the substrate materials using S-HVOF and CVD processes, we need to prepare the substrate surface using grit blasting method for improving the coating adhesion to the substrate. The manufacturing energy of the grit material (#100 mesh alumina) has been estimated based on the rate of production of grit material of 4 kg per hour using a grit manufacturing machine of power 1 kW. Before deposition of coating material using ENP process, grinding linishing method has been used to prepare the substrate surface. The grinding time (120 min), grit material type (SiC), amount of grit material (0.40 kg), power of grinding machine (10 kW) have been considered for evaluating the LCA data of substrate preparation for 1 m$^2$ area through grinding method. Before deposition of coating material onto the carbon steel (S275JR) and stainless steel (316L) using PVD process, surface treatment has been performed using chemical reagents, water, polishing materials, Cr layer formation for adhesion and electrical energy used for cooling and vacuum systems. For 1 m$^2$ area of substrate preparation through grit blasting, grinding linishing and surface treatment methods, the respective data inventories (Tables A2-A4 in the Appendix A) have been used. Based on these primary and secondary data, the LCA data of substrate preparation for 1 m$^2$ area evaluated and are given in Table 4.9.

**Table 4.9 –** Mass, energy and transportation flows for 1 m$^2$ area of substrate surface preparation using grit blasting, grinding linishing and surface treatment methods.

| Processes | Mass | | Transportation | Electrical energy |
|---|---|---|---|---|
| | (kg) | | (tkm) | (kWh) |
| Grit Blasting | 0.627 ($Al_2O_3$) | 0.028 ($TiO_2$) | 0.14 | 0.508 |
| Grinding linishing | 0.400 (SiC) | - | 0.08 | 20.1 |
| Surface treatment | 0.869 (Acetone) | 0.009 (Ar) | 0.66 | 0.279 |
| | 0.864 (Isopropanol) | 0.001 (Cr) | | |
| | 1.097 (Water) | 0.429 (SiC) | | |

The S-HVOF coating deposition process has been carried out with aqueous suspensions of 5 wt% $TiO_2$ nanoparticles using feedstock and fuel source gas flow rates and stand-off distance for developing S-HVOF_$TiO_2$-10 and S-HVOF_$TiO_2$-20 synthesised coatings. Based on the data given in Table A5 of Appendix A and Table 2.2 in section 2, we evaluated the LCA data for these synthesised coatings each of 1 µm thick deposited over 1 m$^2$ area of substrate and are given in Table 4.10.

**Table 4.10 -** Mass, energy and transportation flows for coating deposition of $TiO_2$ nanoparticles.

| Coating ID | Masses (kg) | | | Energy | Transportation |
|---|---|---|---|---|---|
| | Suspension | Hydrogen Fuel | Oxygen | (kWh) | (tkm) |
| S-HVOF_TiO2-10 | 0.02 | 0.13 | 0.8 | 2.67 | 0.19 |
| S-HVOF_TiO2-20 | 0.04 | 0.13 | 0.8 | 2.67 | 0.19 |

MWCNT coatings are being developed during the writing of this report through CVD method which involves Fe catalyst particles, methane gas, inert gases and electrical energy. Based on the data given in Table A6 of Appendix A and assumptions and estimation made, we evaluated the LCA data for these synthesised coatings each of 1 µm thick deposited over 1 m$^2$ area of substrate and are given in Table 4.11.

**Table 4.11 -** Mass, energy and transportation flows for coating deposition of MWCNT coatings.

| Coating ID | Masses (kg) | | | | Energy | Transportation |
|---|---|---|---|---|---|---|
| | Methane | Nitrogen | Argon | Hydrogen | (kWh) | (tkm) |
| CVD_MWCNT | 1.24E-06 | 2.50E-05 | 5.70E-05 | 3.60E-07 | 300 | 11.544 |

Physical vapour deposition (PVD) using DC magnetron sputtering technique has been used to synthesise amorphous metal coatings. All coatings comprised three elements: silicon and tantalum, plus one of aluminium, chromium, iron or titanium. Six samples were prepared for each of the four coatings, making a total of 24 samples. Four candidate coatings (GHX054, GHX028, GHX036 and GHX042) have been down-selected for further testing, from the 24 compositions investigated (Table 2.3). Based on the data given in Table A7 of Appendix A, we evaluated the LCA data for these synthesised coatings each of 1 µm thick deposited over 1 m$^2$ area of substrate and are given in Table 4.12.

**Table 4.12 -** Mass, energy and transportation flows for coating deposition of amorphous metal coatings.

| Sample ID | Masses (kg) | | Energy | Transportation |
|---|---|---|---|---|
| | Coating materials | Argon | (kWh) | (tkm) |
| PVD_Si:Ta:Al (GHX054) | 0.0200 | 0.02624 | 1.3825 | 0.009248 |
| PVD_Si:Ta:Cr (GHX028) | 0.0201 | 0.03608 | 1.5100 | 0.011236 |
| PVD_Si:Ta:Fe (GHX036) | 0.0225 | 0.04920 | 1.9900 | 0.014340 |
| PVD_Si:Ta:Ti (GHX042) | 0.0192 | 0.04100 | 1.8630 | 0.012040 |

To improve the corrosion and scaling performances, the electroless nickel plating (ENP) method has been used to develop Ni-P/Ni-P-PTFE duplex coating on a carbon steel substrate, where in the top layer, PTFE particles were added in the Ni-P matrix to form the Ni-P-PTFE composite coating and in the bottom layer Ni-P coating has been synthesised. A total of 4 sets of samples with varied phosphorous content in bottom layer and top layer have been prepared and tested their performances against corrosion and scaling damages.

- LPLP (Low phosphorous in bottom and top layers)
- LPHP (Low phosphorous in bottom layer and high phosphorous in top layer)
- HPLP (High phosphorous in bottom layer and low phosphorous in top layer)
- HPHP (High phosphorous in bottom and top layers)

Among these, HPLP and HPHP duplex coatings showed better performances against corrosion and scaling damages. Based on the data given in Table A8 of Appendix A, we evaluated the LCA data for these synthesised coatings each of 1 µm thick deposited over 1 m$^2$ area of substrate and are given in Table 4.13.

**Table 4.13 -** Mass, energy and transportation flows for coating deposition of Ni-P/Ni-P-PTFE duplex coatings

| Coating ID | Mass flows (kg) | | | | | Transportation | Energy |
|---|---|---|---|---|---|---|---|
| | Nickel sulphate | Sodium hypophosphite | sodium citrate | Ammonium acetate | PTFE | (tkm) | (kWh) |
| DC_HPLP | 0.1755 | 0.1550 | 0.061425 | 0.13163 | 0.0585 | 0.116415 | 0.75 |
| DC_HPHP | 0.1755 | 0.1755 | 0.061425 | 0.14625 | 0.0585 | 0.123435 | 0.75 |

We have explored inventory data from ecoinvent version 3.6 database for various materials used in SOA, GHS and coating materials and processes. The dataset names have been selected from ecoinvent version 3.6 database for them and are listed in Table 4.14.

**Table 4.14** – Ecoinvent dataset names of materials and processes used.

| Materials/processes | Dataset names |
|---|---|
| C | Carbon black {GLO}\| production \| APOS, U |
| Mn | Manganese {RER}\| production \| APOS, U |
| Si | Silicon, metallurgical grade {RoW}\| production \| APOS, U |
| P | Phosphorus, white, liquid {RER}\| production \| APOS, U |
| S | Sulfite {RER}\| production \| APOS, U |
| N | Nitrogen, liquid {GLO}\| market for \| APOS, U |
| Cr | Chromium {RER}\| production \| APOS, U |
| Ni | Nickel, 99.5% {GLO}\| market for \| APOS, U |
| Fe | Ferrite {GLO}\| production \| APOS, U |
| Nb | Input from nature in ground |
| $TiO_2$ | Titanium dioxide {RER}\| production, chloride process \| APOS, U |
| Water | Water, deionised {Europe without Switzerland}\| water production, deionised \| APOS, U |
| Transportation | Transport, freight, lorry 16-32 metric ton, EURO6 {RER}\| transport, freight, lorry 16-32 metric ton, EURO6 \| APOS, U |
| Electricity | Electricity, medium voltage {GB}\| electricity voltage transformation from high to medium voltage \| APOS, U |
| Iron pellet | Iron pellet {GLO}\| production \| APOS, U |
| Ta | Tantalum, powder, capacitor-grade {GLO}\| production \| APOS, U |
| Aluminium oxide | Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}\| aluminium oxide production \| APOS, U |
| Ti | Titanium, primary {GLO}\| production \| APOS, U |
| Nickel sulfate | Nickel sulfate {GLO}\| production \| APOS, U |
| Sodium phosphate | Sodium phosphate {RER}\| production \| APOS, U |
| Sodium cyanide | Sodium cyanide {RER}\| production \| APOS, U |
| Ammonium thiocyanate | Ammonium thiocyanate {GLO}\| production \| APOS, U |
| PTFE | Tetrafluoroethylene {RER}\| production \| APOS, U |
| SiC | Silicon carbide {RER}\| production \| APOS, U |
| Acetone | Acetone, liquid {RER}\| production \| APOS, U |
| Isopropanol | Isopropanol {RER}\| production \| APOS, U |
| Argon | Argon, liquid {RER}\| production \| APOS, U |
| Hydrogen | Hydrogen, liquid {RER}\| market for \| APOS, U |
| Oxygen | Oxygen, liquid {RER}\| market for \| APOS, U |
| Methane | Methane, 96% by volume {RoW}\| biogas purification to methane 96 vol-% \| APOS, U |

## 4.2.2 LCIA Results of GeoHex Engineered Materials

According to ISO 14040:2006, the Life Cycle Impact Assessment (LCIA) seeks to understand and evaluate the magnitude and significance of potential environmental impacts of a product system or process using the results of the LCI. We have modelled three processes (Figure 3.3) to analyse the environmental impacts for the metal oxide nanoporous, MWCNT, amorphous metal and Ni-P/Ni-P-PTFE duplex coatings synthesised deposited through S-HVOF, CVD, PVD and ENP routes. Using the inventory data given in Tables 4.7-4.13 and the respective ecoinvent datasets (Table 4.14), the cradle to gate LCA analyses for 18 synthesised coatings deposited onto carbon and stainless steel each of 1 µm thick over 1 m$^2$ area have been evaluated and calculated using SimaPro 9.1.1.1 LCA tool considering the impact assessment methodology IMPACT 2002+ version 2.15.

**Metal Oxide Nanoporous Synthesised Coatings deposited through S-HVOF process**

Using the data described in Tables 4.7-4.10 and 4.14, LCA analyses of S-HVOF_$TiO_2$-10 and S-HVOF_$TiO_2$-20 synthesised coatings deposited onto carbon steel and stainless steel substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the environmental footprints in terms of single score for $TiO_2$-10 and $TiO_2$-20 synthesised coatings deposited over carbon steel and stainless steel substrates through S-HVOF process are presented in Figures 4.12 and 4.13, respectively. It is seen from Figure 4.12 that $TiO_2$-10 and $TiO_2$-20 synthesised coatings deposited over carbon steel showed the lower environmental footprints over 4 endpoint damage categories as compared with those of deposited over a stainless steel substrate. The quantification of environmental footprints of over 4 endpoint damage categories for $TiO_2$-10 and $TiO_2$-20 synthesised coatings is listed in Table 4.15.

**Table – 4.15** Quantification of environmental footprints over 4 endpoint damage categories for $TiO_2$-10 and $TiO_2$-20 synthesised coatings each of 1 µm thick over 1 m$^2$ area.

| Endpoint Damage categories | Unit | CS_GB_S-HVOF_TiO2-10 | CS_GB_S-HVOF_TiO2-20 | SS_GB_S-HVOF_TiO2-10 | SS_GB_S-HVOF_TiO2-20 |
|---|---|---|---|---|---|
| Human health | DALY | 0.000197 | 0.000197 | 0.001293 | 0.001293 |
| Ecosystem quality | PDF*m2*yr | 72.461673 | 72.465902 | 668.409469 | 668.413698 |
| Climate change | kg CO2 eq | 65.375010 | 65.385161 | 297.469012 | 297.479163 |
| Resources | MJ primary | 971.218768 | 971.401408 | 4975.425823 | 4975.608463 |

Since the units of environmental footprints such as human health, climate change and others are expressed in their respective units, it is required to convert these units to a common scale to evaluate the total environmental footprints in terms of single score expressed in points (Pt) or millipoints (mPt). The environmental footprints of 4 damage categories in units of mPt for $TiO_2$-10 and $TiO_2$-20 synthesised coatings deposited onto carbon steel and stainless steel substrates is shown in Figure 4.13. It is obtained that the total environmental footprints of $TiO_2$ synthesised coatings deposited onto the stainless steel substrate is about 6.4 times higher than those deposited over carbon steel substrate. From Table 4.15 it has been demonstrated that the carbon footprints of $TiO_2$ synthesised coatings deposited onto the stainless steel substrate is about 4.5 times higher than those deposited over carbon steel substrate.

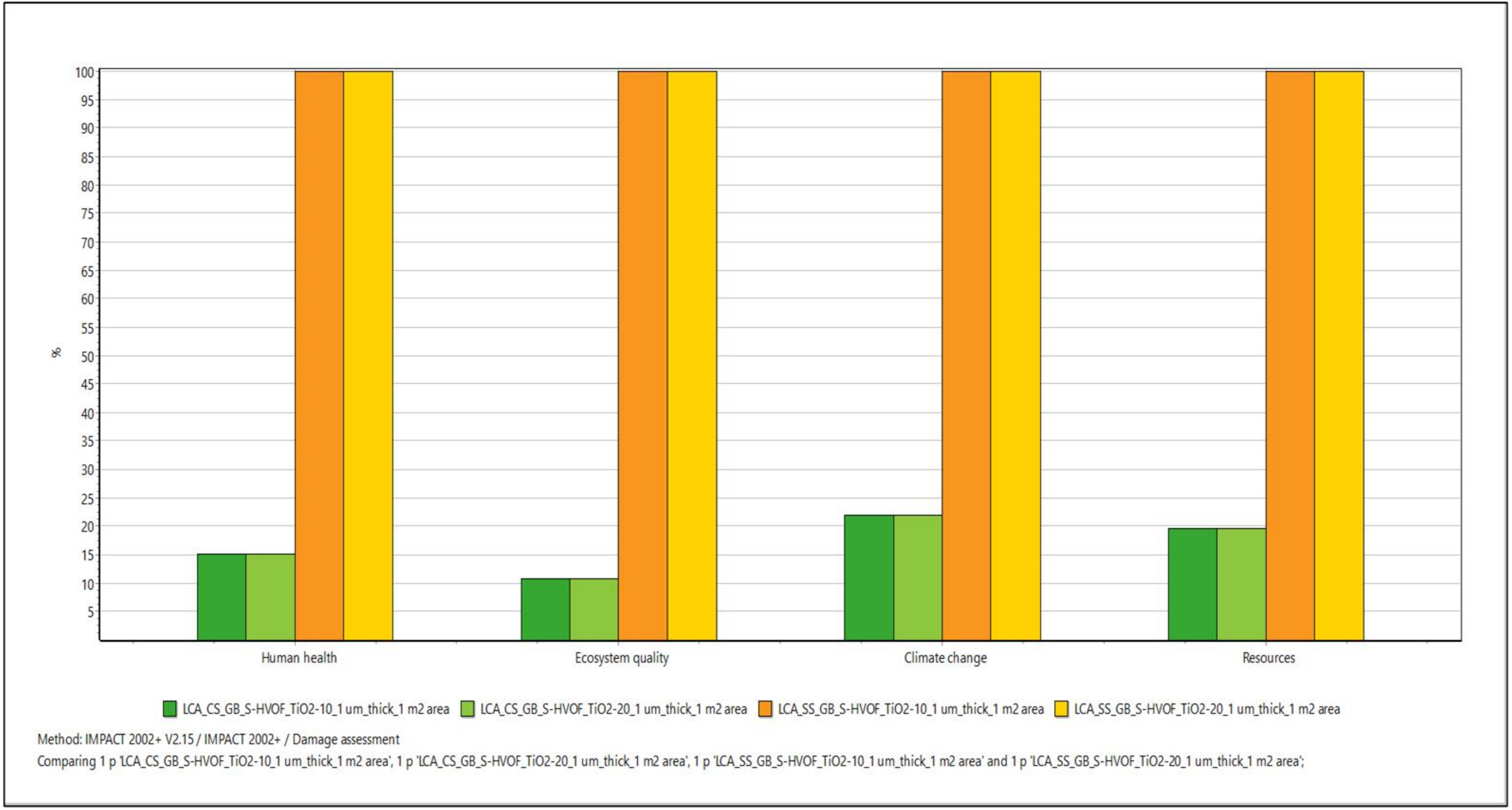


**Figure 4.12 -** Comparisons of 4 endpoint damage categories for $TiO_2$-10 and $TiO_2$-20 synthesised coatings deposited over carbon steel and stainless steel substrates through S-HVOF process.

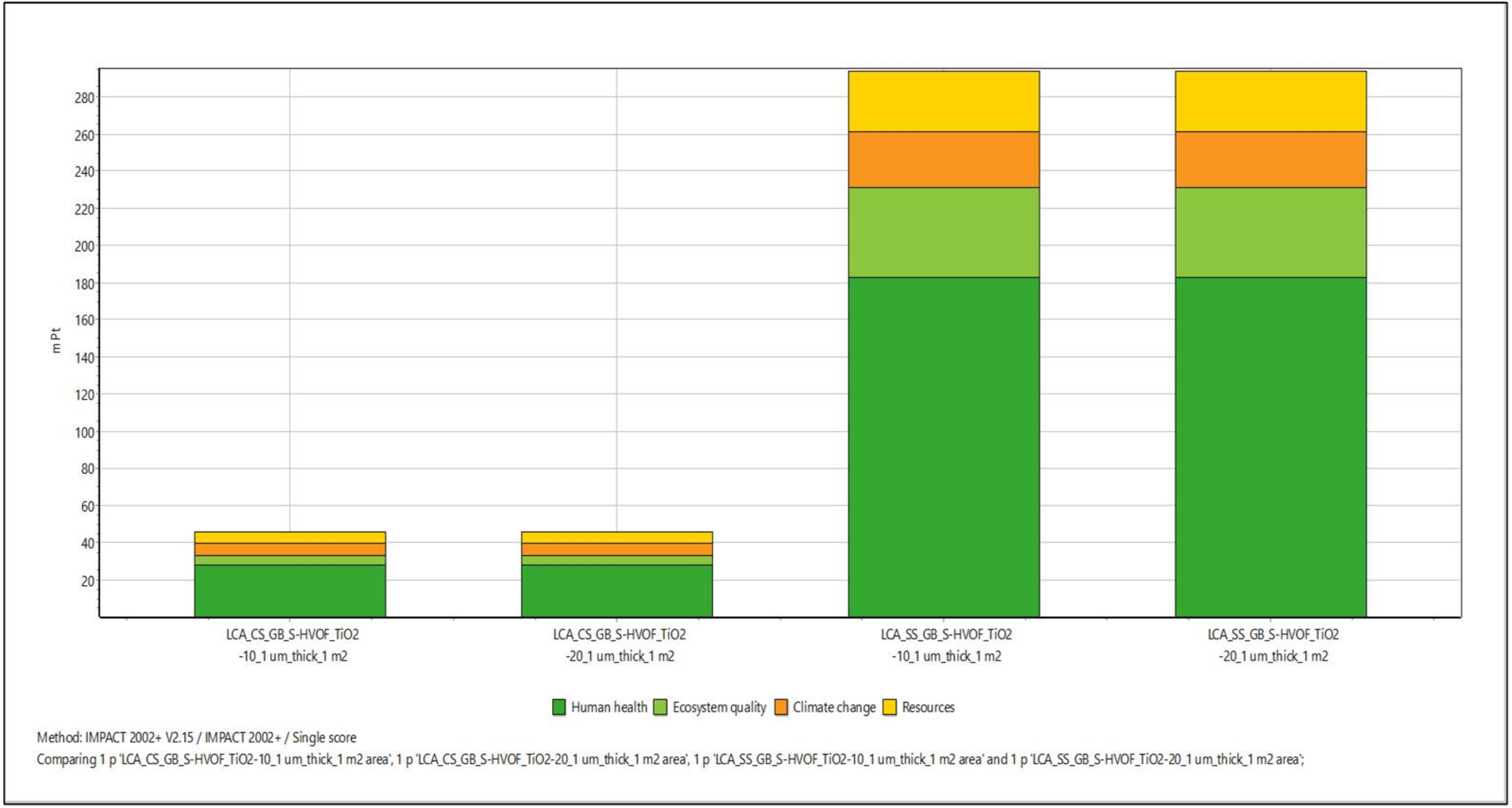


**Figure 4.13 -** Comparisons of single score results for $TiO_2$-10 and $TiO_2$-20 synthesised coatings deposited over carbon steel and stainless steel substrates through S-HVOF process.

### MWCNT Synthesised coatings deposited through CVD process

Using the data described in Tables 4.7-4.9, 4.11 and 4.14, LCA analyses of CVD_MWCNT synthesised coating deposited onto carbon steel and stainless steel substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the environmental impacts in terms of single score for MWCNT synthesised coating deposited over carbon steel and stainless steel substrates through the CVD process are presented in Figures 4.14 and 4.15, respectively. The quantification of environmental footprints of over 4 endpoint damage categories for MWCNT synthesised coatings and is listed in Table 4.16.

**Table – 4.16** Quantification of environmental footprints over 4 endpoint damage categories for MWCNT synthesised coatings each of 1 µm thick over 1 $m^2$ area

| Endpoint Damage categories | Unit | CS_GB_CVD_MWCNT | SS_GB_CVD_MWCNT |
|---|---|---|---|
| Human health | DALY | 0.000244 | 0.001340 |
| Ecosystem quality | PDF*m2*yr | 108.996105 | 704.943901 |
| Climate change | kg CO2 eq | 173.941962 | 406.035963 |
| Resources | MJ primary | 3885.666786 | 7889.873842 |

It is seen from Figure 4.15 that the total environmental footprint of the CS_GB_CVD_MWCNT is about 3.9 times lower than that of the CS_GB_MWCNT synthesised coating. It is also demonstrated from Table 4.16 that the carbon footprint of CS_GB_CVD_MWCNT synthesised coating is about 2.3 times lower than that of SS_GB_CVD_MWCNT synthesised coating.

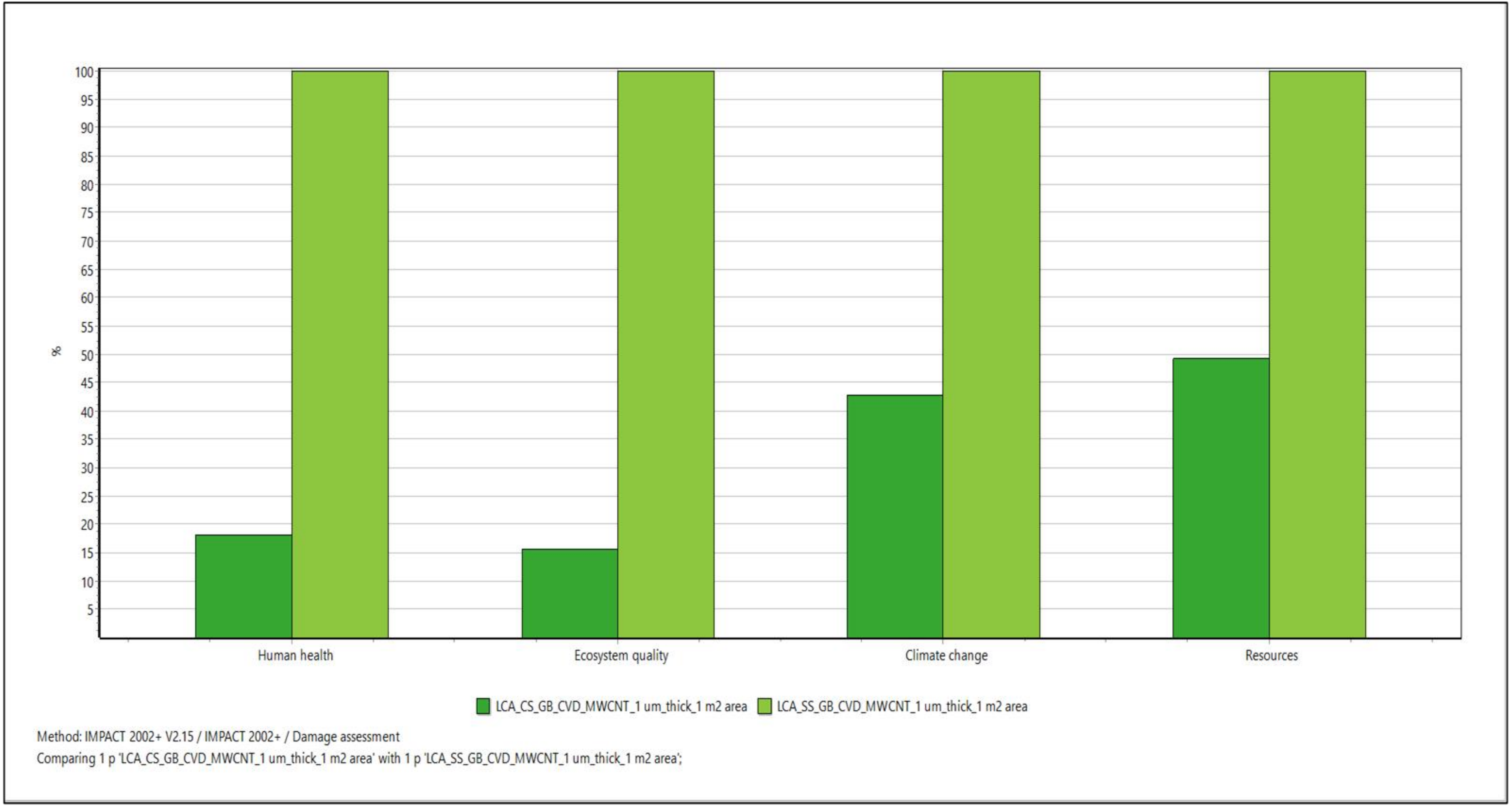


**Figure 4.14 -** Comparisons of 4 endpoint damage categories for MWCNT synthesised coatings deposited over carbon steel and stainless steel substrates through CVD process.

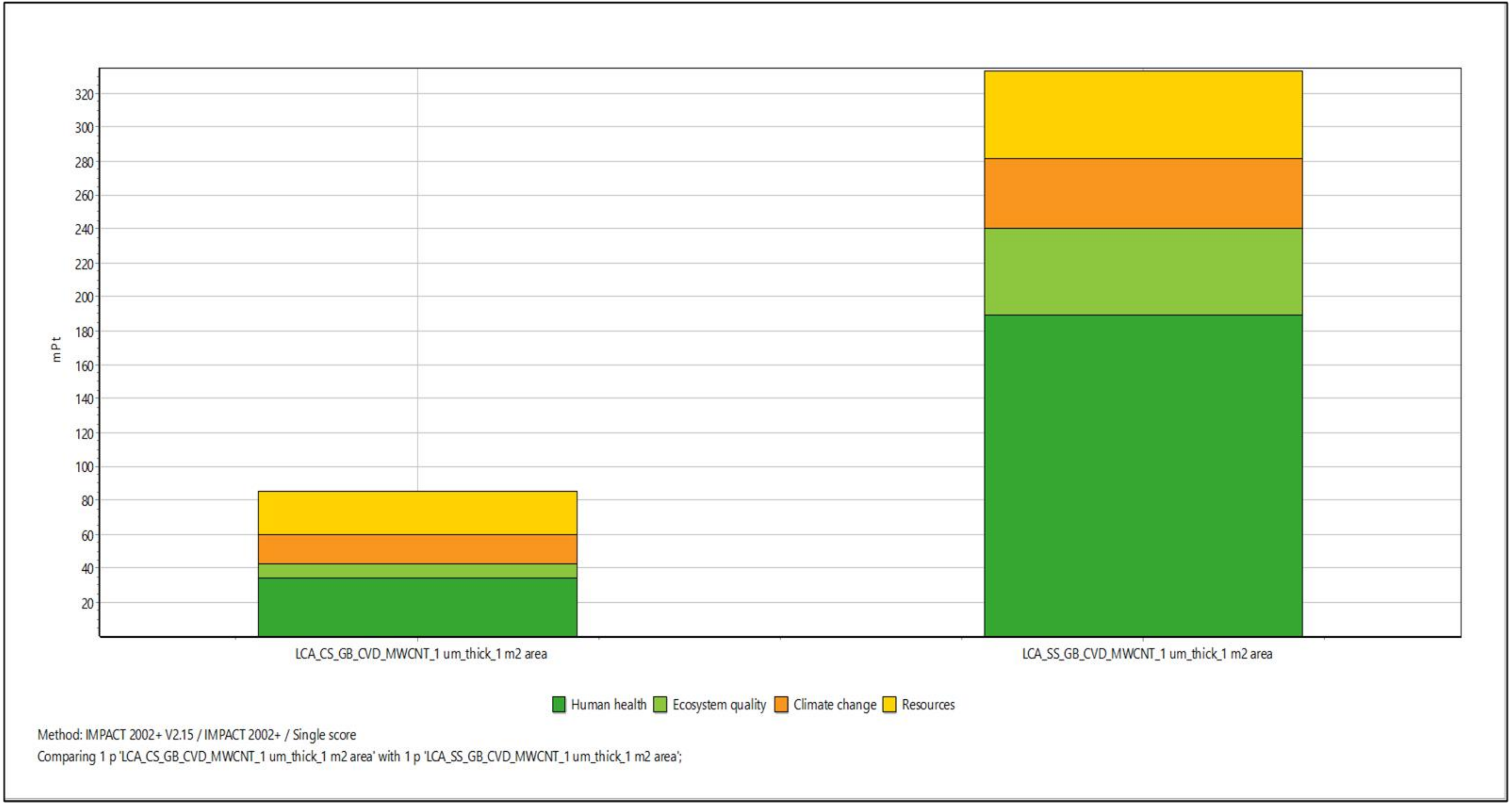


**Figure 4.15 -** Comparisons of single score results for MWCNT synthesised coatings deposited over carbon steel and stainless steel substrates through CVD process.

### Amorphous metal coatings deposited through PVD (Sputtering) process

Using the data described in Tables 4.7-4.9, 4.12 and 4.14, LCA analyses of four amorphous metal synthesised coatings (PVD_Si:Ta:Al, PVD_Si:Ta:Cr, PVD_Si:Ta:Fe and PVD_Si:Ta:Ti) deposited onto carbon steel and stainless steel substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the environmental impacts in terms of single score for these synthesised coatings deposited over carbon steel and stainless steel substrates through CVD process are presented in Figures 4.16 and 4.17, respectively. The quantification of environmental footprints of over 4 endpoint damage categories for these synthesised coatings and is listed in Table 4.17.

**Table – 4.17** Quantification of environmental footprints over 4 endpoint damage categories for amorphous metal synthesised coatings each of 1 µm thick over 1 m$^2$ area

| **Damage category** | **Unit** | **CS_ST_PVD_Si:Ta:Al** | **CS_ST_PVD_Si:Ta:Cr** | **CS_ST_PVD_Si:Ta:Fe** | **CS_ST_PVD_Si:Ta:Ti** | **SS_ST_PVD_Si:Ta:Al** | **SS_ST_PVD_Si:Ta:Cr** | **SS_ST_PVD_Si:Ta:Fe** | **SS_ST_PVD_Si:Ta:Ti** |
|---|---|---|---|---|---|---|---|---|---|
| Human health | DALY | 0.0002 | 0.0002 | 0.0002 | 0.0002 | 0.0013 | 0.0013 | 0.0013 | 0.0013 |
| Ecosystem quality | PDF*m2*yr | 74.6741 | 74.9151 | 76.1186 | 74.7525 | 670.4512 | 670.6922 | 671.8956 | 670.5300 |
| Climate change | kg CO2 eq | 72.6381 | 72.9828 | 74.4723 | 72.9345 | 303.2147 | 303.5594 | 305.0489 | 303.5111 |
| Resources | MJ primary | 1171.5369 | 1178.0861 | 1203.1837 | 1178.0089 | 5123.5907 | 5130.1399 | 5155.2375 | 5130.0627 |

From Table 4.17, it is obtained that the carbon footprint (climate change) of amorphous metal synthesised coatings deposited onto stainless steel is about 4 times higher than those deposited onto carbon steel. It is seen from Figure 4.16 that four amorphous metal synthesised coatings deposited over carbon steel showed the lower environmental footprints over 4 endpoint damage categories as compared with those of deposited over stainless steel substrate. It is also demonstrated from Figure 4.17 that the total environmental footprint of the amorphous metal coatings coated carbon steel is about 6 times lower than that of coated stainless steel.

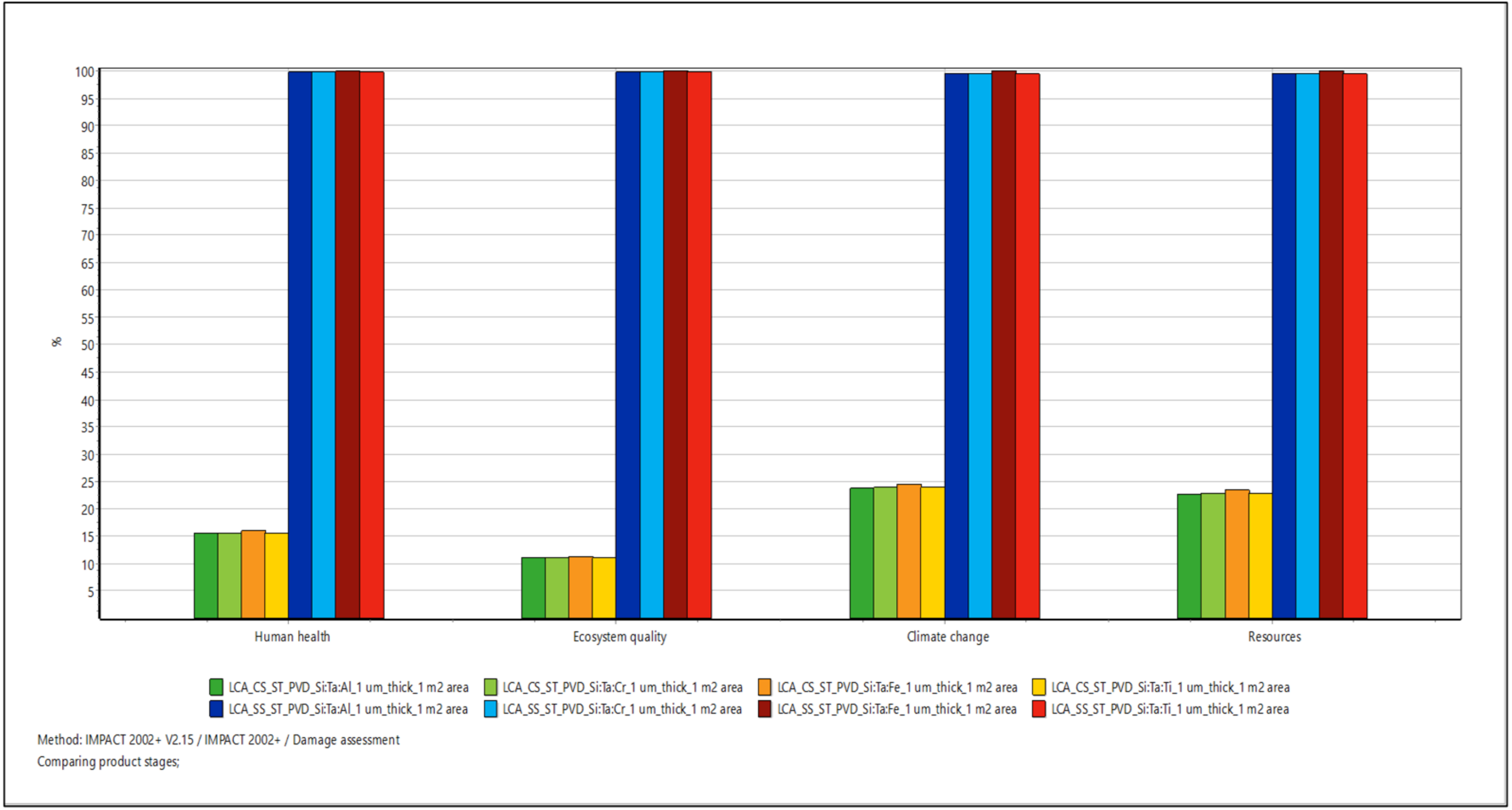


**Figure 4.16 –** Comparisons of 4 endpoint damage categories for amorphous metal synthesised coatings deposited over carbon steel and stainless steel substrates through PVD process

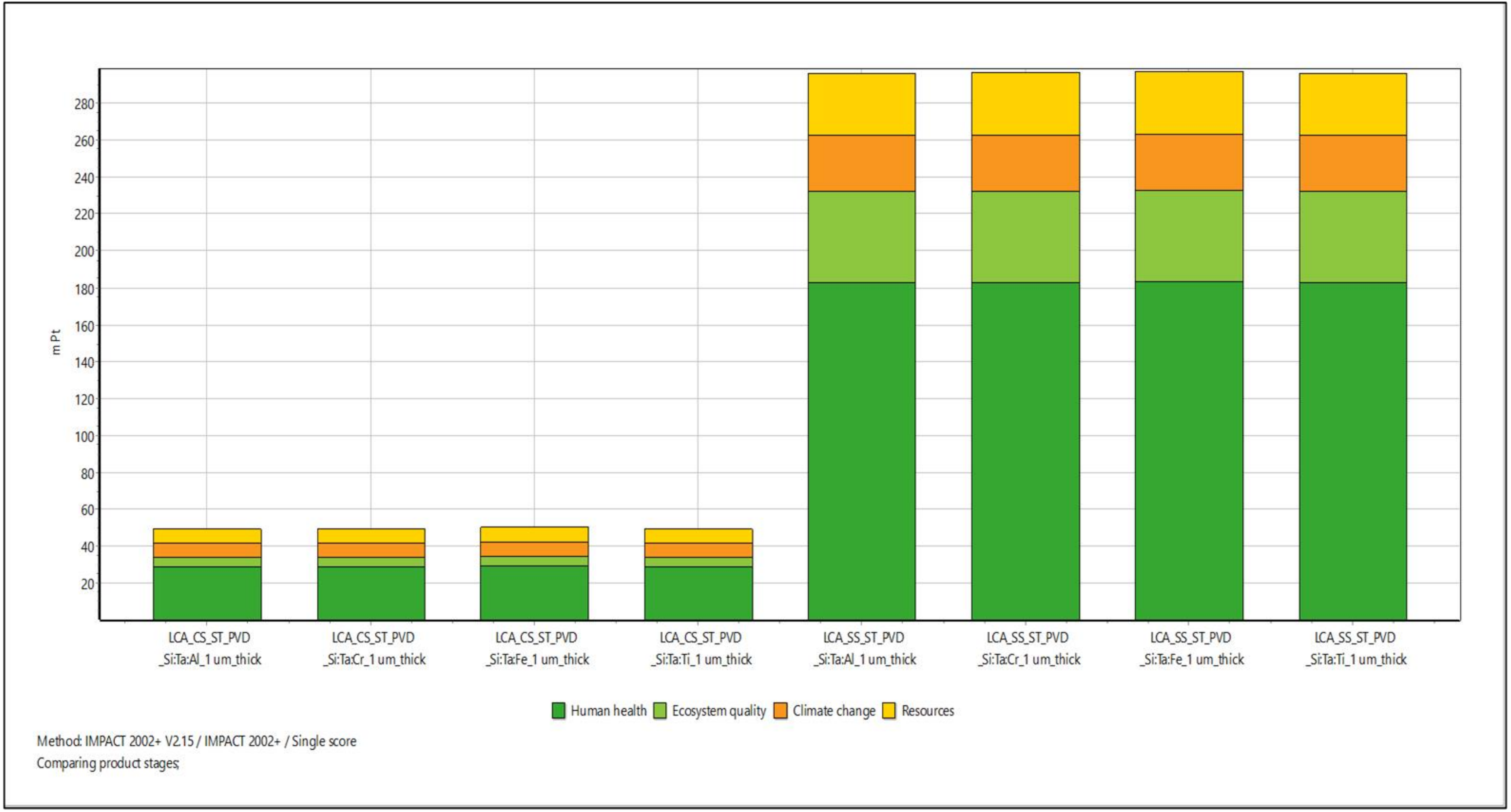


**Figure 4.17 -** Comparisons of single score results for amorphous metal synthesised coatings deposited over carbon steel and stainless steel substrates through PVD process.

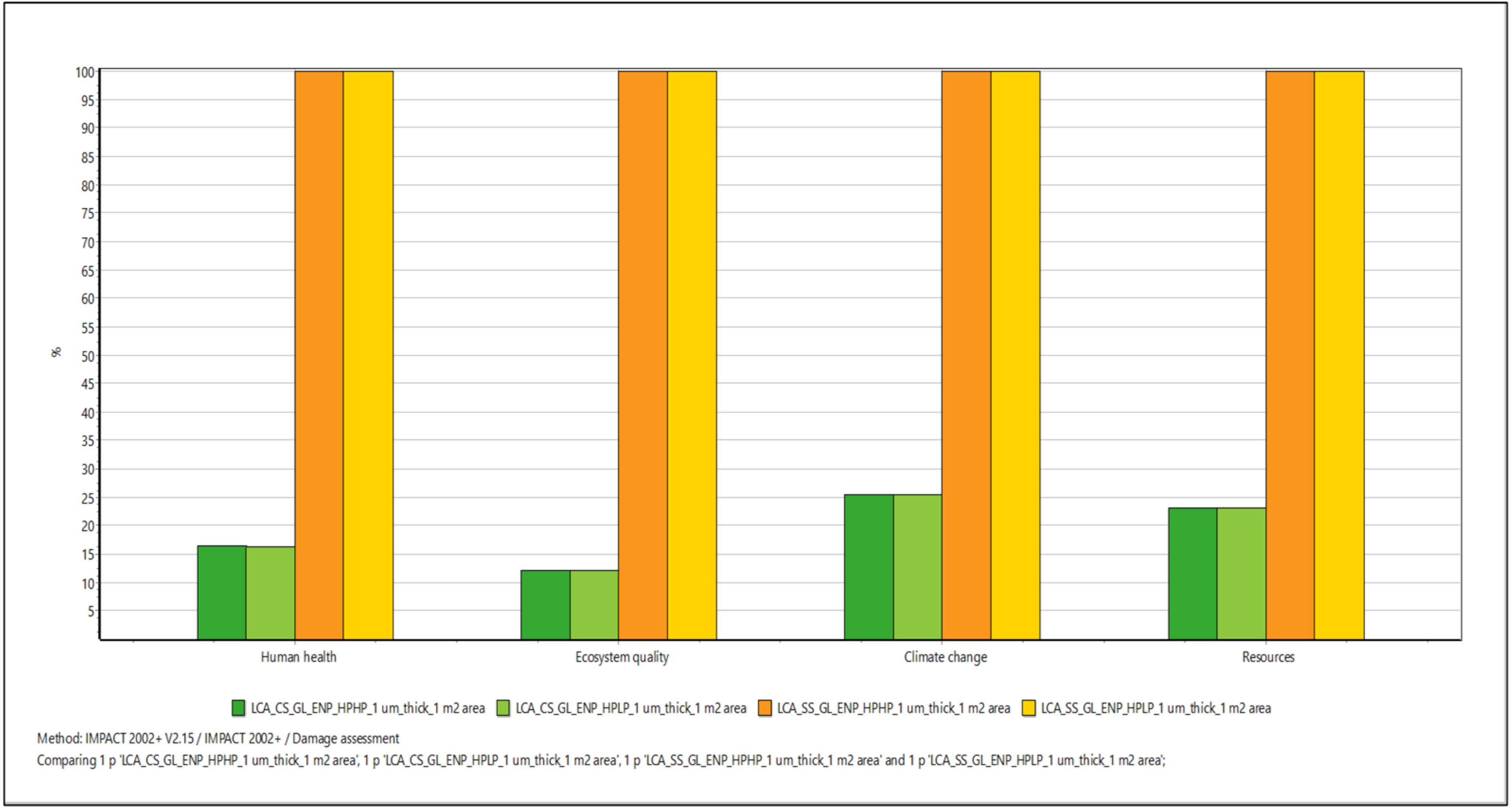
### Ni-P/Ni-P-PTFE Duplex Coatings deposited through ENP process

Using the data described in Tables 4.7-4.9, 4.13 and 4.14, LCA analyses of two Ni-P/NiP-PTFE duplex synthesised coatings (HPLP and HPHP) deposited onto carbon steel and stainless steel substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the environmental impacts in terms of single score for these synthesised coatings deposited over carbon steel and stainless steel substrates through ENP process are presented in Figures 4.18 and 4.19, respectively. The quantification of environmental footprints of over 4 endpoint damage categories for these synthesised coatings and is listed in Table 4.18.

**Table – 4.18** Quantification of environmental footprints over 4 endpoint damage categories for these duplex synthesised coatings each of 1 µm thick over 1 $m^2$ area

| Damage category | Unit | CS_GL_ENP_ HPHP | CS_GL_ENP_ HPLP | SS_GL_ENP_ HPHP | SS_GL_ENP_ HPLP |
|---|---|---|---|---|---|
| Human health | DALY | 0.0002 | 0.0002 | 0.0013 | 0.0013 |
| Ecosystem quality | PDF*m2*yr | 81.7759 | 81.7290 | 677.7237 | 677.6768 |
| Climate change | kg CO2 eq | 79.4463 | 79.3660 | 311.5403 | 311.4600 |
| Resources | MJ primary | 1199.1718 | 1197.8966 | 5203.3788 | 5202.1036 |

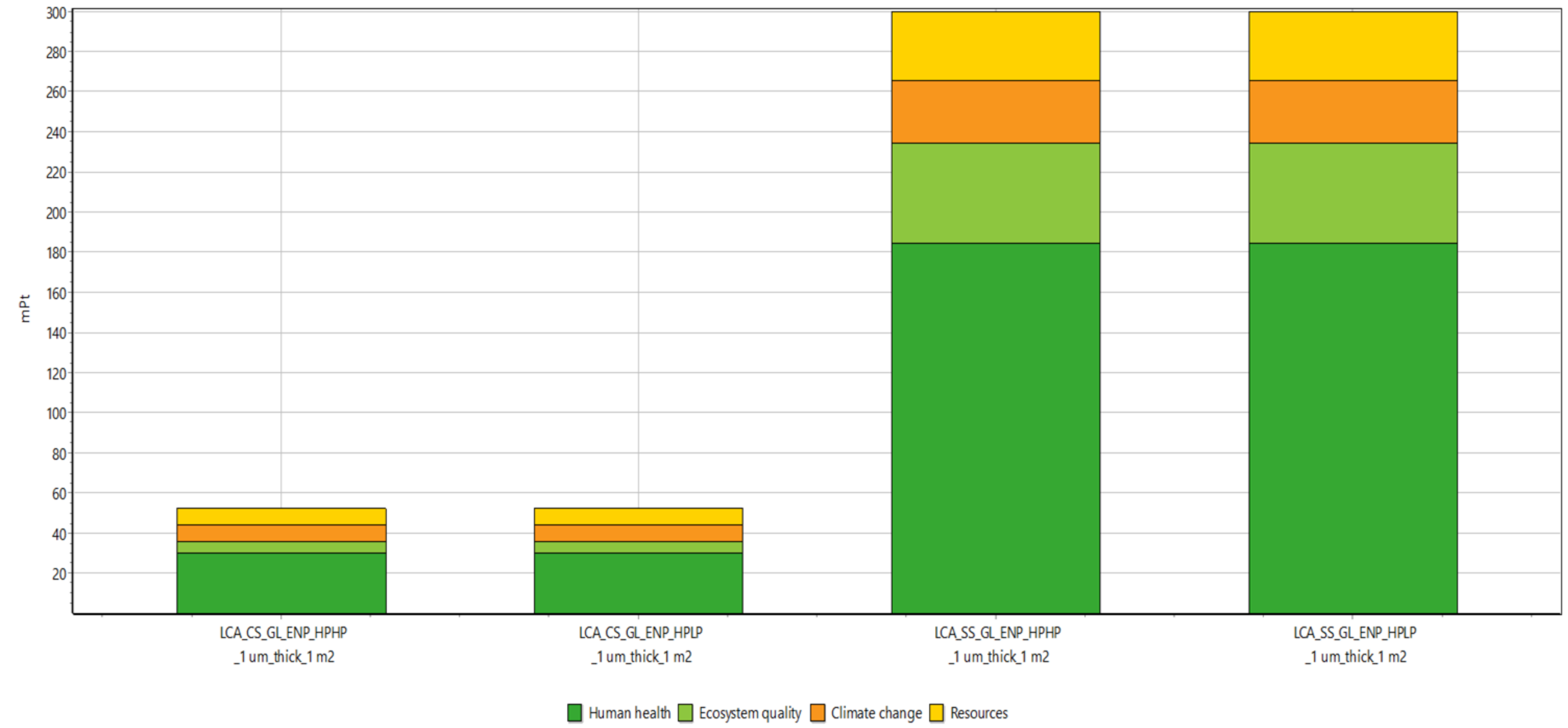
It is seen from Table 4.18 that the carbon footprint (climate change) of duplex synthesised coatings deposited onto stainless steel is about 3.9 times higher than those deposited onto carbon steel. From Figure 4.18, duplex synthesised coatings deposited over carbon steel showed the lower environmental footprints over 4 endpoint damage categories as compared with those of deposited over stainless steel substrate. It is also demonstrated from Figure 4.19 that the total environmental footprint of the duplex coatings coated carbon steel is about 5.7 times lower than that of coated stainless steel.



Method: IMPACT 2002+ V2.15 / IMPACT 2002+ / Damage assessment

Comparing 1 p 'LCA_CS_GL_ENP_HPHP_1 um_thick_1 m2 area', 1 p 'LCA_CS_GL_ENP_HPLP_1 um_thick_1 m2 area', 1 p 'LCA_SS_GL_ENP_HPHP_1 um_thick_1 m2 area' and 1 p 'LCA_SS_GL_ENP_HPLP_1 um_thick_1 m2 area';

**Figure 4.18 –** Comparisons of 4 endpoint damage categories for duplex HPLP and HPHP synthesised coatings deposited over carbon steel and stainless steel substrates through ENP process



Method: IMPACT 2002+ V2.15 / IMPACT 2002+ / Single score
Comparing 1 p 'LCA_CS_GL_ENP_HPHP_1 um_thick_1 m2 area', 1 p 'LCA_CS_GL_ENP_HPLP_1 um_thick_1 m2 area', 1 p 'LCA_SS_GL_ENP_HPHP_1 um_thick_1 m2 area' and 1 p 'LCA_SS_GL_ENP_HPLP_1 um_thick_1 m2 area';

**Figure 4.19 -** Comparisons of single score results for HPLP and HPHP duplex synthesised coatings deposited over carbon steel and stainless steel substrates through ENP process.

## 4.3 DISCUSSIONS

The sustainability assessment of single phase heat exchanger materials has been investigated by combining the costing and environmental performances of four types of coating materials including $TiO_2$, MWCNT, amorphous metal and Ni-P/Ni-P-PTFE duplex deposited onto carbon steel and stainless steel developed for tubes and plates of heat exchangers as an alternative to the state of art materials (SOA) 316L and 254SMO. $TiO_2$ and MWCNT nanoporous coatings are being developed for improving the heat transfer efficiency on the ORC liquid or vapour side of the plates and tubes of 3 different heat exchangers: recuperator, preheater and superheater. Amorphous metal and Ni-P/Ni-P-PTFE duplex coatings are also being developed for combating corrosion and scaling damage on the brine side of the tubes and plates of 2 different heat exchangers: preheater and superheater.

The costs of SOA materials 316L and 254SMO each of dimension 1000mm x 1000 mm x 6 mm have been calculated from the purchased cold rolled sheets' unit cost provided by the partner TWI (Table A1 of Appendix A) and estimated to be €350 and €4020, respectively. Four types of synthesised coatings deposited onto the carbon steel substrate are recommended as alternatives to SOA materials 316L and 254SMO. Using the costing results from the Subsection 4.1.2 and SOA materials, the relative costs of these synthesised coatings deposited onto carbon steel along with the relative costs of SOA materials 316L and 254SMO have been evaluated and are shown in Figures 4.20 and 4.21, respectively. It is seen from Figure 4.20 that only synthesised $TiO_2$ coatings deposited onto carbon steel substrate, offer a cost saving compared to SOA material 316L, with the analysis showing about 57% cost savings.

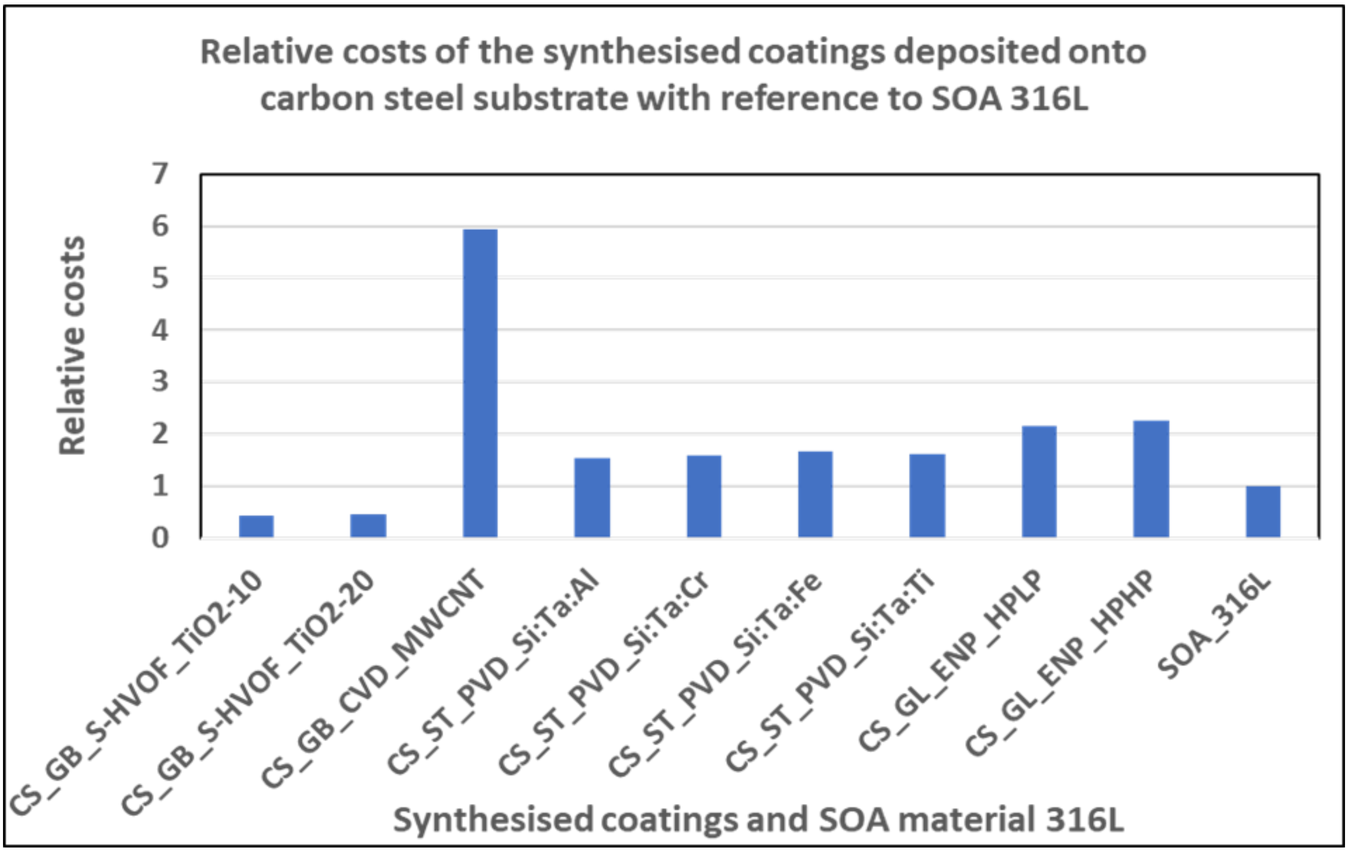


Figure 4.20 – Relative costs of the synthesised coatings deposited onto carbon steel and SOA material 316L.

It is demonstrated from Figure 4.21 that all the synthesised coatings $TiO_2$, MWCNT, amorphous metal Si:Ta:Al and Ni-P-PTFE duplex HPHP materials offer a cost saving when deposited onto carbon steel substrate as an alternative to SOA material 254SMO, giving cost savings of about 96%, 48%, 87%, and 80%, respectively.

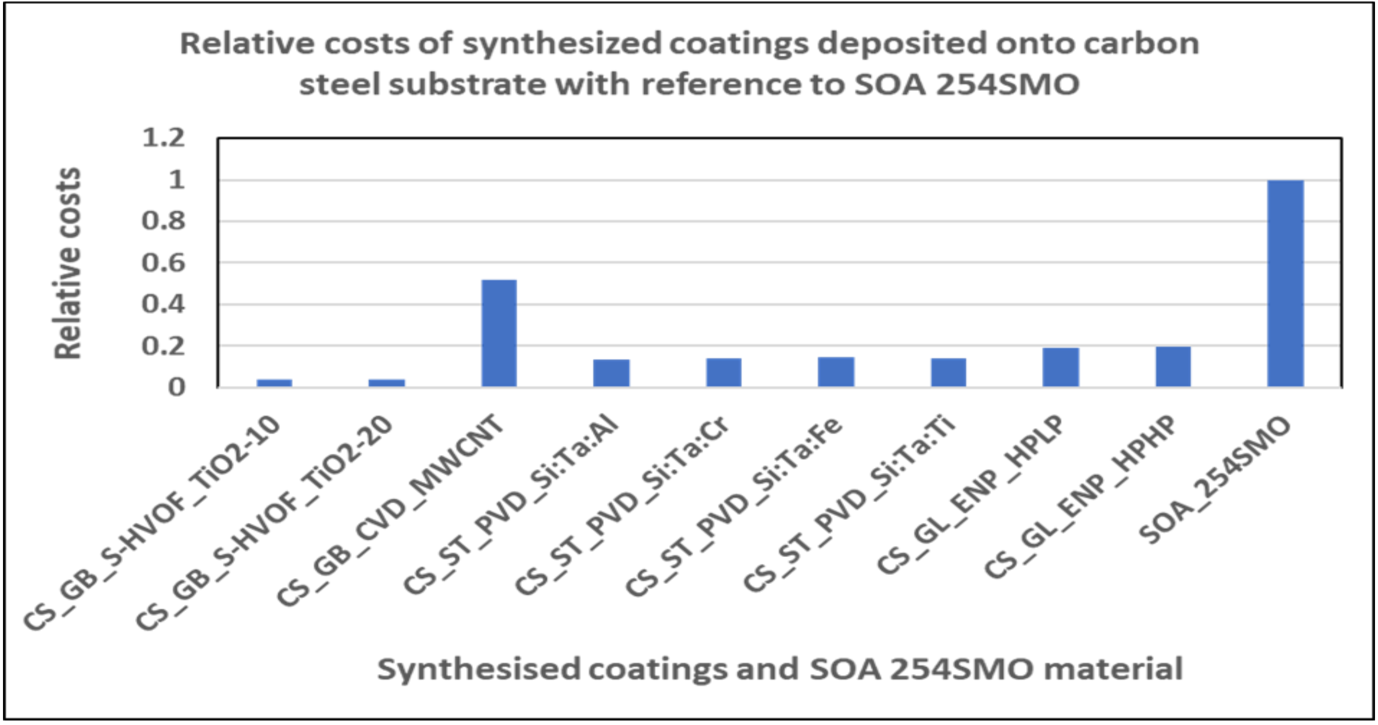


Figure 4.21 - Relative costs of the synthesised coatings deposited onto carbon steel and SOA material 254SMO.

Using the costing results from the Subsection 4.1.2 and SOA material, the relative costs of all the synthesised coatings deposited onto stainless steel (316L) along with the relative costs of SOA material 254SMO have been evaluated and is shown in Figure 4.22.

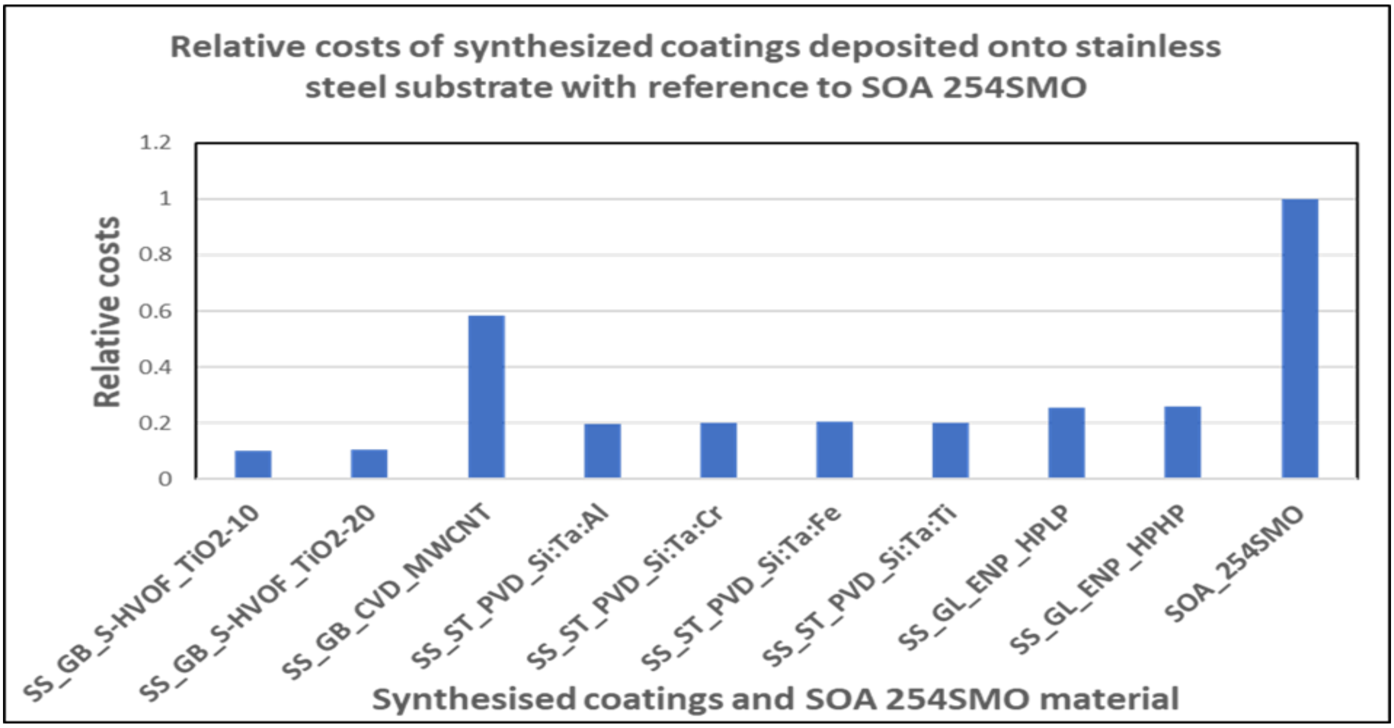


Figure 4.22 – Relative costs of the synthesised coatings deposited onto stainless steel and SOA material 254SMO.

In Figure 4.22, it has been shown that all the synthesised coatings $TiO_2$, MWCNT, amorphous metal Si:Ta:Al and Ni-P-PTFE duplex HPHP materials offer a cost saving when deposited onto stainless steel 316L as an alternative to SOA material 254SMO are about 90%, 42%, 80%, and 74% lower, respectively.

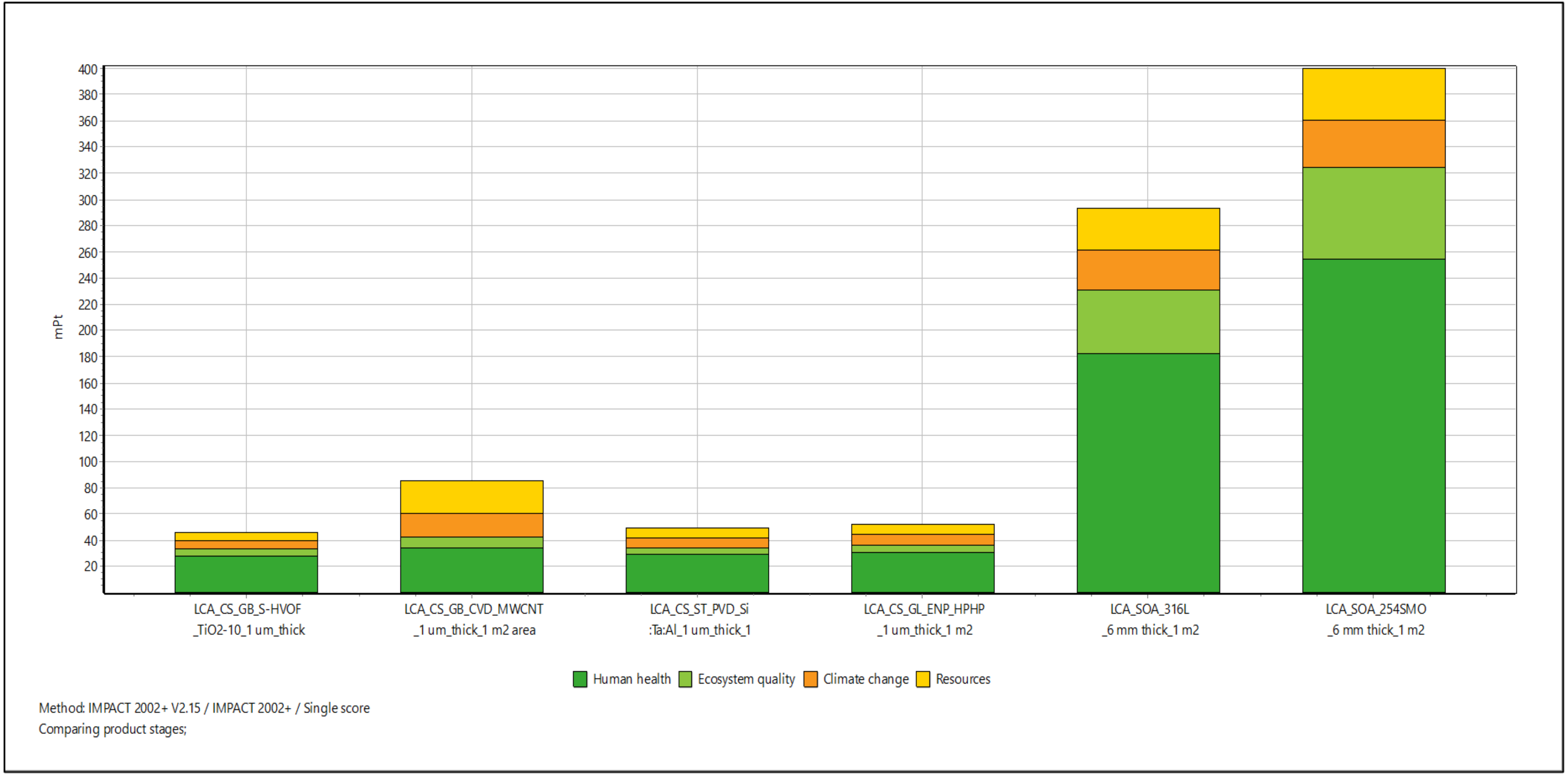
The environmental footprints in units of mPt of four different synthesised coatings ($TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex) each of 1 µm thick deposited onto carbon steel substrate of 1 $m^2$ area for four endpoint damage categories have been compared with that of SOA 316L and 254SMO materials each of 1 $m^2$ area and presented in Figure 4.23. It is clearly seen from the single score results shown in Figure 4.23 that the total environmental footprints of $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex coatings and SOA 316L and 254SMO materials are about 46, 85, 49, 52, 293 and 400 mPt, respectively. The quantification of environmental footprints over 4 endpoint damage categories for these synthesised coatings deposited onto carbon steel and SOA 316L and 254 SMO materials are listed in Table 4.19.

**Table 4.19 –** Quantification of environmental footprints over 4 endpoint damage categories for these synthesised coatings each of 1 µm thick over 1 $m^2$ area and SOA 316L material

| Damage category | Unit | CS_GB_S-HVOF TiO2-10 | CS_GB_CVD_MWCNT | CS_ST_PVD_Si:Ta:Al | CS_GL_ENP_HPHP | SOA_316L | 254SMO |
|---|---|---|---|---|---|---|---|
| Human health | DALY | 0.000197 | 0.000244 | 0.000204 | 0.000214 | 0.001292 | 0.001809 |
| Ecosystem quality | PDF*m2*yr | 72.4617 | 108.9961 | 74.6741 | 81.7759 | 668.7220 | 948.9455 |
| Climate change | kg CO2 eq | 65.3750 | 173.9420 | 72.6381 | 79.4463 | 296.2633 | 357.5835 |
| Resources | MJ primary | 971.22 | 3885.67 | 1171.54 | 1199.17 | 4932.85 | 5988.84 |

It is evident from Table 4.19 that the carbon footprint savings of about 78%, 41%, 75%, 73% for using $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited onto carbon steel, respectively instead of using SOA 316L material and the carbon footprint savings of about 81%, 51%, 80%, 78% for using $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited on to carbon steel, respectively instead of using SOA 254SMO material.

The environmental footprints in units of mPt of four different synthesised coatings ($TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex) each of 1 µm thick deposited onto stainless steel substrate of 1 $m^2$ area for four damage categories have been compared with that of SOA 254SMO material of 1 $m^2$ area and presented in Figure 4.24. It is evident from the single score results shown in Figure 4.24 that the total environmental footprints of $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited onto stainless steel 316L and 254SMO materials are about 294, 333,296, 300, and 400 mPt, respectively.



Method: IMPACT 2002+ V2.15 / IMPACT 2002+ / Single score
Comparing product stages;

Figure 4.23 - Comparisons of single score results for $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex synthesised coatings deposited over carbon steel and SOA 316L and 254SMO materials.

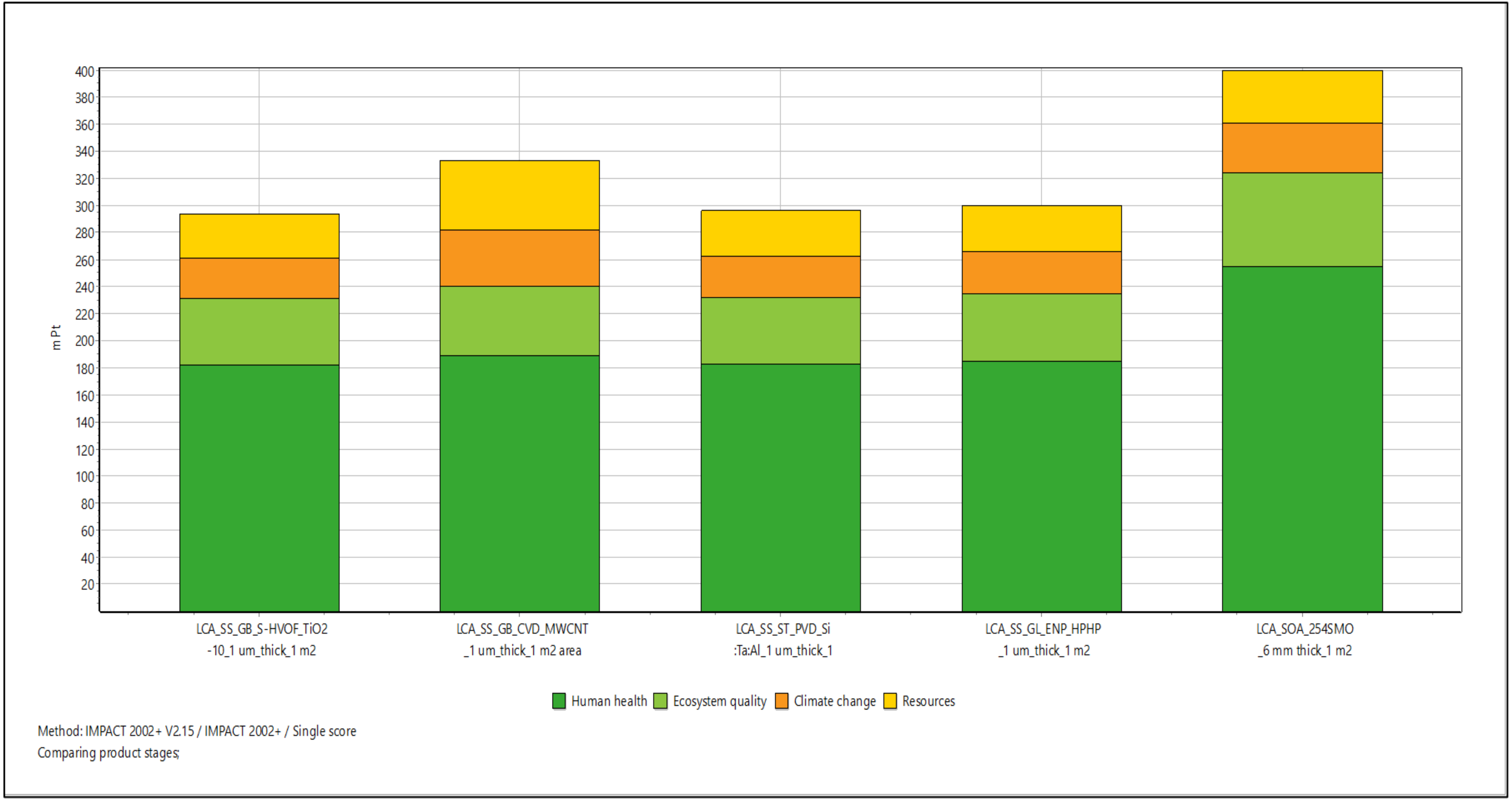


Figure 4.24 - Comparisons of single score results for $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex synthesised coatings deposited over stainless steel and SOA 254SMO material.

# 5. CONCLUSIONS

The aim of this sustainability assessment was to conduct a cradle to gate life cycle assessment and costing analyses of four types of synthesised coatings developed for single phase heat exchangers to help with their decision-making for the applications of GeoHex materials in preheater, superheater and recuperator. The research question was to determine which synthesised coating was the best alternative to SOA material from both environmental and economic points of view. In Figures 4.20-4.21, the relative costs of $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited onto carbon steel and stainless steel developed for heat exchangers along with SOA 316L and 254SMO materials have been demonstrated. The results of environmental footprints in units of mPt of $TiO_2$, MWCNT, Si:Ta:Al and HPHP duplex deposited onto carbon steel substrate of 1 $m^2$ area for four endpoint damage categories is presented in Figure 4.23 along with SOA 316L and 254SMO materials each of 1 $m^2$ area. From these results, the relative costs and the relative environmental footprints of these GeoHex coating materials deposited onto carbon steel with respect to SOA materials have been evaluated and listed in Table 5.1.

**Table 5.1 –** The relative costs and environmental footprints for $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited onto the carbon steel with respect to SOA materials.

| Synthesised coatings and SOA materials ID | Relative costs with respect to SOA material | | Relative environmental footprints with respect to SOA material | |
|---|---|---|---|---|
| | 316L | 254SMO | 316L | 254SMO |
| CS_GB_S-HVOF_$TiO_2$-10 | 0.43 | 0.04 | 0.15 | 0.12 |
| CS_GB_CVD_MWCNT | 5.94 | 0.52 | 0.29 | 0.21 |
| CS_ST_PVD_Si:Ta:Al | 1.54 | 0.13 | 0.17 | 0.12 |
| CS_GL_ENP_HPHP | 2.25 | 0.20 | 0.18 | 0.13 |
| SOA_316L | 1.00 | - | 1.00 | - |
| SOA_254SMO | - | 1.00 | - | 1.00 |

Using GeoHex materials alternative to SOA 316L material, the metal oxide nanoporous coating material $TiO_2$-10 has been demonstrated

- 57% cost savings and
- 85% environmental footprint savings.

It is indicated that the $TiO_2$-10 synthesised coatings deposited onto carbon steel developed for improving the heat transfer efficiency on the ORC liquid or vapour side of the plates and tubes of 3 different heat exchangers: recuperator, preheater and superheater is the best alternative to SOA material 316L from economic and environmental perspectives. It is evident from Table 5.1 that the environmental savings of Si:Ta:Al and HPHP duplex synthesised coatings deposited onto carbon steel alternative to SOA 316L material showed about 83% and 82%, whereas the respective costs are about 1.54 and 2.25 times higher than that of SOA material 316L, respectively.

Using GeoHex materials alternative to SOA 254SMO material, all the GeoHex materials $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex deposited onto carbon steel showed:

- cost savings of about 96%, 48%, 87%, and 80% and
- environmental footprint savings of about 88%, 79%, 88% and 87%, respectively.

The results from Figures 4.22 and 4.24, the relative costs and the relative environmental footprints of these GeoHex coating materials $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex deposited onto stainless steel 316L with respect to SOA material 254SMO have been evaluated and listed in Table 5.2.

**Table 5.2 -** The relative costs and environmental footprints for $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex coatings deposited onto the stainless steel 316L with respect to SOA material 254SMO

| Synthesised coatings and SOA materials ID | Relative costs of GeoHex materials with respect to SOA 254SMO | Relative environmental footprints with respect to SOA 254SMO |
|---|---|---|
| SS_GB_S-HVOF_$TiO_2$-10 | 0.10 | 0.73 |
| SS_GB_CVD_MWCNT | 0.58 | 0.83 |
| SS_ST_PVD_Si:Ta:Al | 0.20 | 0.74 |
| SS_GL_ENP_HPHP | 0.26 | 0.75 |
| SOA_254SMO | 1.00 | 1.00 |

Using GeoHex materials alternative to SOA 254SMO material, all the GeoHex materials $TiO_2$-10, MWCNT, Si:Ta:Al and HPHP duplex deposited onto stainless steel 316L showed:

- cost savings of about 90%, 42%, 80%, and 74% and
- environmental footprint savings of about 27%, 17%, 26% and 25%, respectively.

Based on the sustainability assessment and the conclusions from this study there are some recommendations that are of interest to heat exchanger component manufacturers in their investment decision.

- Water footprint impact category can be included from an environmental perspective.
- The economical evaluation with costing analyses can be improved by conducting a complete life cycle costing analysis.

# APPENDIX A: Inventoried data provided by the partners and cost components calculations

**Table A1 -** Substrate and SOA materials cost calculations[17]

AIM - to determine the cost of 1 m$^2$ area SOA and substrate materials [€/m$^2$], calculated from the purchased cold rolled of 6 mm thick sheet [€/kg]

| Material type | Grade of the materials | Substrate dimension used | Density of the material | Mass of 1 m$^2$ area substrate of 6 mm thick | Unit cost of purchased cold rolled substrate material of 6 mm thick | Cost of substrate material for 1 m$^2$ area of 6 mm thick | Hardware power for cutting 1 m$^2$ area of the substrate | Machining time for cutting 1 m$^2$ area of the substrate | Electrical energy used for cutting | Unit cost of electricity | Electrical energy cost for cutting/ post-machining (calculated) | Labour time/ percentage of processing time | Unit labour cost | Labour cost (calculated) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | [mm x mm x mm] | [kg/m$^3$] | [kg] | [€/kg] | [€] | [kW] | [min] | [kWh] | [€/kWh] | [€] | [min] | [€/h] | [€] |
| Carbon Steel | S275JR, EN 10025-2 | 1000 x 1000 x 6 | 7850 | 47.1 | 1.78 | 83.84 | 20 | 10 | 3.333333 | 0.2 | 0.666666667 | 10 | 28.5 | 4.75 |
| Stainless steel | 316L | 1000 x 1000 x 6 | 7900 | 47.4 | 7.28 | 345.072 | 20 | 10 | 3.333333 | 0.2 | 0.666666667 | 10 | 28.5 | 4.75 |
| stainless steel | 254SMO | 1000 x 1000 x 6 | 8050 | 48.3 | 83.14 | 4015.66 | 20 | 10 | 3.333333 | 0.2 | 0.666666667 | 10 | 28.5 | 4.75 |

**Table A2 -** Substrate surface preparation cost calculations (Grit blasting)[18]

AIM - to determine the substrate surface preparation cost for 1 m$^2$ area using consumables, labour and electrical energy

| Substrate type | Substrate dimension | Grit blasting machine power | Grit blasting time for 1 m$^2$ area substrate | Electrical energy consumption for grit blasting | Cost of electrical energy | Name of grit material | Grit material elemental composition | Grit flow rate | Amount of grit materials used for 1 m$^2$ area | Unit cost of grit material | Resuse factor for grit material | Cost of grit materials (calculated) | Amount of acetone used for 1 m$^2$ area | Unit cost of purchased acetone | Cost of acetone | Labour time/ percentage of processing time | Labour cost |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | [mm x mm x mm] | [kW] | [min] | [kWh] | [€] | | | [g/min] | [g] | [€/kg] | | [€] | [litre] | [€/litre] | [€] | [min] | [€] |
| Carbon steel/stainless | 1000 x 1000 x 6 | 2 | 10 | 0.333333333 | 0.066666667 | #100 mesh white alumina | Al203 | 1400 | 14000 | 2 | 20 | 1.4 | 0.25 | 5 | 1.25 | 15 | 7.13 |

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[17] Primary data provided by TWI, 02 March 2021.

[18] Primary data provided by TWI, 25 Feb 2021

**Table A3 -** Substrate surface preparation cost calculations (Grinding linishing)[19]

AIM - to determine the substrate surface preparation cost for 1 m$^2$ area using consumables, labour and electrical energy

| Substrate material name | Substrate dimension | Surface preparation method | Grinding time per substrate | Amount of grit material used | Name of grit material | Unit cost of grit material | Cost of grit materials (calculated) | Power of the grinding linisher machine | Electrical energy used for 1 m2 area | Electrical energy cost | Labour time/ percentage of processing time | Labour cost |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | [mm] | | [min] | [g] | | [€/kg] | [€] | [kW] | [kWh] | [€] | [min] | [€] |
| Carbon steel | 1000x1000x6 | **Grinding** | **120** | **400** | **SiC** | 2 | 0.8 | **10** | 20 | 4 | **120** | 57 |

**Table A4 -** Substrate surface preparation cost calculations (Surface treatment)[20]

AIM - to determine the substrate surface preparation cost for 1 m$^2$ area using consumables, labour and electrical energy

| Substrate ID | Substrate dimension | Amount of acetone used | Unit cost of acetone | Cost of acetone | Amount of isopropanol used | Unit cost of isopropanol | Cost of isopropanol | Name of the polishing materials | Amount of polishing materials used | Unit cost of polishing material | Cost of polishing materials | Amount of deionised water used | Unit cost of deionised water | Cost of deionised water | Power of ultrasound bath | Duration of ultrasound bath used | Electrical energy used | Electrical energy Cost | labour time | Unit labour cost | labour cost | Cr layer deposition cost for adhesion |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | (mm) | [l] | [€/l] | [€] | [l] | [€/l] | [€] | CarbiMet S | # pcs | [€/100 pcs] | [€] | [litre] | [€/litre] | [€] | (kW) | (min) | (kWh) | [€] | (min) | (€/h) | (€) | (€) |
| 316L | 1000x1000x6 | 1.1 | 6.75 | 7.425 | 1.1 | 21 | 23.1 | P280/P1200/P2500 | 1/1/1/ | 15/203/20 | 6.21 | 1.1 | 0.6 | 0.66 | 1.00E-01 | 10 | 1.67E-02 | 3.33E-03 | 30 | 28.5 | 14.25 | 11.87 |
| S275JR | 1000x1000x6 | 1.6 | 6.75 | 10.8 | 1.6 | 21 | 33.6 | P280/P1200/P2500 | 1/1/1/ | 15/203/20 | 6.21 | 1.6 | 0.6 | 0.96 | 1.00E-01 | 10 | 1.67E-02 | 3.33E-03 | 30 | 28.5 | 14.25 | 11.87 |

**Table A5 –** Coating deposition cost calculations (Metal oxide nanoporous)[21]

AIM - to determine the cost of 1 µm thick coating material deposited over 1 m$^2$ area of substrate based on the data given

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[19] Primary data provided by TWI, 11 March 2021.

[20] Primary data provided by Grein Research, 24 February 2021

[21] Primary data provided by TWI, 25 February 2021

| Sample ID | Coating type | SOD | No. of passes | Hardware power | S-HVOF machine time | Electrical energy used | Unit cost of electricity | Cost of electrical energy | Type of fuel gas used | Fuel gas flow rate | Unit cost of fuel gas | Amount of fuel used | Cost of fuel gas | Oxygen flow rate | Amount of oxygen used | Unit cost of oxygen | Cost of oxygen | Suspension flow rate | Deposition time | Amount of suspension used | Unit cost of suspension | Cost of suspension | Area of the coating | Labour time | Labour cost |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | (mm) | | [kW] | [min] | [kWh] | [€/kWh] | [€] | | [litre/min] | [€/m$^3$] | [m$^3$] | [€] | [litre/min] | [m$^3$] | [€/m$^3$] | [€] | [ml/min] | [min] | [l] | [€/l] | [€] | [m$^2$] | [min] | [€] |
| S-HVOF_TiO2-10 | $TiO_2$ | 150 | 30 | 80 | 40 | 53.33333 | 0.2 | 10.66667 | Hydrogen | 788 | 4.8 | 31.52 | 151.296 | 280 | 11.2 | 1.3 | 14.56 | 10 | 40 | 0.4 | 245 | 98 | 1 | 120 | 57 |
| S-HVOF_TiO2-20 | $TiO_2$ | 150 | 30 | 80 | 40 | 53.33333 | 0.2 | 10.66667 | Hydrogen | 788 | 4.8 | 31.52 | 151.296 | 280 | 11.2 | 1.3 | 14.56 | 20 | 40 | 0.8 | 245 | 196 | 1 | 120 | 57 |

## **Table A6 –** Coating deposition cost calculations (MWCNT)[22]

AIM - to determine the cost of 1 µm thick coating material deposited over 1 m$^2$ area of substrate based on the data given below and assumptions made.

| Catalyst | Cost of Iron catalyst | Name of active gas | Active gas flow rate | Unit cost of active gas | Cost of active gas | Hardware power of CVD reactor | Deposition time | Electrical energy used for CVD reactor | Unit cost of electricity | Cost of electrical energy for CVD reactor | Name of carrier (inert) gas | Carrier gas flow rate | Unit cost of carrier gas | Cost of carrier gas | Area of the coating | Thickness of the coating | Labour cost | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | [€] | | cm3 | [€/cm3] | [€] | [kW] | [h] | [kWh] | [€/kWh] | [€] | | [cm3] | [€/cm3] | [€] | [cm$^2$] | [µm] | [€] | | | |
| Fe | ? | Methane | 0.043 | 35 | **1.505** | 25 | 6 | 150 | 0.2 | **30** | Nitrogen | 0.5 | 3.5 | 1.75 | 225 | ? | 1 PhD: 40 hx 30€= 1200€ | | | |
| | ? | ? | ? | ? | | ? | | | | | Argon | 0.8 | 4.5 | 3.6 | | ? | 1 Tehnnician: 8 hx15€ = 120€ | | | |
| | ? | ? | ? | ? | | ? | | | | | Hydrogen | 0.1 | 10 | 1 | | ? | Overhead costs: Labor costs x 50% = 96.5 | | | |
| | | | | | | | | | | | | | | | | | 247.5 | | | |

## **Table A7 –** Coating deposition cost calculations (Amorphous metal coatings)[23]

AIM - to determine the cost of 1 µm thick coating material deposited over 1 m$^2$ area of substrate based on the data given below

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[22] Primary data provided by UoB, 09 March 2021

[23] Primary data provided by Grein Research, 24 February 2021

| Coating name | Coating composition | Hardware power of vacuum system | Duration vacuum system left running | Electrical energy used for vacuum | Unit cost of electricity | Cost of electrical energy for vacuum | Hardware power of cooling system | Duration of cooling | Electrical energy used for cooling | Cost of electrical energy for cooling | Type of inert gas used | inert gas used | Unit cost of inert gas | Cost of inert gas | Area of the coating | Thickness of the coating | labour time | labour cost | PVD target cost for 6 mm thick and target diameter of 102 mm | PVD target cost for 1 um thick coating over 1 m2 area | Coating material unit cost | Volume of the coating material | Density of the coating material | Mass of the coating material with 50% waste | Cost of the coating material for 1 um thick 1 m2 area |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | [kW] | [min] | [kWh] | [€/kWh] | [€] | [kW] | [min] | [kWh] | [€] | | [l] | [€/l] | [€] | [cm2] | [µm] | (min) | (€) | [€] | [€] | [€/kg] | [m3] | [kg/m3] | [kg] | [€] |
| GHX054 | Si:Ta:Al | 6.00E-01 | 325 | 3.25E+00 | 0.2 | **0.65** | 5.50E-02 | 225 | 2.06E-01 | **0.04** | Ar(5N) | 80 | 0.471 | **37.68** | 10000 | 1 | 300 | **142.5** | 1678 | 100.68 | 500.71 | 0.000001 | 13301.25 | 0.0200 | 9.99 |
| GHX028 | Si:Ta:Cr | 6.00E-01 | 350 | 3.50E+00 | 0.2 | **0.70** | 5.50E-02 | 300 | 2.75E-01 | **0.06** | Ar(5N) | 110 | 0.471 | **51.81** | 10000 | 1 | 300 | **142.5** | 1740 | 104.4 | 508.79 | 0.000001 | 13402.8 | 0.0201 | 10.23 |
| GHX036 | Si:Ta:Fe | 6.00E-01 | 460 | 4.60E+00 | 0.2 | **0.92** | 5.50E-02 | 410 | 3.76E-01 | **0.08** | Ar(5N) | 150 | 0.471 | **70.65** | 10000 | 1 | 300 | **142.5** | 1678 | 100.68 | 801.03 | 0.000001 | 14996.24 | 0.0225 | 18.02 |
| GHX042 | Si:Ta:Ti | 6.00E-01 | 435 | 4.35E+00 | 0.2 | **0.87** | 5.50E-02 | 335 | 3.07E-01 | **0.06** | Ar(5N) | 125 | 0.471 | **58.88** | 10000 | 1 | 300 | **142.5** | 1740 | 104.4 | 562.24 | 0.000001 | 12814.34 | 0.0192 | 10.81 |

## **Table A8 –** Coating deposition cost calculations (Ni-P/Ni-P-PTFE duplex coatings)[24]

AIM - to determine the cost of 1 µm thick coating material deposited over 1 m$^2$ area of substrate based on the data given below

| Sample ID | Topcoat/undercoat coatings (TC/UC) | Phosphorus levels | Coating composition | Minimum bath volume | Flow of Nickel Sulphate ($NiSO_4.6H_2O$) | Nickel Sulphate ($NiSO_4.6H_2O$) amount | Unit cost of Nickel Sulphate ($NiSO_4.6H_2O$) | Cost of Nickel Sulphate ($NiSO_4.6H_2O$) | Flow of Sodium hypophosphite ($NaH_2PO_2.H_2O$) | Sodium hypophosphite ($NaH_2PO_2.H_2O$) amount | Unit cost of Sodium hypophosphite ($NaH_2PO_2.H_2O$) | Cost of Sodium hypophosphite ($NaH_2PO_2.H_2O$) | Flow of Sodium citrate dyhydrate ($C_6H_5Na_3O_7.2H_2O$) | Sodium citrate dyhydrate ($C_6H_5Na_3O_7.2H_2O$) amount | Unit cost of Sodium citrate dyhydrate ($C_6H_5Na_3O_7.2H_2O$) | Cost of Sodium citrate dyhydrate ($C_6H_5Na_3O_7.2H_2O$) | Flow of Ammonium acetate ($NH_4CH_3COO$) | Ammonium acetate ($NH_4CH_3COO$) | Unit cost of Ammonium acetate ($NH_4CH_3COO$) | Cost of Ammonium acetate ($NH_4CH_3COO$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | [litre] | [g/l] | [kg] | [€/kg] | [€] | [g/l] | [kg] | [€/kg] | [€] | [g/l] | [kg] | [€/kg] | [€] | [g/l] | [kg] | [€/kg] | [€] |
| HPLP | UC3 | HP | Ni-P | **2925** | **30** | 87.75 | 119 | 10442.25 | 30 | 87.75 | 80 | 7020 | 10.5 | 30.7125 | 47 | 1443.4875 | 25 | 73.125 | 102 | 7458.75 |
| | TC3 | LP | Ni-P-PTFE | **2925** | **30** | 87.75 | 119 | 10442.25 | 23 | 67.275 | 80 | 5382 | 10.5 | 30.7125 | 47 | 1443.4875 | 20 | 58.5 | 102 | 5967 |
| HPHP | UC4 | HP | Ni-P | **2925** | **30** | 87.75 | 119 | 10442.25 | 30 | 87.75 | 80 | 7020 | 10.5 | 30.7125 | 47 | 1443.4875 | 25 | 73.125 | 102 | 7458.75 |
| | TC4 | HP | Ni-P-PTFE | **2925** | **30** | 87.75 | 119 | 10442.25 | 30 | 87.75 | 80 | 7020 | 10.5 | 30.7125 | 47 | 1443.4875 | 25 | 73.125 | 102 | 7458.75 |

| Phosphorus levels | Coating composition | Thiourea ($CH_4N_2S$) amount | Flow of Polytetrafluoroethylene or PTFE $(C_2F_4)_n$ | Polytetrafluoroethylene or PTFE $(C_2F_4)_n$ amount | Unit cost of Polytetrafluoroethylene or PTFE $(C_2F_4)_n$ | Cost of Polytetrafluoroethylene or PTFE $(C_2F_4)_n$ | Flow of Fluorocarbon or FC4 ($C_{20}H_{20}F_{23}N_2O_4I$) or CTAB | Fluorocarbon or FC4 ($C_{20}H_{20}F_{23}N_2O_4I$) amount | Unit cost of Fluorocarbon or FC4 ($C_{20}H_{20}F_{23}N_2O_4I$) amount | Cost of Fluorocarbon or FC4 ($C_{20}H_{20}F_{23}N_2O_4I$) amount | 50% ammonium hydroxide $NH_4OH$, 10% sulfuric acid $H_2SO_4$ amount | Unit cost of 50% ammonium hydroxide $NH_4OH$, 10% sulfuric acid $H_2SO_4$ | Cost of 50% ammonium hydroxide $NH_4OH$, 10% sulfuric acid $H_2SO_4$ amount | Total cost of consumables (calculated) | Coating thickness (maximum) | Immersion time | Labour time | Total labour cost (calculated) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | [ppm] | [g/l] | [kg] | [€/kg] | [€] | [g/l] | [kg] | [€/kg] | [€] | [ml] | €/l | [€] | [€] | [µm] | [min] | [min] | [€] |
| HP | Ni-P | | | | | | | | | | **500** | **31** | **15.5** | 26379.9875 | **25** | **90** | **120** | 57 |
| LP | Ni-P-PTFE | 1 | 10 | 29.25 | 162 | 4738.5 | 0.1 | 0.2925 | 360 | 105.3 | **500** | **31** | **15.5** | 28094.0375 | **25** | **90** | **120** | 57 |
| HP | Ni-P | | | | | | | | | | **500** | **31** | **15.5** | 26379.9875 | **25** | **90** | **120** | 57 |
| HP | Ni-P-PTFE | | 10 | 29.25 | 162 | 4738.5 | 0.1 | 0.2925 | 360 | 105.3 | **500** | **31** | **15.5** | 31223.7875 | **25** | **90** | **120** | 57 |

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[24] Primary data provided by TWI, 11 March 2021.