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### D5.4 Sustainability assessment of phase change HX material

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<b>Abstract</b>	This document provides the sustainability assessment of GeoHex phase change heat exchanger (HX) materials by combining the cost analysis and environmental impacts of these materials developed for evaporators and condensers.		

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## Executive Summary

This document provides the sustainability assessment of GeoHex phase change heat exchanger (HX) materials by combining the cost analysis and environmental impacts of these materials developed for evaporators and condensers. The high-performance GeoHex materials such as superhydrophobic & superoleophobic materials with silica based nanoparticles and functionalised hi-mesh materials are being developed for promoting robust dropwise condensation for water and ORC working fluid in condensers of geothermal steam and ORC-based power plants. For evaporators, the GeoHex materials such as doped and undoped  $\text{Al}_2\text{O}_3\text{-TiO}_2$  composite coatings and hydrophilic amorphous metal coatings are being developed for promoting robust nucleate boiling for ORC working fluid. These GeoHex materials will be deposited onto carbon steel, stainless steel and other substrates as alternatives to the state of the art materials (SOA) 316L and 254SMO used for the plates and tubes of condensers and evaporators. 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 these GeoHex materials. Parametric cost modelling has been used to evaluate the total costs of production of 20 synthesised coatings accounting for the substrate, substrate surface preparation, coating deposition and overhead costs. The cradle to gate LCA analyses of these 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 performance is 1 m<sup>2</sup> flat GeoHex engineered surfaces developed with 20 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 in GeoHex D5.3 will be used for evaluating the cost and environmental impacts in terms of 1 kW capacity for respective types of GeoHex enabled HXs those are being developed in WP7 through the proposed manufacturing route and design considerations.

## Objectives Met

The deliverable contributed towards the work package objectives:

- To model environmental and cost performances of the HX materials developed in WP3 and WP4.
- To model environmental and cost performances of the HXs developed through the proposed route.

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## 1. INTRODUCTION

One of the GeoHex goals is to develop heat exchanger materials that protect the phase change heat exchangers from degradation due to corrosion and scaling damage in evaporators and another goal is to enhance heat transfer and durability performance in both evaporators and condensers. These developments will lead to smaller, more efficient, cost effective heat exchanger systems for geothermal sectors and beyond with lower environmental footprints. Silica based hydrophobic coatings such as Sharc sapphire SMS35 333 HMDS 25:75 (ShS-SMS35) and Sharc sapphire Gelest 25:75 (ShS-Gelest) will be deposited onto carbon steel (CS), Stainless steel (SS), Copper (Cu) and Aluminium (Al) substrates are being developed for ORC and steam condensers promoting dropwise and sucking flow condensation. For increasing the robustness of the condensing surface, amorphous metal coating composition Zr:Si:Nd (GHX072) deposited onto CS, SS, Al and Cu substrates are also being developed. Superhydrophobic functionalised hierarchical mesh-covered surface coated with Tutoprom™ Bright (Tutoprom) using low-cost and commercially available woven metal micro-meshes such as CS and SS micro meshes (for CS and SS substrates respectively) are being developed for promoting sucking flow condensation. Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite materials without and with doping of Fe (HSP-0 and HSP-3.6) deposited onto CS and SS substrates are being developed for promoting robust nucleate boiling on the ORC working fluid side of evaporator and also developing amorphous metal coating composition Zr:Si:La (GHX099) for optimising the bi-oleophilic surfaces to enhance both heat transfer coefficient (HTC) and critical heat flux (CHF).

We have investigated both environmental and economic performance of these GeoHex materials developed for phase change 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 these materials and processes. We have used LCA tool SimaPro 9.1.1.1 (commercial LCA software which includes ecoinvent version 3.6 and other databases and several impact assessment methodologies) software; the following relevant standards are followed: LCA framework of ISO 14040<sup>2</sup> and 14044<sup>3</sup> standards, International Reference Life Cycle Data System (ILCD)<sup>4</sup>.

The LCA modelling includes mass, energy and transportation flows of these phase change GeoHex materials considering cradle to gate approach. The LCA tool assessed the energy and resources consumed for a functional unit of synthesised coatings (1 m<sup>2</sup> flat surface area) for a specific surface material developed for heat exchangers. Based on the energy and resource 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.

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<sup>2</sup> ISO 14040: 2006 – Environmental management – Life cycle assessment – Principles and framework; Geneva. (2006a).

<sup>3</sup> ISO 14044: 2006 – Environmental management – Life cycle assessment – Requirements and guidelines; Geneva. (2006b).

<sup>4</sup> 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.

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.
- Development of GeoHex technology and consumables with minimum environmental impact.

In addition to the evaluation of environmental performance, parametrised cost modelling has been used to evaluate the cost performance of various materials developed for phase change heat exchangers. The parametric cost model accounts for the substrate material, substrate surface preparation, coating deposition and overhead costs and quantifies the total costs of the GeoHex materials over 1 m<sup>2</sup> substrate area. The combined results of the cost and environmental impacts of GeoHex materials developed providing the sustainability assessment. Therefore, the environmental and cost 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 material development and allow them to further optimise materials and processes.

For assessing the sustainability of HX materials, the total costing for different types of GeoHex materials deposited onto carbon steel and other substrates through different deposition processes and the respective environmental impacts have been quantified and analysed. In this study, we are dealing with 4 different phase change GeoHex materials, 3 deposition processes, and 7 different substrates (S275JR, P355NH, 304L, 316L, Al 3003, Al-46, Cu C103). A total of 20 synthesised coatings have been considered and evaluated, which accounts for the total costs using parametric cost modelling and environmental impacts using LCA modelling for deposition of a functional unit of 1 m<sup>2</sup> flat surface area.

Table 1.1 lists the total number of synthesised coatings using the Dip coating, PVD and S-HVOF deposition processes with GeoHex materials deposited onto carbon steel and other substrates. The naming of the 20 synthesised coatings follows the sequence as [substrate type]\_[coating material types]. Before applying deposition of coating materials, grit blasting and other surface treatments have been carried out. In addition, the costing and environmental impacts of SOA materials (316L and 254SMO) each of 1 m<sup>2</sup> area of 6 mm thick have been evaluated.

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

Coating types	Substrate types	Surface Preparation methods	Coating types	Deposition processes
CS_ShS-SMS35	CS: P355NH	Grit blasting & others	Sharc Sapphire/SMS35 333HMDS 25/75	Dip coating
CS_ShS-Gelest	CS: P355NH	Grit blasting & others	Sharc Sapphire/Gelest 25/75	Dip coating
SS_ShS-SMS35	SS: 304L	Grit blasting & others	Sharc Sapphire/SMS35 333HMDS 25/75	Dip coating
SS_ShS-Gelest	SS: 304L	Grit blasting & others	Sharc Sapphire/Gelest 25/75	Dip coating
Al_ShS-SMS35	Al Q-panel: Al-46	Grit blasting & others	Sharc Sapphire/SMS35 333HMDS 25/75	Dip coating
Al_ShS-Gelest	Al Q-panel: Al-46	Grit blasting & others	Sharc Sapphire/Gelest 25/75	Dip coating

Coating types	Substrate types	Surface Preparation methods	Coating types	Deposition processes
Cu_ShS-SMS35	Cu: C103	Grit blasting & others	Shar c Sapphire/SMS35 333HMDS 25/75	Dip coating
Cu_ShS-Gelest	Cu: C103	Grit blasting & others	Shar c Sapphire/Gelest 25/75	Dip coating
CS_Tutoprom	CS: P355NH	UDB, Grit blasting & others	Tutoprom™ Bright	Dip coating
SS_Tutoprom	SS: 316L	UDB, Grit blasting & others	Tutoprom™ Bright	Dip coating
CS_GHX072	CS: S275JR	Grit blasting & others	GHX072-Zr:Si:Nd	PVD
SS_GHX072	SS: 316L	Grit blasting & others	GHX072-Zr:Si:Nd	PVD
Al_GHX072	Al: 3003	Grit blasting & others	GHX072-Zr:Si:Nd	PVD
Cu_GHX072	Cu: C103	Grit blasting & others	GHX072-Zr:Si:Nd	PVD
CS_HSP-0	CS: S275JR	Grit blasting & others	TiO <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub>	S-HVOF
CS_HSP3.6	CS: S275JR	Grit blasting & others	TiO <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub> (Fe)	S-HVOF
SS_HSP-0	SS: 316L	Grit blasting & others	TiO <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub>	S-HVOF
SS_HSP-3.6	SS: 316L	Grit blasting & others	TiO <sub>2</sub> -Al <sub>2</sub> O <sub>3</sub> (Fe)	S-HVOF
CS_GHX099	CS: S275JR	Grit blasting & others	GHX099-Zr:Si:La	PVD
SS_GHX099	SS: 316L	Grit blasting & others	GHX099-Zr:Si:La	PVD

Section 2 describes four types of materials developed for phase change 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 briefly in Section 3. Cost and LCA modelling results of GeoHex engineered materials are presented and discussed in Section 4. Finally, we conclude the results and findings in Section 5.

## 2. PHASE CHANGE HEAT EXCHANGER MATERIALS

### 2.1 Silica based hydrophobic materials

An important aspect of condensation heat transfer is the wetting of solids by liquids since this can have a substantial impact on heat transfer efficiency. Dropwise condensation (DwC) is a method where condensed droplets form on cooled surfaces then rapidly depart, which in turn stops liquid films forming on the surface. This event occurs when the pinning forces on the surface is overcome by gravity, which happens when droplet radius becomes comparable to a liquid's capillary length.<sup>5</sup> The formation of liquid films would rapidly increase thermal resistance and hence reduce heat transfer performance. Therefore, one such method to promote dropwise condensation is the use of hydrophobic coatings.<sup>6</sup> These hydrophobic coatings form liquid droplets on the surfaces of the substrates rather than films due the condensing liquids forming contact angles more than 150° (this makes the surface non-wetting). Commercially available coating (Sharc Sapphire) and silica-based additives (SMS35 and Gelest) were down-selected as hydrophobic layer on four different substrates Al, Cu, CS and SS (shown in Table 1.1). The silica additive enhances the hydrophobic properties of the Sharc Sapphire coating, by increasing the surface roughness, which in turn greatly increases the heat transfer properties of heat exchangers when compared to SOA materials. Table 2.1 lists two down-selected silica based hydrophobic materials.

**Table 2.1** – Down-selected silica based hydrophobic coating systems

Coating ID	Coating type	Coating name	Hydrophobicity achieved through
ShS-Gelest	Sharc Sapphire (25%wt) + Gelest particles (75%wt)	Sharc Sapphire Gelest 25:75	Surface chemistry and hierarchical roughness
ShS-SMS35	Sharc Sapphire (25%wt) + SMS35 particles (dual functionalised) (75%wt)	Sharc Sapphire SMS35 333 HMDS 25:75	Surface chemistry and hierarchical roughness

These coatings were then deposited onto the substrates using dip coating method with a speed of 100 mm/min after undertaken the substrate surface treatment steps such as grit blasting, degreasing, etching and anodising. These two down-selected hydrophobic coating systems will be used for further testing of the heat transfer and durability performance.

### 2.2 Functionalised hierarchical mesh-covered hydrophobic materials

Similarly, to silica based hydrophobic coatings, functionalised hierarchical mesh covered surfaces can also promote dropwise condensation. These mesh materials were joined onto substrates by uniaxial diffusion bonding (UDB). This direct metallurgical bonding of mesh materials to substrates formed interconnected channels which provided passages for condensed liquids to flow.<sup>7</sup> Thus, by promoting more DwC on substrate surfaces, the heat transfer performance of a heat exchanger can be

<sup>5</sup> S. Adera, L. Naworski, A. Davitt, N.K. Mandsberg, A.V. Shneidman, J. Alvarenga, and J. Aizenberg, *Sci Rep*, 2021, **11**, 10675.

<sup>6</sup> R. Parin, M. Rigon, S. Bortolin, A. Martucci, and D. Del Col, *Materials*, 2020, **13**, 878.

<sup>7</sup> R. Wen, W. Liu, X. Ma, and R. Yang, *iScience*, 2021, Volume **24**, Issue 6, 102531.

Date: 30 June 2021

increased.<sup>8</sup> The use of commercially available high mesh materials (made of pure materials) will significantly reduce costs as well as improve anti corrosion/anti scaling properties of ORC-based heat exchangers. In the GeoHex project in addition to the mesh materials, a superhydrophobic coating Tutoprom™ Bright (Tutoprom) was applied by dip coating method with speed of 100 mm/min. The hydrophobic coating allows droplets to form (due to the high contact angle of liquids on the surface) and then the interconnected channels formed by the mesh let condensed fluids drain away from the substrate (sucking flow condensation). The coated mesh materials also act as an addition barrier to reduce corrosion/scaling/damage on the heat exchanger substrates therefore using such materials would greatly increase the longevity, damage resistance and thermal transfer properties of heat exchanger components. The best performing superhydrophobic Tutoprom coated and mesh bonded stainless steel substrate-SS mesh and carbon steel substrate-MS mesh samples have been down-selected for further tests of heat transfer performance and durability in a representative environment.

### 2.3 Robust hydrophobic and hydrophilic amorphous metal coating materials

Metals such as steel sheets are typically used within heat exchangers. Steel sheets are polycrystals, which are composed of varying crystalline orientations joined by grain boundaries. The grain boundaries are known to be one possible means by which corrosion can occur on such materials. Additionally, the corrosion resistance of a metal can also be dictated by a native oxide layer which forms on the metal surface when exposed to air. Hence, corrosive species damage metals by penetrating through both oxide layer and grain boundaries. There are certain metal combinations which can form structures in which no grain boundaries develop. These are known as amorphous metals or metallic glass. In this study, five elements: Silicon (Si), Zirconium (Zr), Lanthanum (La), Samarium (Sm) and Neodymium (Nd) were used as the amorphous metal coatings. The thin film ternary compositions were mapped out by using a compositional model and of these ratios three different compositions were found to have favourable properties (shown in Table 2.2 below).

**Table 2.2** - The ternary composition at the centre of each of the 36 samples in wt%

Sample no.	Ternary composition of the samples in wt%								
	Si:Zr:Nd			Si:Zr:La			Si:Zr:Sm		
	Si	Zr	Nd	Si	Zr	La	Si	Zr	Sm
1	34	33	33	34	33	33	34	33	33
2	60	20	20	60	20	20	60	20	20
3	20	60	20	20	60	20	20	60	20
4	20	20	60	20	20	60	20	20	60

The sample GHX072 (Si:Zr:Nd) was down-selected and deposited on various substrates (shown in Table 1.1). These coatings were applied by physical vapour deposition (PVD) method (DC magnetron sputtering). This coating was found to show promise as a hydrophobic coating with potential applications in condensing heat exchangers. Also the amorphous coating GHX099 (Si:La:Zr) was tested on steel substrates (CS and SS, shown in Table 1.1). This amorphous metal coating showed promise to be used in hydrophilic coating with potential applications in evaporating heat exchangers.

<sup>8</sup> R. Wen, S. Xu, D. Zhao, L. Yang, X. Ma, W. Liu, Y. Lee, R. Yang, *National Science Review*, 2018, Volume 5, Issue 6, 878–887.

Furthermore, to the steel substrates an adhesion layer of chromium was added prior to amorphous metal coatings being deposited by PVD. These two down-selected coatings will be applied to various substrates for further testing of the heat transfer and durability properties.

## 2.4 Doped and undoped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite materials

In heat exchangers that use boiling as a mechanism for heat transfer, the greater the number of boiling nucleation sites on the surface of a substrate the greater the heat transfer. The use of coating materials to form such nucleation sites would enhance the efficiency of heat exchangers through passive techniques. Passive techniques do not require any external power (here the technique used is inner/outer surface modification of the heat exchanger components). Whereas active techniques do require external power (this would significantly increase costs for maintenance and upkeep).<sup>9</sup>

In this study, composite coatings of aluminium and titanium oxides (undoped and iron doped) were used on two different steel substrates (shown in Table 1.1) to achieve enhanced heat transfer. The deposition method to apply the composite coatings was suspension high velocity oxy-fuel (S-HVOF) thermal spraying and the following variables were considered: standoff distance, ethanol-water ratio, precursor concentration and feedstock flow rates. The variable deposition parameters considered for S-HVOF allow tuning of the micro and nano features of the coating (such as pores or thickness). This in turn enhances the critical heat flux and heat transfer coefficient of the heat exchanger system. Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> coating samples with and without iron doped deposited on substrates with finalised parameters will be sent for further testing of heat transfer and durability performances.

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<sup>9</sup> M. Sheikholeslami, M. Gorji-Bandpy, and D.D. Ganji, *Renewable and Sustainable Energy Reviews*, 2015, **49**, 444-469.

### 3. SUSTAINABILITY ASSESSMENT METHODS

#### 3.1 Cost Modelling

A parametric cost model that accounts for the substrate material, substrate preparation, coating deposition and overhead costs used to produce the new and innovative GeoHex materials developed in a laboratory scale. Overhead cost usually includes items such as services, insurances, taxes, facilities maintenance, and the depreciation of the equipment. This cost analysis study is a part of a laboratory-scale and modelling efforts to develop coating materials and methods that can be used for practical, large-scale applications, and applied to the phase change heat exchanger tubes & plates those are in contact with geofluid and ORC fluid. For this analysis, we aim to develop a parametric cost modelling of synthesised coatings in terms of the total costs of the synthesised coatings for  $\mu\text{m}^2$  area [ $\text{€ m}^{-2}$ ]. The parametric cost model quantifies the cost of the coating layer on a  $1 \text{ m}^2$  substrate area with different deposition techniques with four different GeoHex materials. A general equation for the total costing ( ${}^x_a C_T$ ) in  $\text{€}$  for a coating material (say,  $x$ ) deposited over  $1 \text{ m}^2$  area of substrate (say,  $y$ ) using a deposition process (say,  $a$ ) is given by:

$${}^x_a C_T = SM^y + SP_z + CD_a + OH \quad (3.1)$$

Here,  $SM^y$  = substrate material cost for  $1 \text{ m}^2$  area of  $6 \text{ mm}$  thick in  $\text{€}$ ;  $SP_z$  = substrate preparation cost for  $1 \text{ m}^2$  area in  $\text{€}$  using a surface preparation method (say,  $z$ );  $CD_a$  = coating deposition cost for  $1 \text{ m}^2$  area in  $\text{€}$ ;  $OH$  = overhead cost per  $\text{m}^2$  area of coating and given by

$$OH (\text{€}) = \text{overhead cost factor} \times \text{total labour cost} (\text{€}) \quad (3.2)$$

Where, overhead cost factor is assumed to be 0.5. However, this factor will be tuned to match with the large-scale applications.

Other cost components in equation (3.1) have been elaborated and the costing equations for the costs of substrate material, substrate surface preparation, coating deposition have also been deduced in section 3.1.2 of GeoHex D5.3.

#### 3.2 LCA Modelling

The formal components of Life Cycle Assessment (LCA) such as goal and scope, inventory analysis, impact assessment and interpretation have been used to evaluate the environmental footprints of phase change GeoHex materials deposited onto carbon steel, stainless steel and other substrates through S-HVOF, PVD, and Dip coating 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 GeoHex materials have been studied throughout the cradle-to-gate life cycle approach. The LCA framework and its description are given in the subsection 3.2.1 of GeoHex D5.3.

##### Goal of the study

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

- Quantify and evaluate the environmental footprints of the phase change GeoHex materials
- Use the study results for these materials' 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

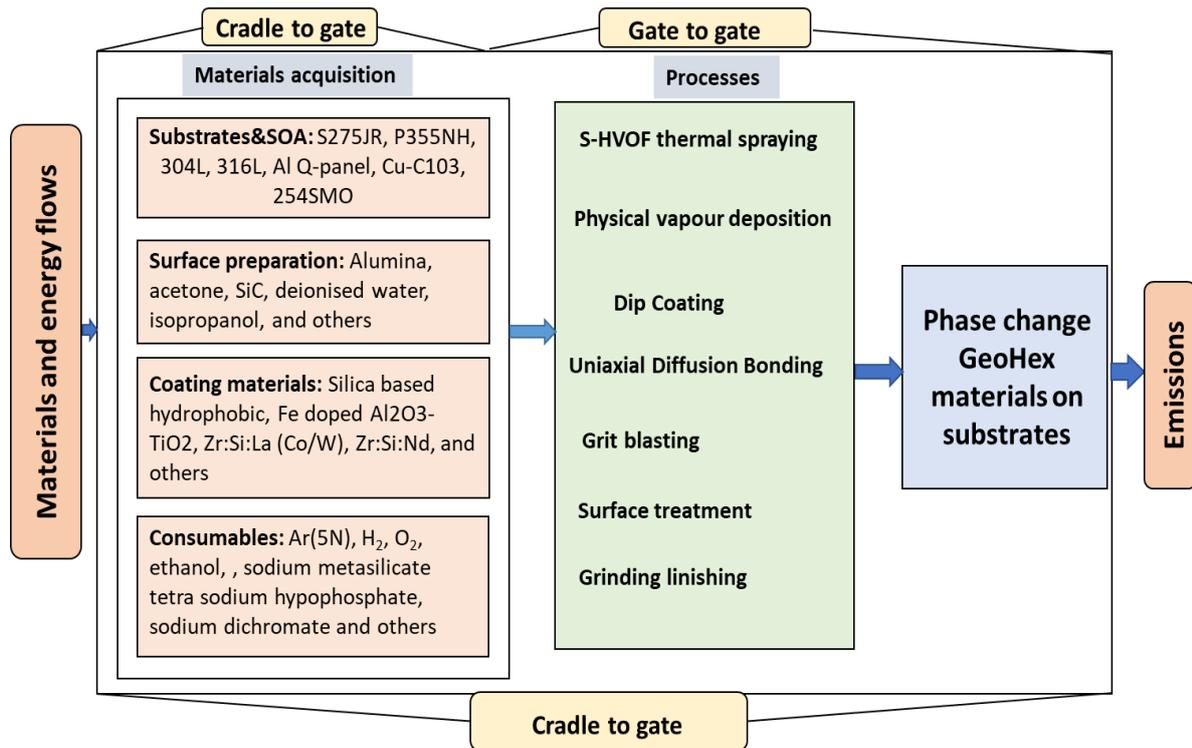
### Scope the study

The scope of the study is to establish the baseline information to produce synthesised coatings and materials 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 material deposition and other processes involved includes:

- Substrate and its preparation processes: grit blasting, grinding finishing and surface treatment (excluding the manufacturing of the infrastructure materials of grit blasting and grinding machines);
- Coating elements and/or compounds and consumables used to manufacture phase change GeoHex materials: silica based hydrophobic materials, doped and undoped  $\text{Al}_2\text{O}_3\text{-TiO}_2$ , ethanol, sodium metasilicate, sodium dichromate, Argon inert gas and others (excluding the manufacturing of the infrastructure materials and others);
- Coating deposition and other processes used: Suspension High Velocity Oxy-Fuel (S-HVOF) Thermal spraying, Physical Vapour Deposition (PVD), Uniaxial Diffusion Bonding (UDB) and Dip Coating (DC). 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 phase change GeoHex materials (Figure 3.1) will be focused to:

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



**Figure 3.1** - A scope of study for the LCA studies of phase change GeoHex materials

### Functional unit

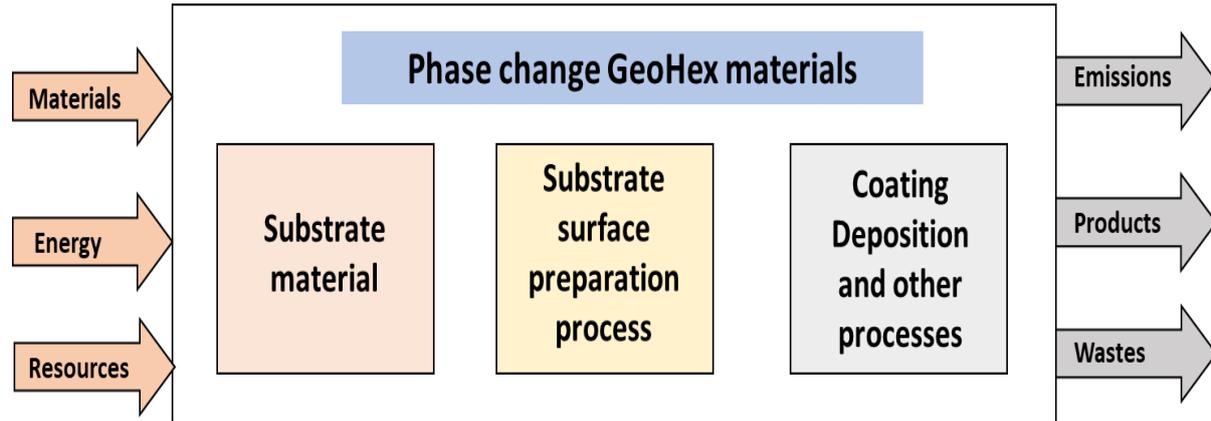
The functional unit of the cradle to gate LCA study is GeoHex materials deposited on a 1 m<sup>2</sup> area of the plates/tubes of phase change heat exchangers.

### 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.

### LCA modelling of phase change GeoHex materials

For a certain thickness of coating over 1m<sup>2</sup> area, Life Cycle Inventory (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 3.2.



**Figure 3.2** – Components of LCA modelling of phase change GeoHex materials

### Data collection and Data sources

The product phase change GeoHex materials' LCI data were mainly collected from primary sources. Some data have been 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 the materials deposited over 1 m<sup>2</sup> 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

The ecoinvent version 3.6 & other databases and several life cycle impact assessment (LCIA) methodologies are linked to SimaPro 9.1.1.1 LCA tool. 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 LC database in Europe, and the data are valid for Swiss and Western European conditions. The available LCIA methodologies 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 LCIA methodology IMPACT 2002+ version 2.15 has been considered for assessing the environmental impacts of the GeoHex materials under the study.

The sustainability assessment of heat exchanger materials developed for phase change 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.

## 3.3 Cost and LCA Models for Phase change GeoHex enabled Heat Exchangers

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 kW capacity of phase change 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 phase change heat exchangers (evaporator and condenser) 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 following 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 of certain capacity (say, 10 kW), the total surface area of the tubes and plates in m<sup>2</sup> will be evaluated where the GeoHex materials applied for enhancing the heat transfer and durability performances. Therefore, the costs of the respective HXs made with GeoHex enabled and SOA materials in units of € per kW will be evaluated and compared.

### **LCA model**

The functional unit of the LCA studies for phase change heat exchangers made with phase change GeoHex enabled and SOA materials is 1 kW capacity of heat exchanger. 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 a phase change heat exchangers of certain capacity (say, 10 kW) whose tubes and plates 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 footprint and economic performances for GeoHex enabled phase change HXs and compared these results with representative HXs using SOA materials in units of Pt per kW and € per kW capacity.

## 4. RESULTS AND DISCUSSIONS

### 4.1 Cost Modelling Results

#### 4.1.1 Data inventories

Data inventories of materials, substrate and its preparation, coating deposition using S-HVOF thermal spraying, Physical vapour deposition, Dip coating deposition techniques for a certain area and others were obtained from discussions with experts from consortium partners. 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 factor and consumable factor 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<sup>10</sup>.

**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<sup>11</sup>. We convert it into € using a conversion factor of 1 GBP = 1.20 €. We estimated the average unit rate of electricity as € 0.20 per kWh.

#### 4.1.2 Costing Results of GeoHex Engineered Materials

Using the data provided by the partners (Tables A1-A5 of Appendix A) and the unit costs of electricity, labour, and coating materials and others described in the section 4.1.1, the costing of substrate and SOA materials, substrate surface preparation cost subcomponents in € have been calculated and estimated for 1 m<sup>2</sup> area of substrates and listed in Tables 4.1-4.5.

**Table 4.1** – Cost subcomponents for substrates and SOA materials

Material type	Grade of the materials	Substrate dimension used	Unit cost	Cost of substrate specimen	Electrical energy cost	Labour cost	Total cost
		[mm]	[€/kg]	[€]	[€]	[€]	[€]
Carbon Steel	S275JR, EN 10025-2	1000 x 1000 x 6	1.78	83.84	0.67	4.75	89.26
Carbon Steel	P355NH	1000 x 1000 x 6	8.97	420	0.67	4.75	425.42
Stainless steel	316L	1000 x 1000 x 6	10.13	480	0.67	4.75	485.42
Stainless steel	254SMO	1000 x 1000 x 6	83.14	4015.80	0.67	4.75	4021.22
Stainless steel	304L	1000 x 1000 x 6	11.45	600	0.67	4.75	605.42

<sup>10</sup> [https://ec.europa.eu/eurostat/statistics-explained/index.php/Wages\\_and\\_labour\\_costs](https://ec.europa.eu/eurostat/statistics-explained/index.php/Wages_and_labour_costs); accessed on 02 April 2021.

<sup>11</sup> [https://www.ukpower.co.uk/home\\_energy/tariffs-per-unit-kwh/](https://www.ukpower.co.uk/home_energy/tariffs-per-unit-kwh/); accessed on 02 April 2021.

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Material type	Grade of the materials	Substrate dimension used	Unit cost	Cost of substrate specimen	Electrical energy cost	Labour cost	Total cost
		[mm]	[€/kg]	[€]	[€]	[€]	[€]
Aluminium Q-panel	Al-46	1000 x 1000 x 6	28.35	464.40	0.67	4.75	469.15
Copper	C103	1000 x 1000 x 6	16.07	858	0.67	4.75	863.42
Aluminium	Al-3003	1000 x 1000 x 6	102.56	1680	0.67	4.75	1685.42

**Table 4.2** – Substrate surface preparation cost subcomponents before silica based hydrophobic coating material deposition using Dip coating method

Substrate type	Substrate dimension	Electrical energy cost	Cost of grit materials	Cost of consumables	Labour cost	Substrate surface preparation cost
	[mm]	[€]	[€]	[€]	[€]	[€]
P355NH	1000 x 1000 x 6	0.32	4.5	14.5	28.5	47.82
304L	1000 x 1000 x 6	0.45	4.5	69.75	16.63	91.33
Al-46	1000 x 1000 x 6	0.50	4.5	87.01	16.63	108.64
C103	1000 x 1000 x 6	0.45	4.5	91.25	19	115.20

**Table 4.3** - Substrate surface preparation cost subcomponents before uniaxial diffusion bonding and Tutoprom bright materials deposition using Dip coating method

Substrate type	Substrate dimension	Electrical energy cost	Cost of grit materials	Cost of consumables	Labour cost	Substrate surface preparation cost
	[mm]	[€]	[€]	[€]	[€]	[€]
Carbon steel/stainless steel	1000 x 1000 x 6	0.85	4.5	127	28.5	160.85

**Table 4.4** – Substrate surface preparation cost subcomponents before amorphous metal coatings deposition using PVD method

Substrate type	Substrate dimension	Consumables cost	Cleaning cost	Labour cost	Adhesion cost	Surface preparation cost
		[€]	[€]	[€]	[€]	[€]
S275JR	1000 x 1000 x 6	51.57	-	14.25	18.69	84.51
316L	1000 x 1000 x 6	37.37	-	14.25	18.69	70.31
Al-3003	1000 x 1000 x 6	37.37	64.89	14.25	18.69	135.20
Cu-C103	1000 x 1000 x 6	37.37	29.25	14.25	18.69	99.56

**Table 4.5** – Substrate surface preparation cost subcomponents before deposition of Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coating materials using S-HVOF method

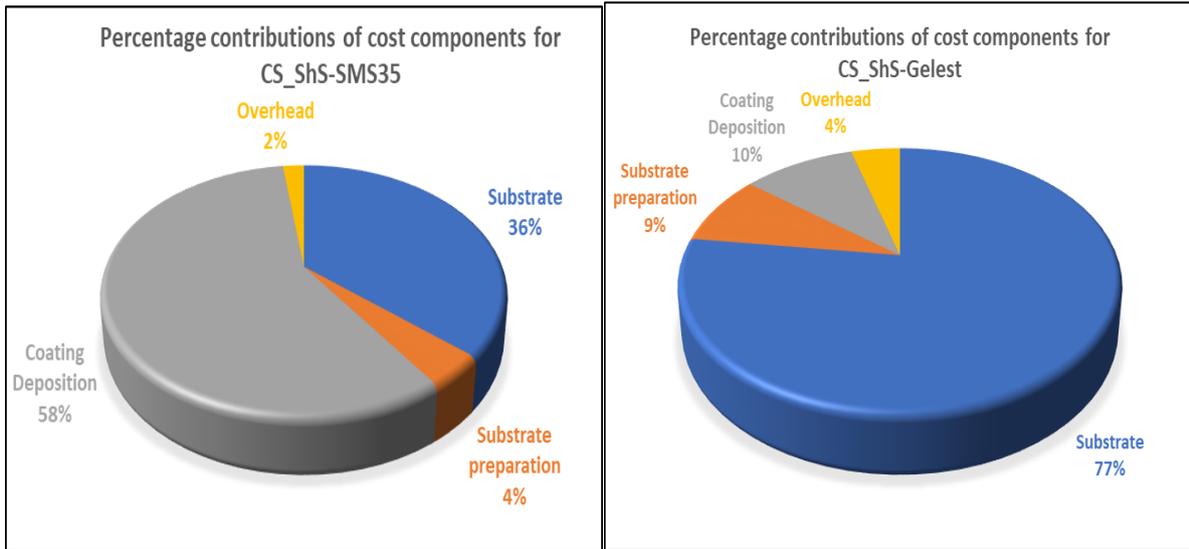
Substrate type	Substrate dimension	Electrical energy cost	Cost of grit materials	Cost of consumables	Labour cost	Substrate surface preparation cost
	[mm]	[€]	[€]	[€]	[€]	[€]
Carbon steel/stainless steel	1000 x 1000 x 6	0.07	1.4	1.25	7.12	9.84

The dip coating deposition method has been used to deposit coating materials Sharc Sapphire/SMS35 333HMDS (ShS-SMS35) and Sharc Sapphire-Gelest (ShS-Gelest) onto the substrates. The cost components of substrate, surface preparation, coating deposition and overhead for these materials deposited onto carbon steel (P355NH), stainless steel (304L), aluminium (Al-46) and Copper (C103) substrates of 1 m<sup>2</sup> area have been evaluated using the data given in Tables 4.1 & 4.2 and Tables A7 of Appendix A and listed in Table 4.6.

**Table 4.6** – Cost components of substrate, surface preparation, coating deposition, overhead and the total costs for the materials deposited over 1 m<sup>2</sup> area of the substrates using Dip coating method

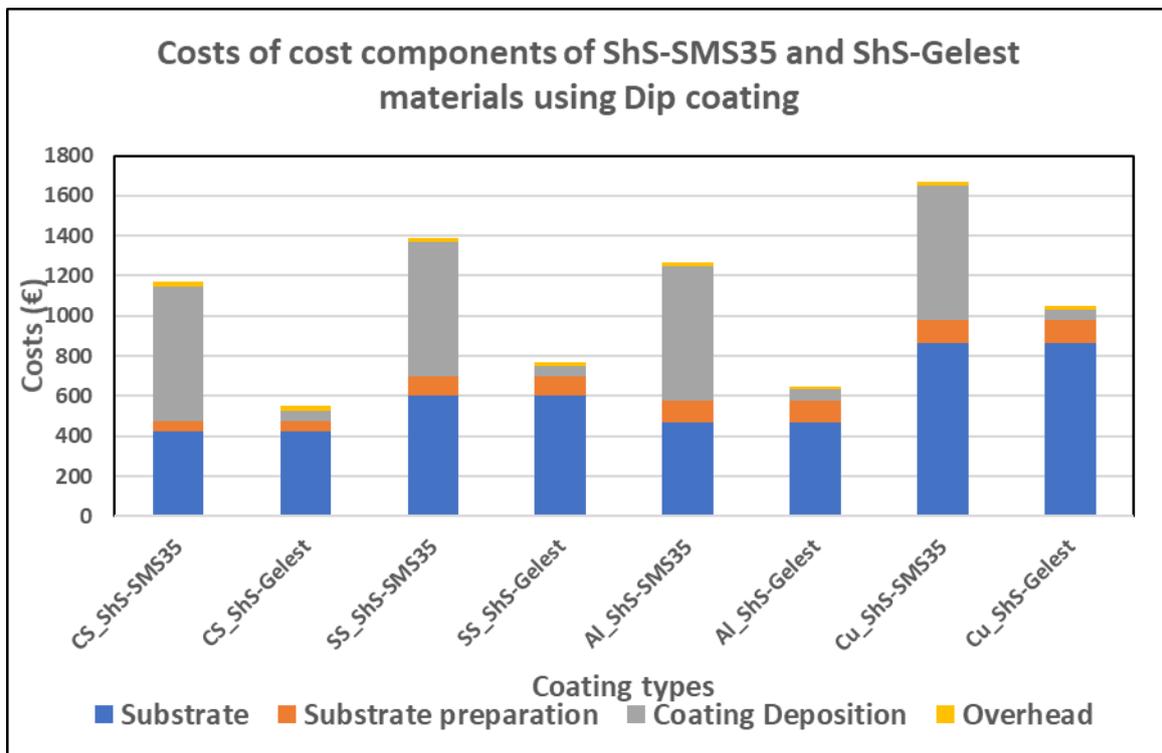
Coating ID	Costs of				
	Substrate	Substrate preparation	Coating Deposition	Overhead	Total
CS_SP_ShS-SMS35_DC	425.42	47.82	673.17	23.75	<b>1170</b>
CS_SP_ShS-Gelest_DC	425.42	47.82	54.73	23.75	<b>552</b>
SS_SP_ShS-SMS35_DC	605.42	91.33	673.17	17.82	<b>1388</b>
SS_SP_ShS-Gelest_DC	605.42	91.33	54.73	17.82	<b>769</b>
Al_SP_ShS-SMS35_DC	469.15	108.64	673.17	17.82	<b>1269</b>
Al_SP_ShS-Gelest_DC	469.15	108.64	54.73	17.82	<b>650</b>
Cu_SP_ShS-SMS35_DC	863.42	115.20	673.17	19.00	<b>1671</b>
Cu_SP_ShS-Gelest_DC	863.42	115.20	54.73	19.00	<b>1052</b>

The percentage contributions of the cost components for ShS-SMS35 and ShS-Gelest onto carbon steel are shown in Figures 4.1(a) and 4.1(b), respectively.



**Figure 4.1** – Cost component contributions for deposition of ShS-SMS35 and ShS-Gelest materials onto carbon steel.

Figure 4.2 shows the costs of cost components for both coatings deposited onto carbon steel, stainless steel, aluminium and Copper substrates.



**Figure 4.2** - Costs of four cost components for coatings deposited onto carbon steel, stainless steel, aluminium and Copper substrates.

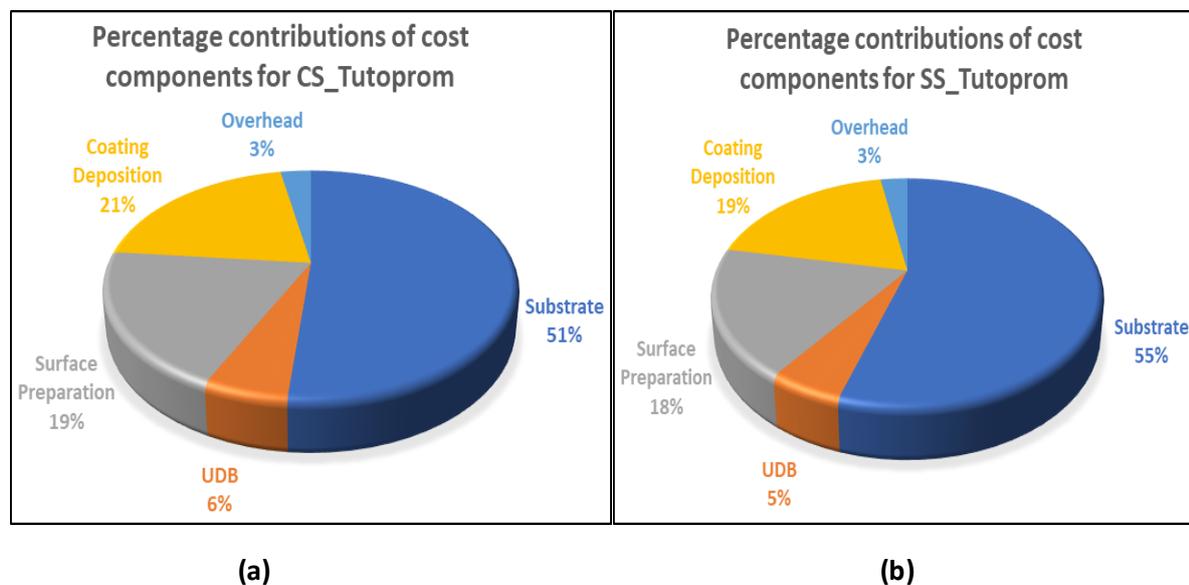
The dip coating deposition method has been used to deposit coating material Tutoprom™ bright onto the carbon steel and stainless steel substrates. The cost components of substrate, surface bonding, surface preparation, coating deposition and overhead for the material deposited onto carbon steel

(P355NH), stainless steel (316L) substrates of 1 m<sup>2</sup> area have been evaluated using the data given in Tables 4.1 & 4.3 and Tables A6 & A8 of Appendix A and listed in Table 4.7.

**Table 4.7** – Cost components of substrate, surface bonding, surface preparation, coating deposition, overhead and the total costs for the materials deposited over 1 m<sup>2</sup> area of the substrates using Dip coating method

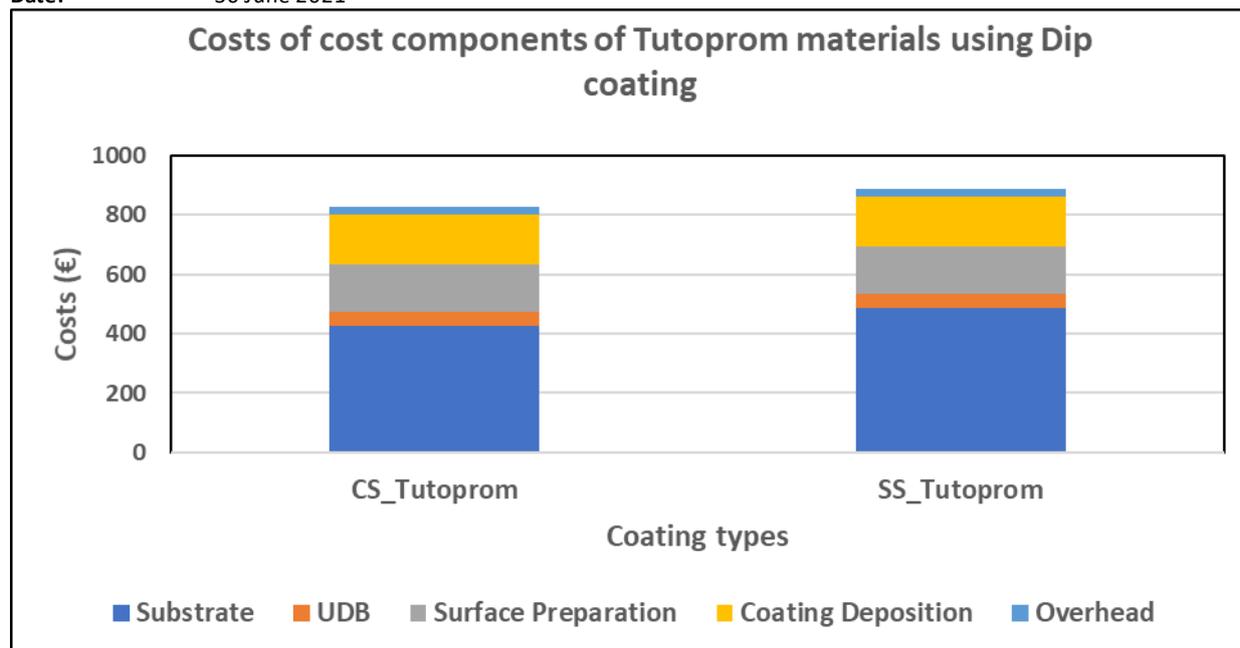
Coating ID	Cost of					
	Substrate	Surface Bonding	Surface Preparation	Coating Deposition	Overhead	Total
CS_UDB_SP_Tutoprom_DC	425.42	46.38	160.85	169.58	23.75	<b>826</b>
SS_UDB_SP_Tutoprom_DC	485.42	46.38	160.85	169.58	23.75	<b>886</b>

The percentage contributions of the cost components for Tutoprom materials onto carbon steel and stainless steel are shown in Figures 4.3(a) and 4.3(b), respectively.



**Figure 4.3** – Cost component contributions for deposition of Tutoprom bright materials onto (a) carbon steel and (b) stainless steel substrates.

Figure 4.4 shows the costs of cost components of Tutoprom materials deposited onto carbon steel and stainless steel substrates.



**Figure 4.4** – Costs of cost component contributions for deposition of Tutoprom bright materials onto carbon steel and stainless steel substrates.

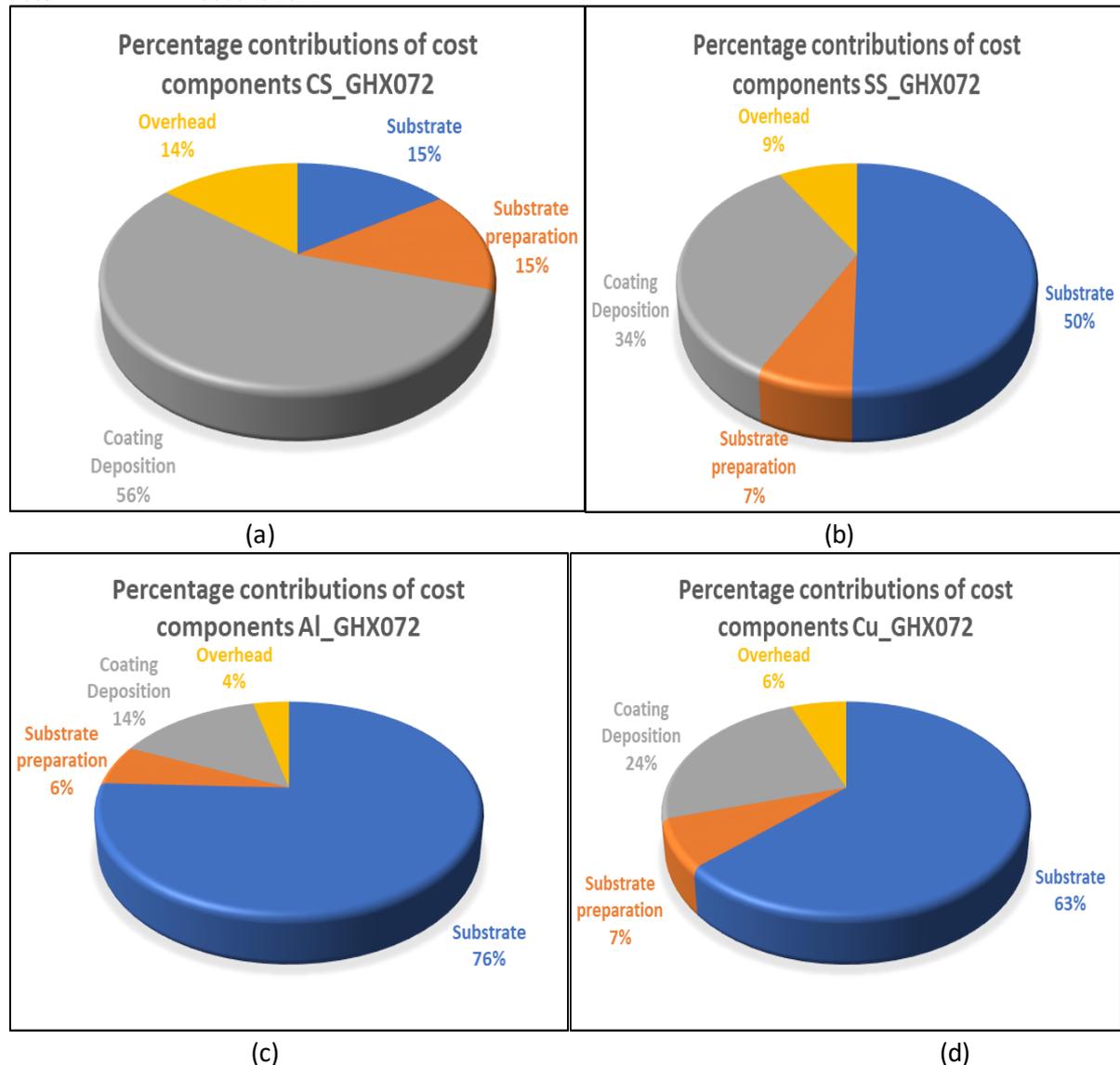
The physical vapour deposition (PVD) method has been used to deposit the amorphous metal coating material GHX072 onto the substrates. The cost components of substrate, surface preparation, coating deposition and overhead for these materials deposited onto carbon steel (S275JR), stainless steel (316L), aluminium (3003) and Copper (C103) substrates of 1 m<sup>2</sup> area have been evaluated using the data given in Tables 4.1 & 4.4 and Table A9 of Appendix A and listed in Table 4.8.

**Table 4.8** – Cost components of substrate, surface preparation, coating deposition, overhead and the total costs for the materials deposited over 1 m<sup>2</sup> area of the substrates using PVD method

Coating ID	Costs of				
	Substrate	Substrate preparation	Coating Deposition	Overhead	Total
CS_SP_GHX072_PVD	89.26	84.51	343.03	80.75	<b>598</b>
SS_SP_GHX072_PVD	485.42	70.31	343.03	83.125	<b>982</b>
Al_SP_GHX072_PVD	1685.42	135.20	343.03	80.75	<b>2244</b>
Cu_SP_GHX072_PVD	863.42	99.56	343.03	80.75	<b>1387</b>

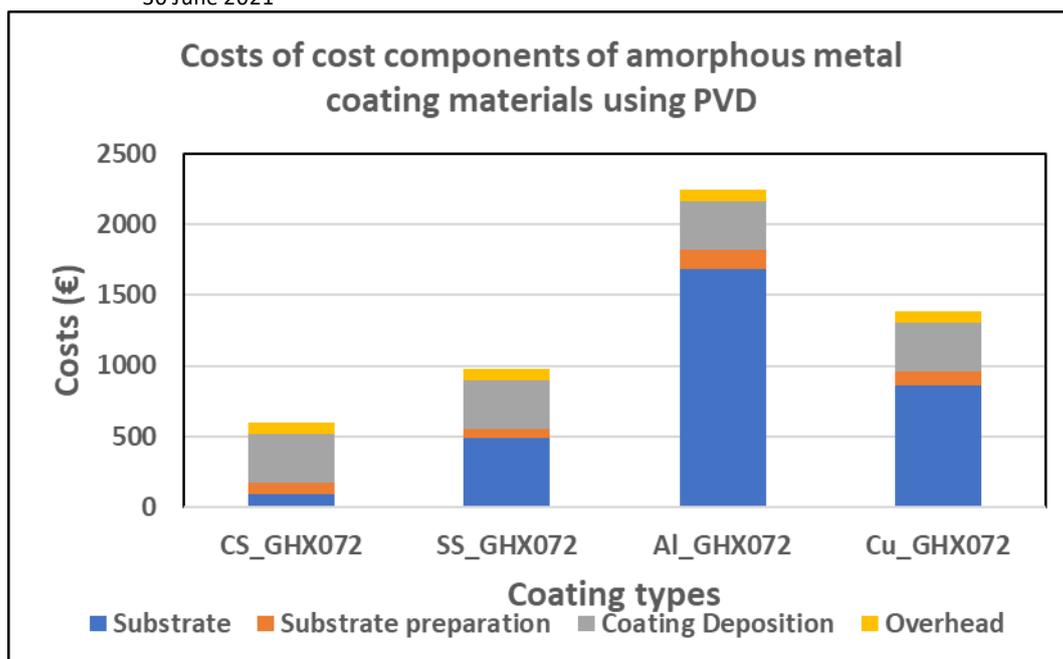
The percentage contributions of the cost components for GHX072 amorphous metal coatings onto carbon steel (CS), Stainless steel (SS), aluminium (Al) and Copper (Cu) substrates are shown in Figures 4.5(a)-(d), respectively.

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**Figure 4.5** - Cost component contributions for deposition of GHX072 materials onto (a) carbon steel (b) stainless steel (c) aluminium and (d) copper substrates.

Figure 4.6 shows the costs of cost components of amorphous metal coating materials deposited onto carbon steel, stainless steel, aluminium and copper substrates.



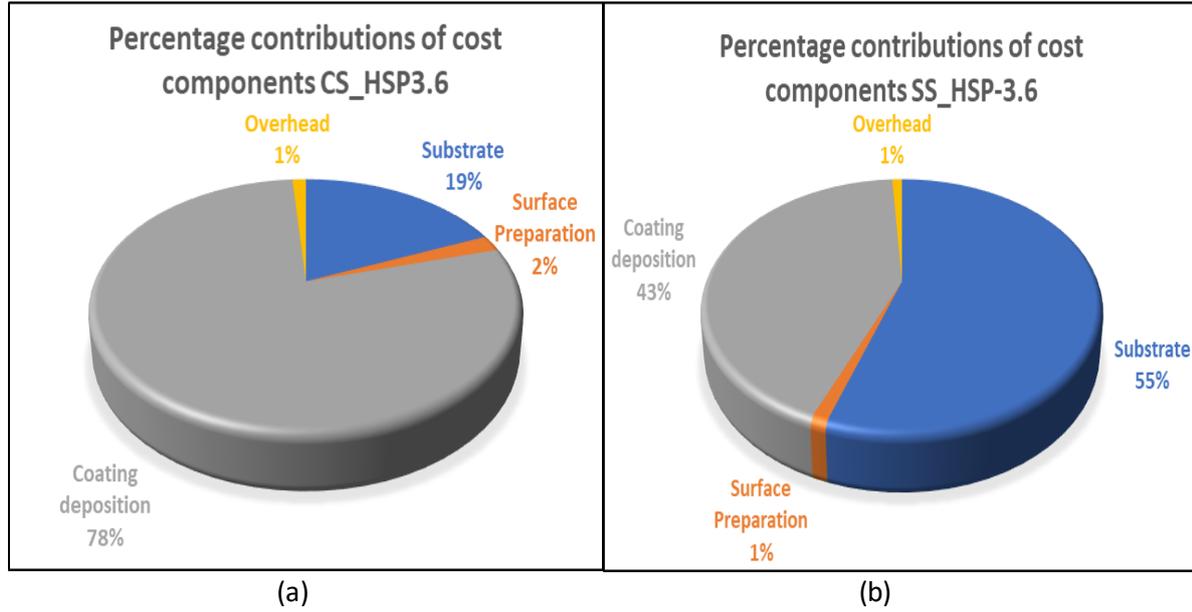
**Figure 4.6** - The costs of cost components of amorphous metal coating materials GHX072 deposited onto carbon steel, stainless steel, aluminium and copper substrates.

The S-HVOF coating deposition method has been used to deposit coating material Fe-doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> onto the carbon steel and stainless steel substrates. The cost components of substrate, surface preparation, coating deposition and overhead for the materials deposited onto carbon steel (S275JR) and stainless steel (316L) substrates of 1 m<sup>2</sup> area have been evaluated using the data given in Tables 4.1 & 4.5 and Table A10 of Appendix A and listed in Table 4.9.

**Table 4.9** – Cost components of substrate, surface preparation, coating deposition, overhead and the total costs for the materials deposited over 1 m<sup>2</sup> area of the substrates using S-HVOF deposition method

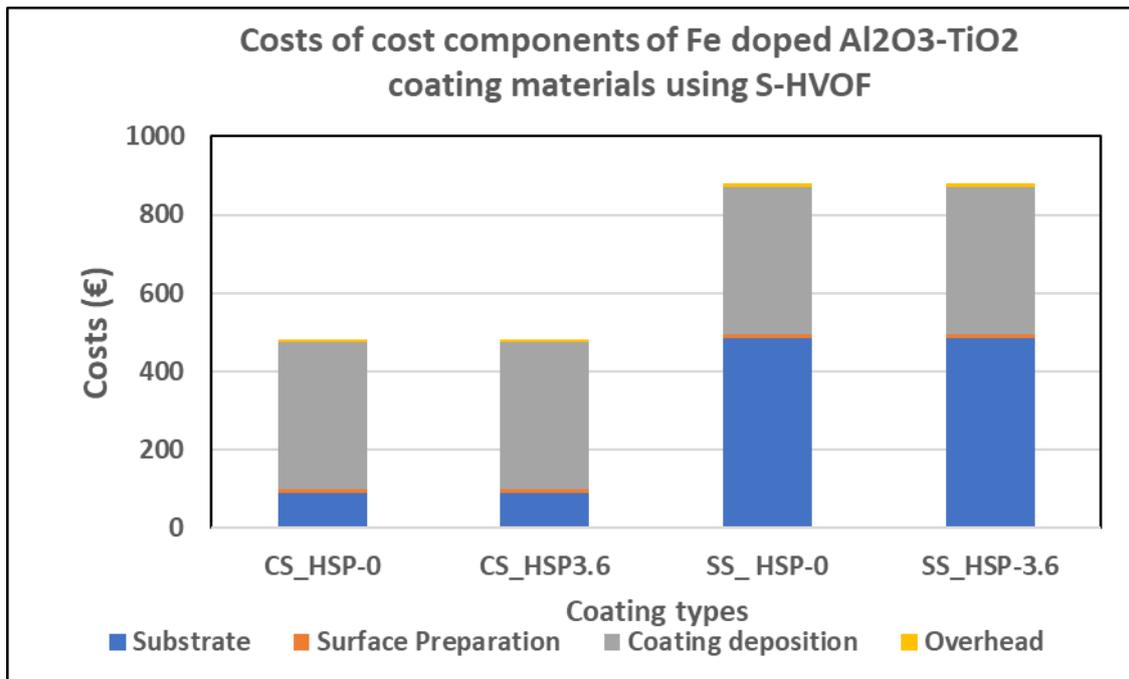
Coating ID	Costs of				
	Substrate	Surface Preparation	Coating deposition	Overhead	Total
CS_SP_HSP-0_S-HVOF	89.25	9.84	376.11	34.44	509.64
CS_SP_HSP3.6_S-HVOF	89.25	9.84	376.27	34.44	509.81
SS_SP_HSP-0_S-HVOF	485.42	9.84	376.11	36.82	908.18
SS_SP_HSP-3.6_S-HVOF	485.42	9.84	376.27	36.82	908.35

The percentage contributions of the cost components for Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> coating (HSP-3.6) materials onto carbon steel and stainless steel are shown in Figures 4.7(a) and (b), respectively.



**Figure 4.7** - Cost component contributions for deposition of Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> (HSP-3.6) coating materials onto (a) carbon steel and (b) stainless steel substrates.

Figure 4.8 shows the costs of cost components of undoped and doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> (HSP-0 and HSP-3.6) coating materials deposited onto carbon steel and stainless steel substrates.



**Figure 4.8** - Costs of cost component contributions for deposition of Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> coating materials onto carbon steel and stainless steel substrates.

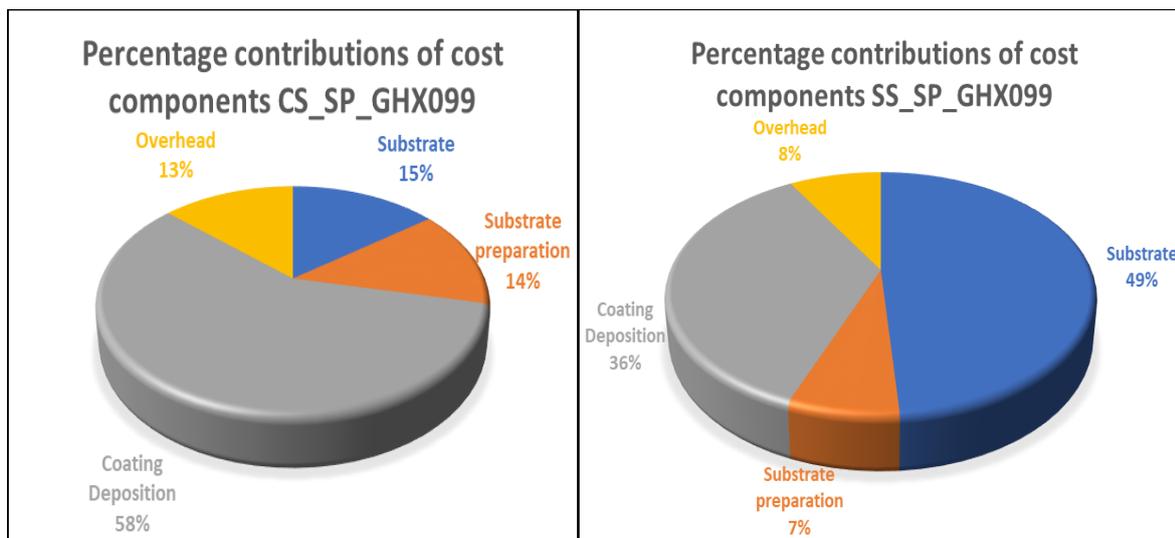
The physical vapour deposition (PVD) method has been used to deposit the amorphous metal coating material GHX099 onto the substrates. The cost components of substrate, surface preparation, coating deposition and overhead for these materials deposited onto carbon steel (S275JR) and stainless steel

(316L) substrates of 1 m<sup>2</sup> area have been evaluated using the data given in Tables 4.1 & 4.4 and Table A9 of Appendix A and listed in Table 4.10.

**Table 4.10** – Cost components of substrate, surface preparation, coating deposition, overhead and the total costs for the materials deposited over 1 m<sup>2</sup> area of the substrates using PVD method

Coating ID	Costs of				
	Substrate	Substrate preparation	Coating Deposition	Overhead	Total
CS_SP_GHX099_PVD	89.26	84.51	355.21	80.75	<b>610</b>
SS_SP_GHX099_PVD	485.42	70.31	355.21	83.125	<b>994</b>

The percentage contributions of the cost components for GHX099 amorphous metal coatings onto carbon steel (CS) and Stainless steel (SS) substrates are shown in Figures 4.9 (a)-(b), respectively.



(a)

(b)

**Figure 4.9** - Cost component contributions for deposition of GHX099 materials onto (a) carbon steel (b) stainless steel.

Figure 4.10 shows the costs of cost components of amorphous metal coating materials GHX099 deposited onto carbon steel and stainless steel substrates.

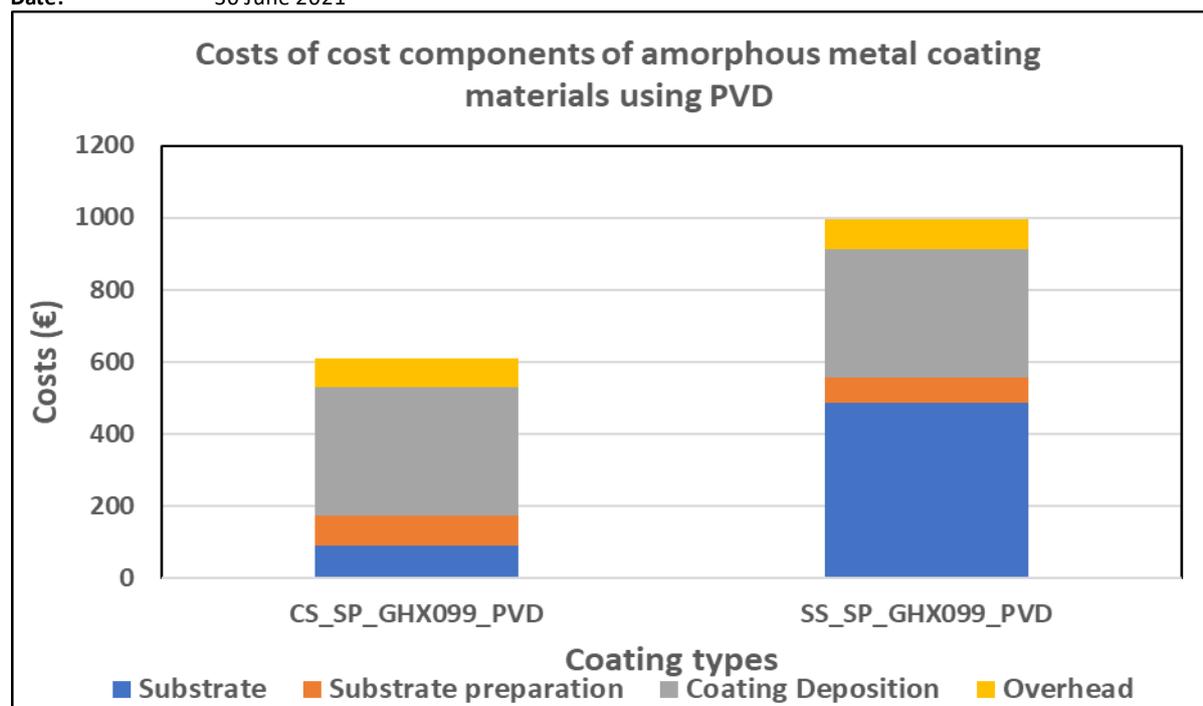


Figure 4.10 - The costs of cost components of amorphous metal coating materials GHX099 deposited onto carbon steel and stainless steel substrates.

## 4.2 LCA Modelling Results

### 4.2.1 Data inventories

The cradle to gate LCA study of phase change GeoHex materials used for condensers and evaporators has been performed in terms of a functional unit of 1 m<sup>2</sup> surface area of tubes and plates of these 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 GeoHex substrate materials used for HX tubes and plates before deposition of phase change GeoHex materials are given in Table 4.11.

Table 4.11 - Elemental composition of relevant GeoHex substrate materials in wt%

Element name	Elemental composition (wt%) of GeoHex Substrate materials			
	Al_3003	Cu_C103	SS_304L	CS_P355NH
C	-	-	0.035	0.18
Mn	1.5	-	2	1.60
Si	0.6	-	1	0.50
P	-	-	0.045	0.025
S	-	-	0.03	0.015
N	-	-	-	0.012
Cu	0.2	99.95	-	0.30
Cr	-	-	19	0.30
Ni	-	-	10	0.50
Fe	0.7	0.044	67.89	96.338

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Element name	Elemental composition (wt%) of GeoHex Substrate materials			
	Al_3003	Cu_C103	SS_304L	CS_P355NH
Al	96.9	-	-	0.02
Mo	-	-	-	0.08
Nb	-	-	-	-
Ti	-	-	-	0.03
V	-	-	-	0.10
Pb	-	0.005	-	-
Bi	-	0.001	-	-
Zn	0.1	-	-	-

The mass, energy and transportation flows for carbon steel, stainless steel, copper and aluminium materials each of 1 m<sup>2</sup> 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<sup>2</sup> area of 6 mm thick have been evaluated and given in Table 4.12.

**Table 4.12** – Mass, energy and transportation flows for carbon steel and stainless steel, copper and aluminium

Material grade	Dimension	Mass	Energy	Transportation
	(mm)	(kg)	(kWh)	(tkm)
Al_3003	1000x1000x6	16.38	0.67	3.28
Cu_C103	1000x1000x6	53.4	0.67	10.68
SS_304L	1000x1000x6	52.4	0.67	10.48
CS_P355NH	1000x1000x6	46.8	0.67	9.36

Before applying coating materials onto the substrate materials using S-HVOF, Dip Coating and PVD processes, we need to prepare the substrate surface using grit blasting and other methods for improving the coating adhesion to the substrate. For 1 m<sup>2</sup> area of substrate surface preparation through grit blasting, grinding finishing and surface treatment methods, the respective data inventories (Tables A2-A6 in the Appendix A) have been used. Based on these primary and secondary data, the LCA data of substrate surface preparation for 1 m<sup>2</sup> area evaluated and are given in Tables 4.13-4.15 before applying Dip coating, PVD and S-HVOF deposition processes, respectively.

**Table 4.13** – Mass, energy and transportation flows for 1 m<sup>2</sup> area of substrate surface preparation for Aluminium, copper, stainless steel and carbon steel surfaces before using Dip coating deposition method.

Surfaces	Masses		Transportation (tkm)	Electrical energy (kWh)
	(kg)			
Al, Cu, 304L, P355NH, 316L	1.44 (Al <sub>2</sub> O <sub>3</sub> )	0.06 (TiO <sub>2</sub> )	-	-
Al	3.00 (METFIN AK 16)	0.95 (sulfuric acid)	1.212	2.875
	0.25 (sodium dichromate)	0.36 (orthophosphoric acid)		
Cu, 304L, P355NH	0.5 (Alkaline solution)	5 (de-ionised water)	-	-
Cu	0.25 (Ammonium persulfate)	-	1.45	2.638
304L	1 (Oxalic acid)	-	1.6	2.638
P355NH	1 (Phosphoric acid)	-	1.6	2.638
316L	0.25 (Tetra sodium pyrophosphate)	1 (Sodium hydroxide)	1.9	4.625
	0.25 (Sodium metasilicate)	1 (Phosphoric acid)		

**Table 4.14** – Mass, energy and transportation flows for 1 m<sup>2</sup> area of substrate surface preparation for Aluminium, copper, stainless steel and carbon steel surfaces before using PVD deposition method.

Surfaces	Masses		Transportation (tkm)	Electrical energy (kWh)
	(kg)			
Al, Cu, 316L	0.8690 (Acetone)	0.8635 (Isopropanol)	1.95	1.327
	1.0967 (deionised water)	0.0098 (Ar)		
	0.00144 (Cr)	0.36 (orthophosphoric acid)		
	0.5 (Alkaline solution)	0.4294 (SiC)		
S275JR	1.264 (Acetone)	1.256 (Isopropanol)	2.25	1.327
	1.5952 (deionised water)	0.0098 (Ar)		
	0.00144 (Cr)	0.4294 (SiC)		

**Table 4.15** – Mass, energy and transportation flows for 1 m<sup>2</sup> area of substrate surface preparation for stainless steel (SS) and carbon steel (CS) surfaces before using S-HVOF deposition method.

Surfaces	Masses		Transportation (tkm)	Electrical energy (kWh)
	(kg)			
SS/CS	0.25 (Acetone)	-	0.14	0.508
	0.672 (Al <sub>2</sub> O <sub>3</sub> )	0.028 (TiO <sub>2</sub> )		

The S-HVOF coating deposition process has been carried out with 0% and 3.6% Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coating materials using gas flow rates and stand-off distance for developing HSP-0 and HSP-

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3.6 synthesised coatings onto carbon steel and stainless steel substrates. Based on the data given in Table A10 of Appendix A, we evaluated the LCA data for these synthesised coatings deposited over 1 m<sup>2</sup> area of substrate and are given in Table 4.16.

**Table 4.16** - Mass, energy and transportation flows for coating deposition of HSP-0\_S-HVOF and HSP-3.6\_S-HVOF synthesised coatings

Coating types	Precursor solution (litre)	Masses (kg)		Energy	Transportation
		Hydrogen Fuel	Oxygen	(kWh)	(tkm)
HSP-0	1.2	2.64	16.00	53.33	3.73
HSP-3.6	1.2	2.64	16.00	53.33	3.73

Silica based hydrophobic coatings have been developed and deposited onto four substrates such as aluminium (Al-46), copper (C103), stainless steel (304L) and carbon steel (P355) for enhancing heat transfer performances on condensing surfaces of heat exchangers. A number of commercially available coating materials such as sharc sapphire Gelest 25/75 (ShS\_Gelest\_25/75) and sharc sapphire SMS35 333 HMDS 25/75 (ShS\_SMS\_25/75) were selected to achieve superhydrophobic behaviour. All these coatings were applied using dip coating method with a speed of 100 mm min<sup>-1</sup> and the curing method has been undertaken subsequently as per manufacturer's guidance. Based on the data given in Table A7 of Appendix A, we evaluated the LCA data for these synthesised coatings deposited over 1 m<sup>2</sup> area of substrate and are given in Table 4.17.

**Table 4.17** - Mass, energy and transportation flows for coating deposition of ShS\_SMS35\_25/75 and ShS\_Gelest\_25/75 synthesised coatings using dip coating method

Coating ID	Masses (kg)	Energy	Transportation
		(kWh)	(tkm)
ShS-SMS35	0.817625	2.65	0.163525
ShS-Gelest	0.863750	2.65	0.172750

Superhydrophobic and functionalised hierarchical mesh-covered surfaces have been developed to enable sucking flow condensation for expediting both droplet growth and surface refreshing. Commercially available woven micro meshes of mild steel (MS) and stainless steel (316L) have been metallurgically joined to carbon steel (P355NH) and stainless steel (316L) substrates using uniaxial diffusion bonding process. These two categories of mesh bonded substrates were successfully developed coated with a polysilazane based coating material Tutoprom™ Bright – a commercially available hydrophobic coating material. This coating material was applied using dip coating method with a speed of 100 mm min<sup>-1</sup> and the curing method has been undertaken subsequently as per manufacturer's guidance. Based on the data given in Table A8 of Appendix A, we evaluated the LCA data for these synthesised coatings deposited over 1 m<sup>2</sup> area of substrate and are given in Table 4.18.

**Table 4.18** - Mass, energy and transportation flows for coating deposition of Tutoprom™ Bright (TutopromB) coatings using dip coating method

Coating type	Mass	Energy	Transportation
	(kg)	(kWh)	(tkm)
Tutoprom	0.43	2.65	0.086

Physical vapour deposition (PVD) using DC magnetron sputtering technique has been used to synthesise amorphous metal coatings. All coatings comprised three elements: silicon (Si) and zirconium (Zr), plus one of neodymium (Nd) or lanthanum (La). Two candidate coatings (GHX072 and GHX099) have been down-selected for further testing, from the compositions investigated (Table 2.2). Based on the data given in Table A9 of Appendix A, we evaluated the LCA data for these synthesised coatings deposited over 1 m<sup>2</sup> area of substrate and are given in Table 4.19.

**Table 4.19** - Mass, energy and transportation flows for coating deposition of amorphous metal coatings

Coating types	Masses (kg)		Energy	Transportation
	Coating material	Argon	(kWh)	(tkm)
GHX072	0.0041	0.1804	3.275	0.03689
GHX099	0.0052	0.1804	3.2750	0.03711

We have explored inventory data from ecoinvent version 3.6 database and other databases for various materials used in SOA, substrate and coating materials and processes. The dataset names have been selected from the databases for them and are listed in Table 4.20.

**Table 4.20** – 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
Cu	Copper {RER}   production, primary   APOS, U
Ni	Nickel, 99.5% {GLO}   market for   APOS, U
Fe	Ferrite {GLO}   production   APOS, U
Nb	Input from nature in ground
Mo	Molybdenum {RER}   production   APOS, U
Ti	Titanium, primary {GLO}   production   APOS, U
V	Input from nature in ground
Al	Aluminium, primary, ingot {IAI Area, EU27 & EFTA}   production   APOS, U
Zn	Zinc oxide {RER}   production   APOS, U
Pb	Lead {GLO}   primary lead production from concentrate   APOS, U
Bi	Input from nature in ground

Date: 30 June 2021

Materials/processes	Dataset names
Nd	Neodymium oxide {RoW}   rare earth oxides production from bastnasite concentrate   APOS, U
La	Lanthanum oxide {RoW}   rare earth oxides production from bastnasite concentrate   APOS, U
TiO <sub>2</sub>	Titanium dioxide {RER}   production, chloride process   APOS, U
ZrO	Zirconium oxide {RoW}   production   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
Ar	Argon, liquid {RER}   production   APOS, U
Aluminium oxide	Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}   aluminium oxide production   APOS, U
Ethanol	Ethanol, without water, in 99.7% solution state, from ethylene {RER}   ethylene hydration   APOS, U
HCl	Hydrochloric acid, without water, in 30% solution state {RER}   allyl chloride production, reaction of propylene and chlorine   APOS, U
H <sub>2</sub> SO <sub>4</sub>	Sulfuric acid {RER}   production   APOS, U
H <sub>3</sub> PO <sub>4</sub>	Phosphoric acid, industrial grade, without water, in 85% solution state {RER}   purification of wet-process phosphoric acid to industrial grade, product in 85% solution state   APOS, U
Sodium dichromate	Sodium dichromate {RER}   production   APOS, U
Sodium pyrophosphate	Sodium pyrophosphate {GLO}   production   APOS, U
Acetylene	Acetylene {RER}   market for acetylene   APOS, U
Iron sulfate	Iron sulfate {RER}   production   APOS, U
Ammonium sulfate	Ammonium sulfate, as N {RER}   ammonium sulfate production   APOS, U
Dimethyldichlorosilane	Dimethyldichlorosilane {GLO}   dimethyldichlorosilane production   APOS, U
Hexamethyl disilazane	Hexamethyl disilazane {GLO}   amination of chlorosilane   APOS, U
Silica particles	Activated silica {GLO}   production   APOS, U
SiC	Silicon carbide {RER}   production   APOS, U
Acetone	Acetone, liquid {RER}   production   APOS, U
Isopropanol	Isopropanol {RER}   production   APOS, U
Isobutyl acetate	Isobutyl acetate {RER}   production   APOS, U
Potassium hydroxide	Potassium hydroxide {RER}   production   APOS, U
Sodium hydroxide	Sodium hydroxide, chlor-alkali production mix, at plant/RER
Sodium metasilicate	Sodium metasilicate pentahydrate, 58% active substance, powder {RER}   production   APOS, U
Hydrogen	Hydrogen, liquid {RER}   market for   APOS, U
Oxygen	Oxygen, liquid {RER}   market for   APOS, U

#### 4.2.2 LCIA Results of GeoHex Engineered Materials

We have modelled three processes (substrate material, substrate surface preparation and coating material deposition) shown in Figure 3.2 to analyse the environmental impacts for the phase change GeoHex materials deposited through S-HVOF, PVD and Dip coating processes. Using the inventory data

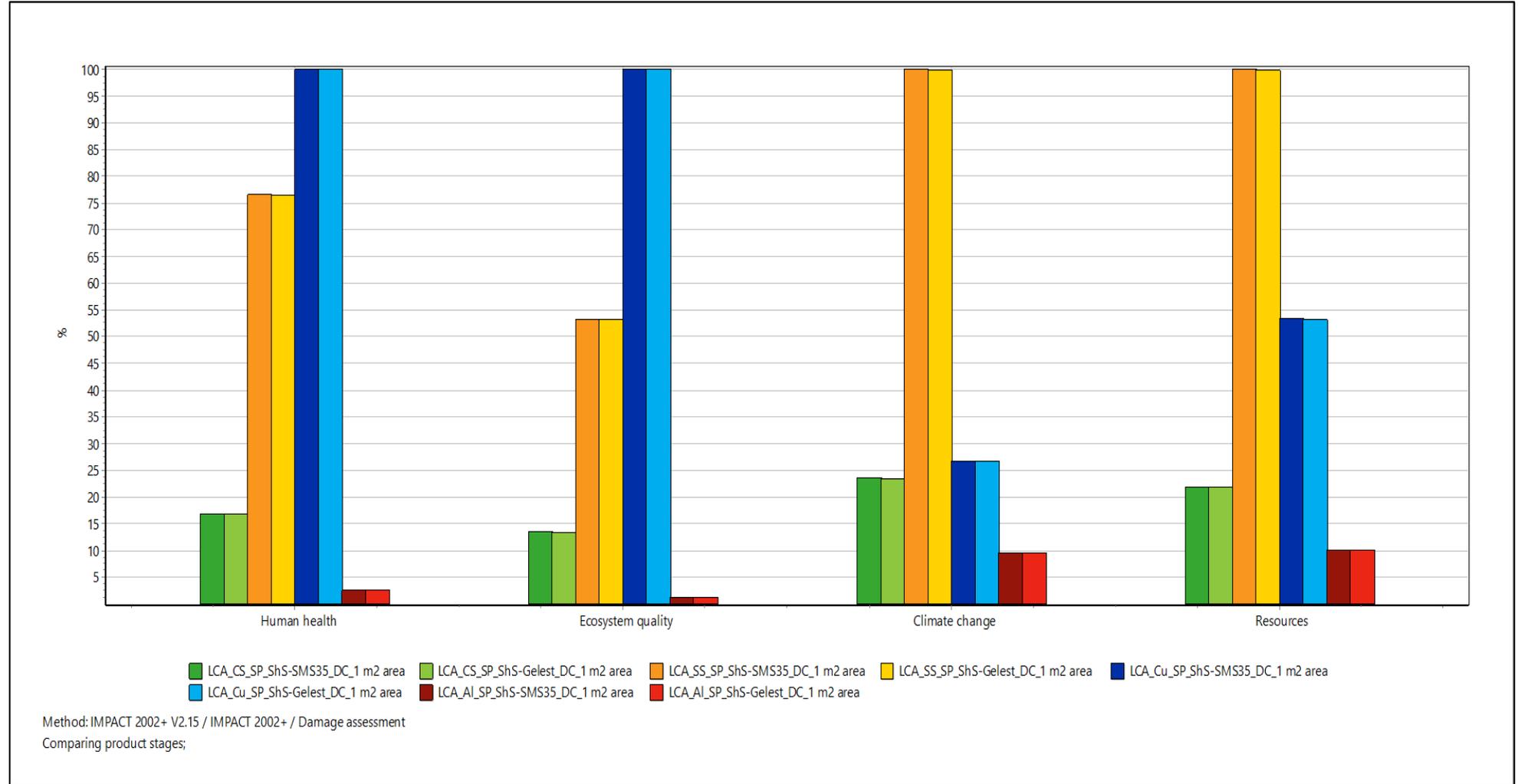
given in Tables 4.11-4.20, the cradle to gate LCA analyses for 20 synthesised coatings over 1 m<sup>2</sup> area have been evaluated and calculated using SimaPro 9.1.1.1 LCA tool considering the impact assessment methodology IMPACT 2002+ version 2.15.

### Silica based hydrophobic materials deposited through Dip coating process for condensers

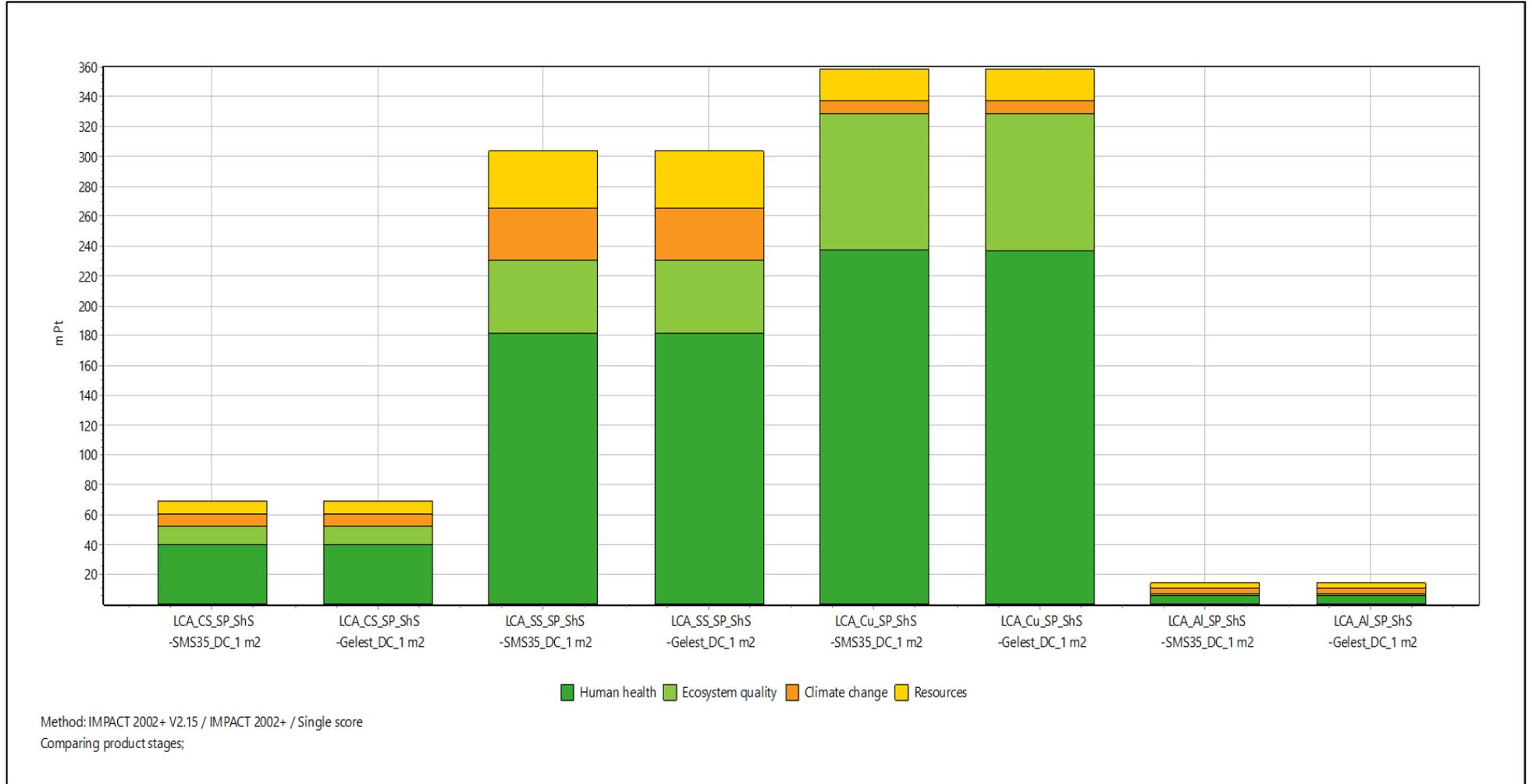
Silica based hydrophobic materials such as the sharc sapphire with SMS35 333 HMDS (ShS-SMS35) and sharc sapphire Gelest silica particles (ShS-Gelest) have been deposited over 1 m<sup>2</sup> area of four different substrates (carbon steel, stainless steel, aluminium and copper) through dip coating process. Using the data described in Tables 4.11-4.13, 4.17 and 4.20, LCA analyses of ShS-SMS35 and ShS-Gelest coating systems deposited onto the substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the overall environmental footprints in terms of single score for these synthesised coatings are presented in Figures 4.11 and 4.12, respectively. It is seen from Figure 4.11 that ShS-SMS35 and ShS-Gelest synthesised coatings deposited over aluminium substrate showed the lower environmental footprints over 4 endpoint damage categories as compared with those of deposited over other substrates. The quantification of environmental footprints of over 4 endpoint damage categories for ShS-SMS35 and ShS-Gelest synthesised coatings and is listed in Table 4.21.

**Table – 4.21** Quantification of environmental footprints over 4 endpoint damage categories for ShS-SMS35 and ShS-Gelest synthesised coatings over 1 m<sup>2</sup> area.

Endpoint Damage categories	Unit	Coating types							
		CS_ShS-SMS35	CS_ShS-Gelest	SS_ShS-SMS35	SS_ShS-Gelest	Cu_ShS-SMS35	Cu_ShS-Gelest	Al_ShS-SMS35	Al_ShS-Gelest
Human health	DALY	0.0003	0.0003	0.0013	0.0013	0.0017	0.0017	0.0000	0.0000
Ecosystem quality	PDF*m2*yr	169.23	169.18	666.09	666.04	1251.50	1251.45	15.98	15.93
Climate change	kg CO2 eq	82.21	81.83	348.57	348.18	93.10	92.72	33.70	33.31
Resources	MJ primary	1279.64	1272.69	5860.54	5853.59	3124.73	3117.78	599.41	592.46



**Figure 4.11** - The percentage contribution of environmental footprints of ShS-SMS35 and ShS-Gelest materials deposited onto carbon steel, stainless steel, copper and aluminium substrates materials each of 1 m<sup>2</sup> area for four endpoint damage categories.



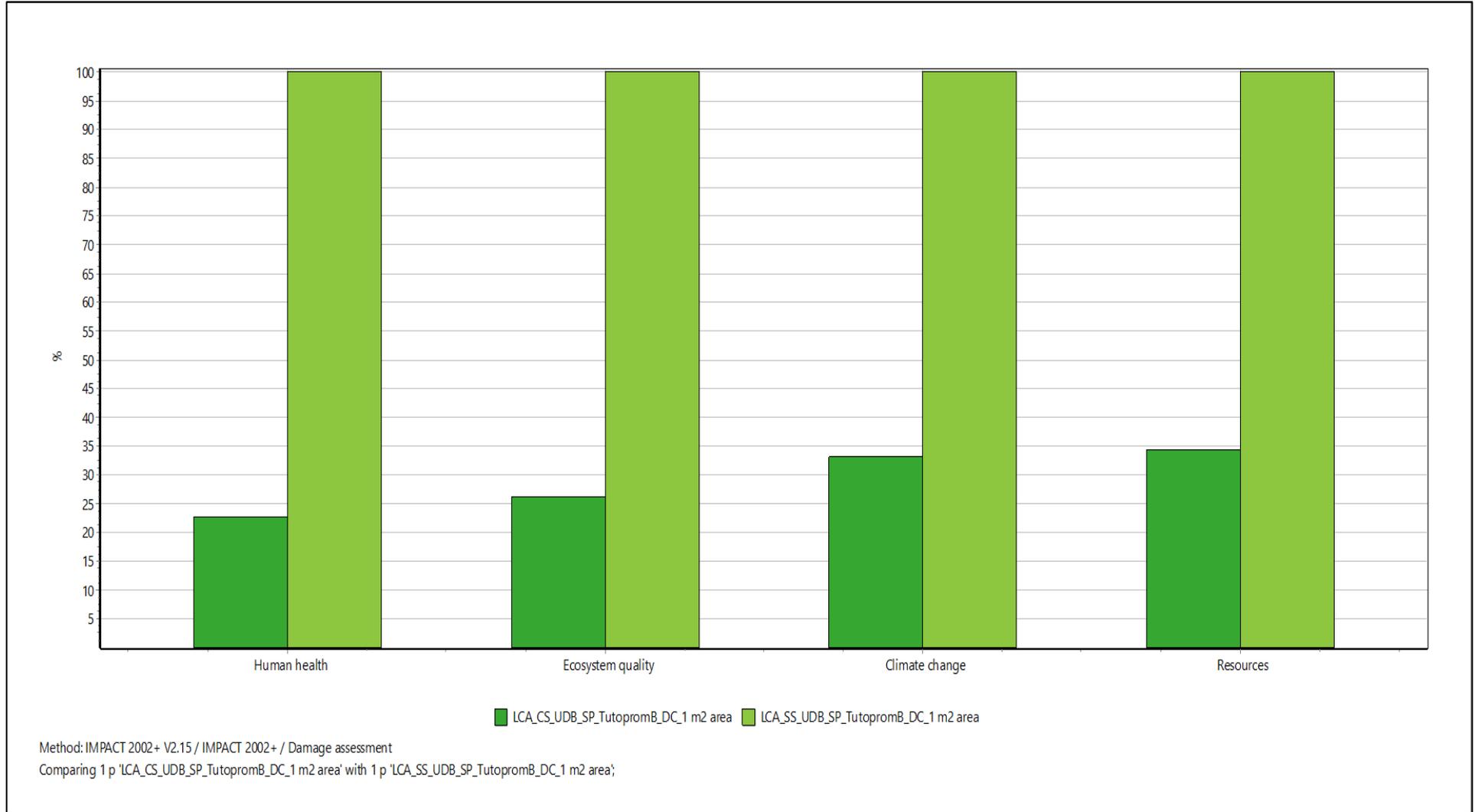
**Figure 4.12** - Single score results of environmental footprints of ShS-SMS35 & ShS-Gelest materials deposited onto carbon steel, stainless steel, copper and aluminium substrates each of 1 m<sup>2</sup> area in units of mPt for four endpoint damage categories.

**Superhydrophobic and functionalised hi-mesh materials using Dip coating process for condensers**

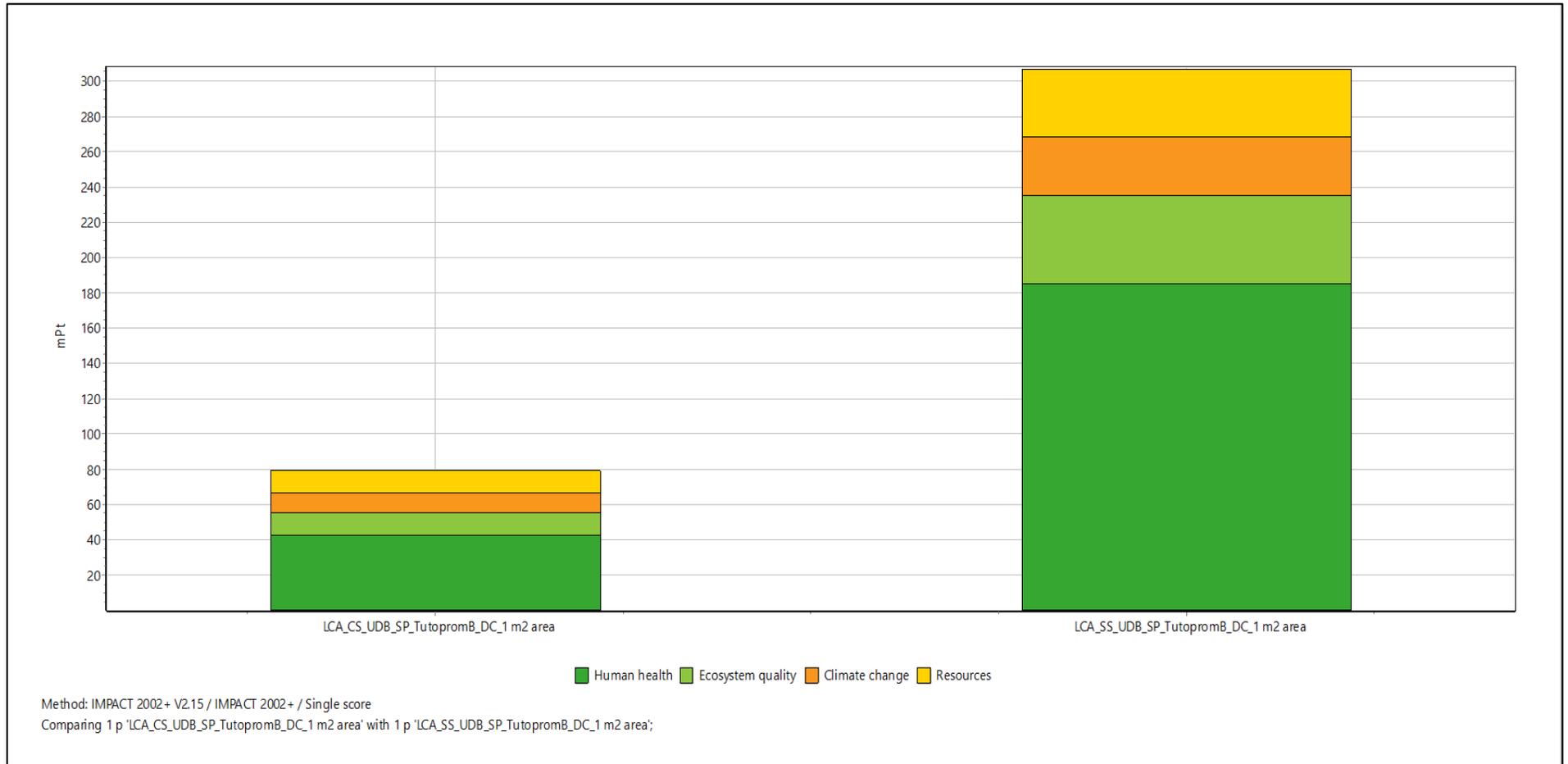
Commercially available woven micro meshes of mild steel (MS) and stainless steel (316L) have been metallurgically joined to carbon steel (P355NH) and stainless steel (316L) substrates were successfully developed coated with a polysilazane based coating material Tutoprom™ Bright (Tutoprom) – a commercially available hydrophobic coating material. Using the data described in Tables 4.11-4.13, 4.18 and 4.20, LCA analyses of Tutoprom coating systems deposited onto the substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the overall environmental footprints in terms of single score for these synthesised coatings are presented in Figures 4.13 and 4.14, respectively. It is seen from Figure 4.13 that Tutoprom materials deposited over carbon steel substrate showed the lower contributions of environmental footprints over 4 endpoint damage categories as compared with those of deposited over stainless steel substrate. The quantification of environmental footprints of Tutoprom materials deposited onto carbon steel and stainless steel substrates for over 4 endpoint damage categories and is listed in Table 4.22.

**Table – 4.22** Quantification of environmental footprints over 4 endpoint damage categories for TutopromB synthesised coatings over 1 m<sup>2</sup> area.

Coating types	Endpoint Damage categories			
	Human health	Ecosystem quality	Climate change	Resources
	DALY	PDF*m2*yr	kg CO2 eq	MJ primary
CS_Tutoprom	0.0003	178.95	109.79	1991.60
SS_Tutoprom	0.0013	681.48	331.24	5793.32



**Figure 4.13** – The percentage contribution of environmental footprints of Tutoprom materials deposited onto carbon steel and stainless steel substrates materials each of 1 m<sup>2</sup> area for four endpoint damage categories.



**Figure 4.14** – Single score results of environmental footprints of Tutoprom materials deposited onto carbon steel and stainless steel substrates each of 1 m<sup>2</sup> area in units of mPt for four endpoint damage categories.

**Doped and undoped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite materials using S-HVOF process for evaporators**

Doped and undoped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coating materials using gas flow rates and stand-off distance for developing HSP-0 and HSP-3.6 synthesised coatings have been deposited onto carbon steel and stainless steel substrates using S-HVOF method. Using the data described in Tables 4.15, 4.16 and 4.20, LCA analyses of these composite coating systems deposited onto the substrates have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the overall environmental footprints in terms of single score for these synthesised coatings are presented in Figures 4.15 and 4.16, respectively. It is seen from Figure 4.15 that synthesised coatings deposited over carbon steel substrate showed the lower contributions of environmental footprints over 4 endpoint damage categories as compared with those of deposited over stainless steel substrate. The quantification of environmental footprints of over 4 endpoint damage categories for these synthesised coatings (HSP-0 and HSP-3.6) and is listed in Table 4.23.

**Table – 4.23** Quantification of environmental footprints over 4 endpoint damage categories for doped and undoped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coatings over 1 m<sup>2</sup> area.

Endpoint Damage categories	Unit	Coating types			
		CS_HSP-0	CS_HSP-3.6	SS_HSP-0	SS_HSP-3.6
Human health	DALY	0.0002	0.0002	0.0013	0.0013
Ecosystem quality	PDF*m2*yr	89.49	89.48	685.45	685.44
Climate change	kg CO2 eq	114.94	114.92	347.05	347.02
Resources	MJ primary	2329.16	2328.80	6333.52	6333.16

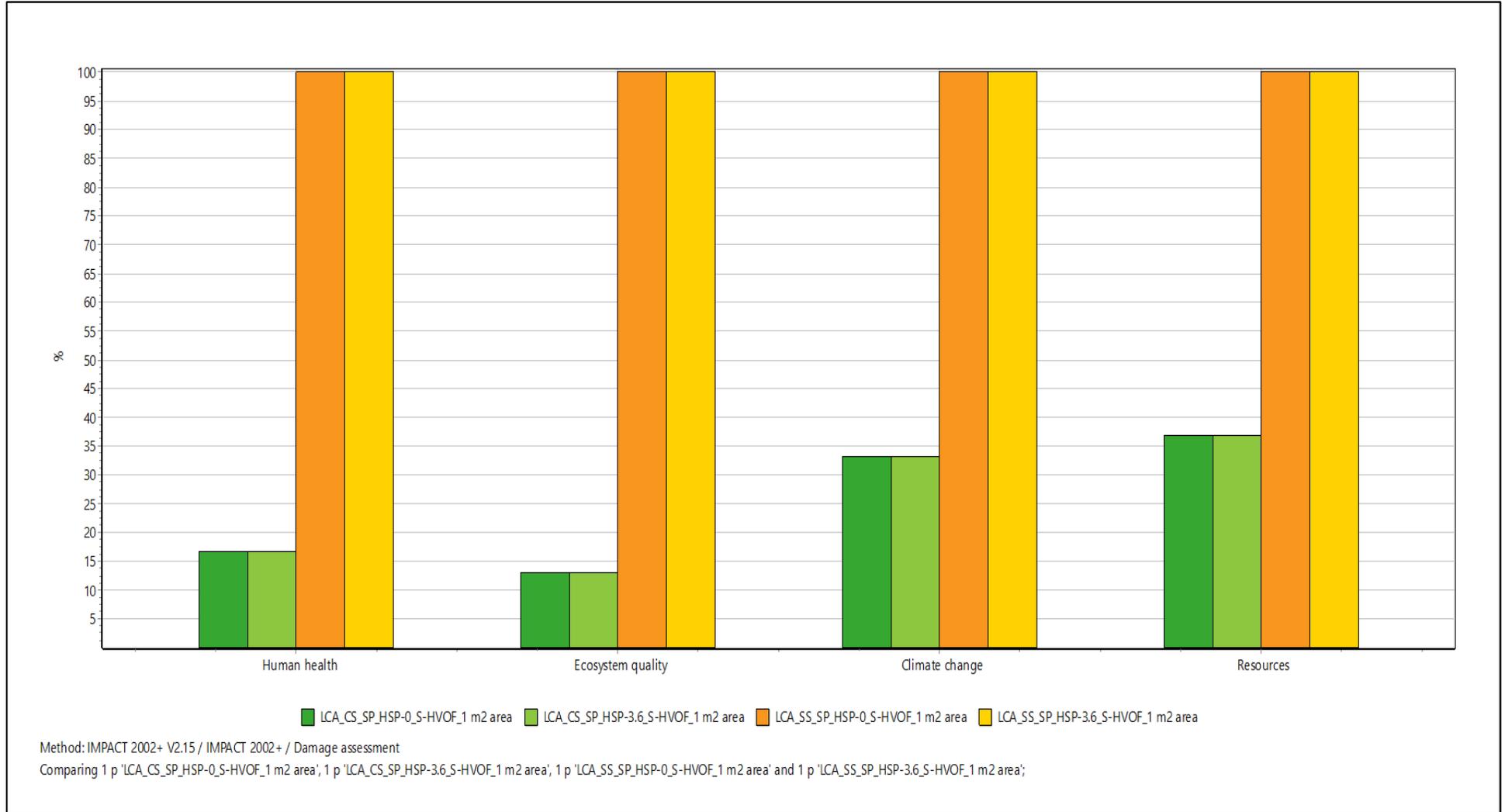
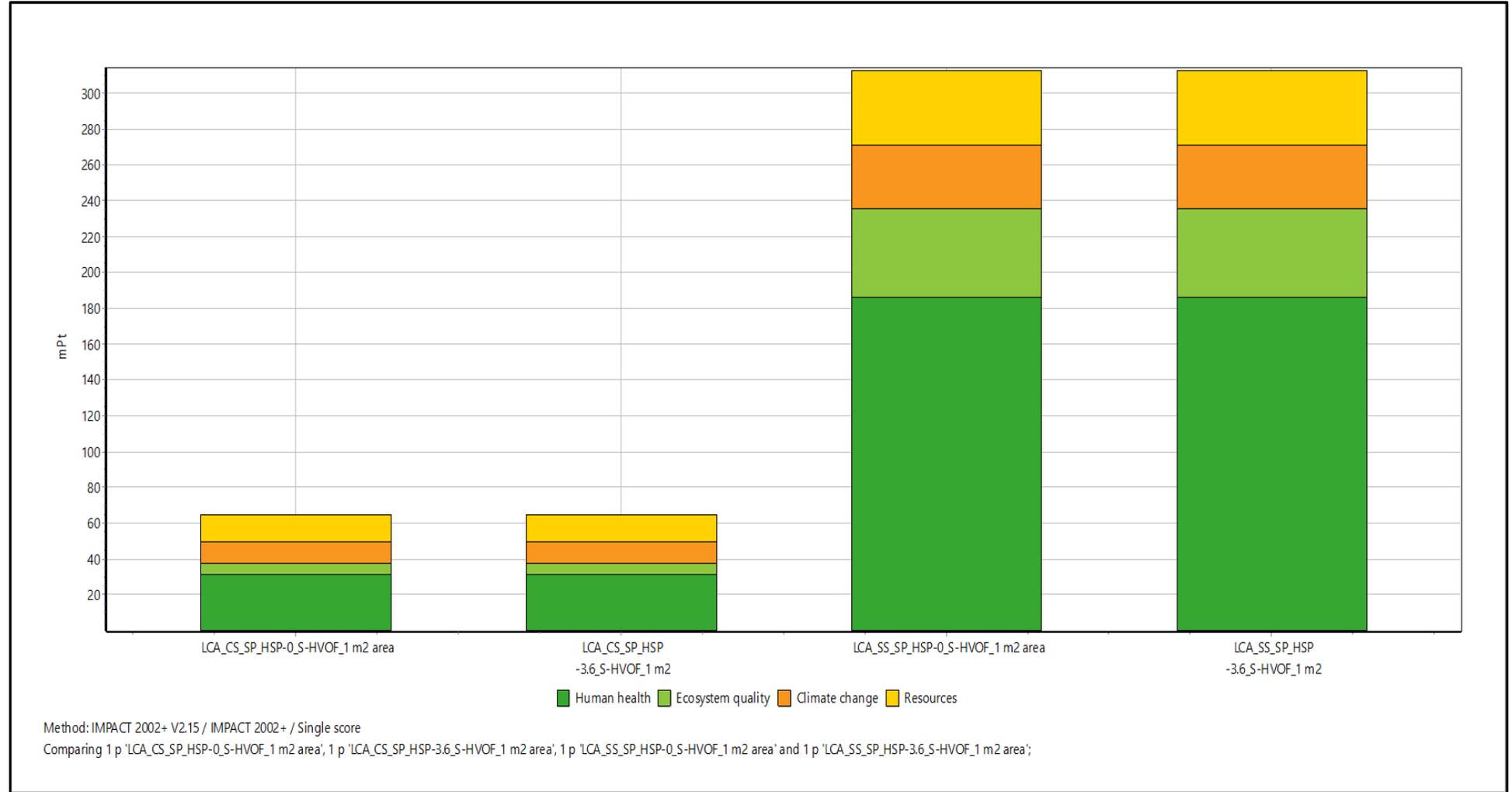


Figure 4.15 – The percentage contribution of environmental footprints of HSP-0 and HSP-3.6 materials deposited onto carbon steel and stainless steel substrates materials each of 1 m<sup>2</sup> area for four endpoint damage categories.



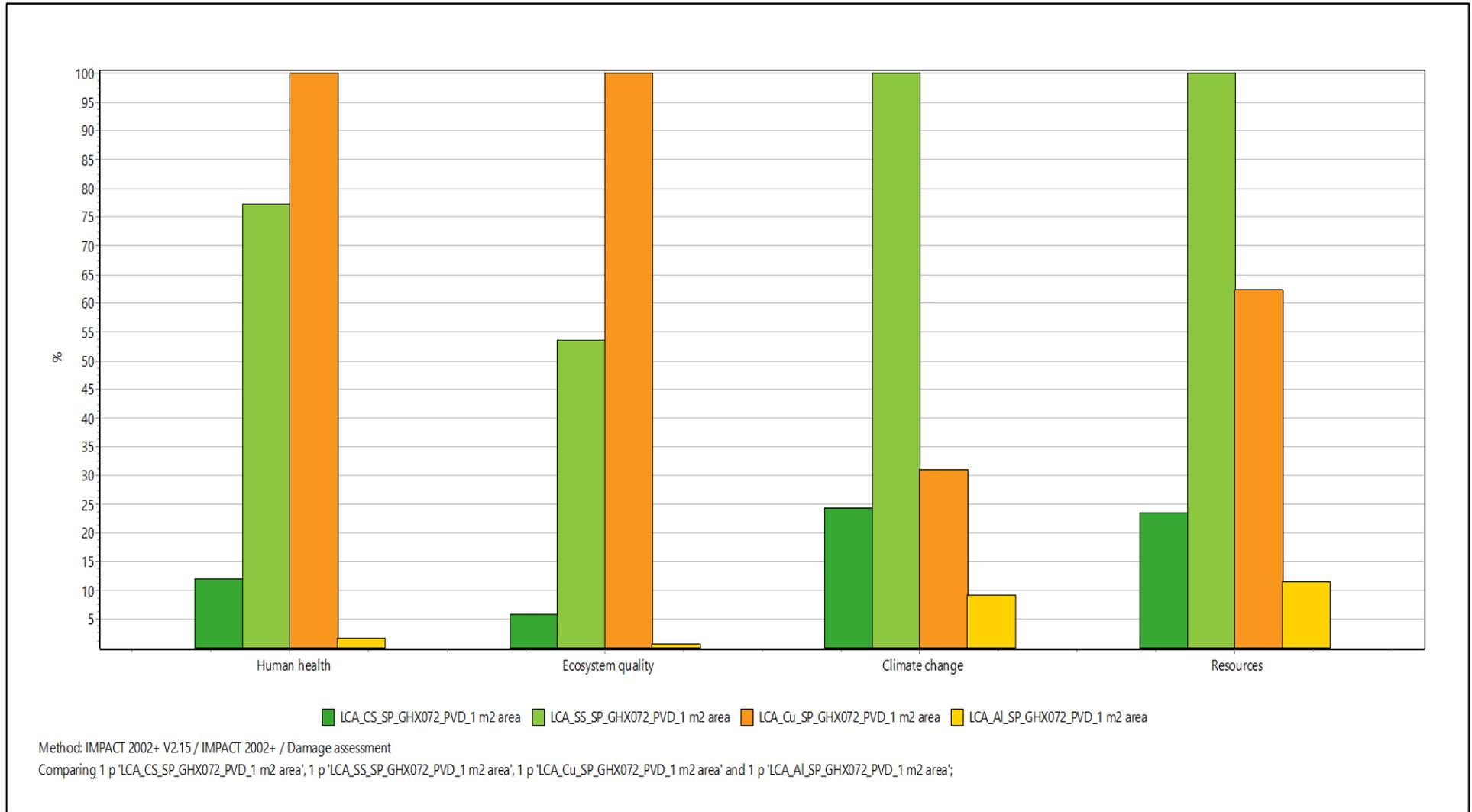
**Figure 4.16** – Single score results of environmental footprints of HSP-0 and HSP-3.6 materials deposited onto carbon steel and stainless steel substrates each of 1 m<sup>2</sup> area in units of mPt for four endpoint damage categories.

**Amorphous metal coating materials using PVD method for condensers**

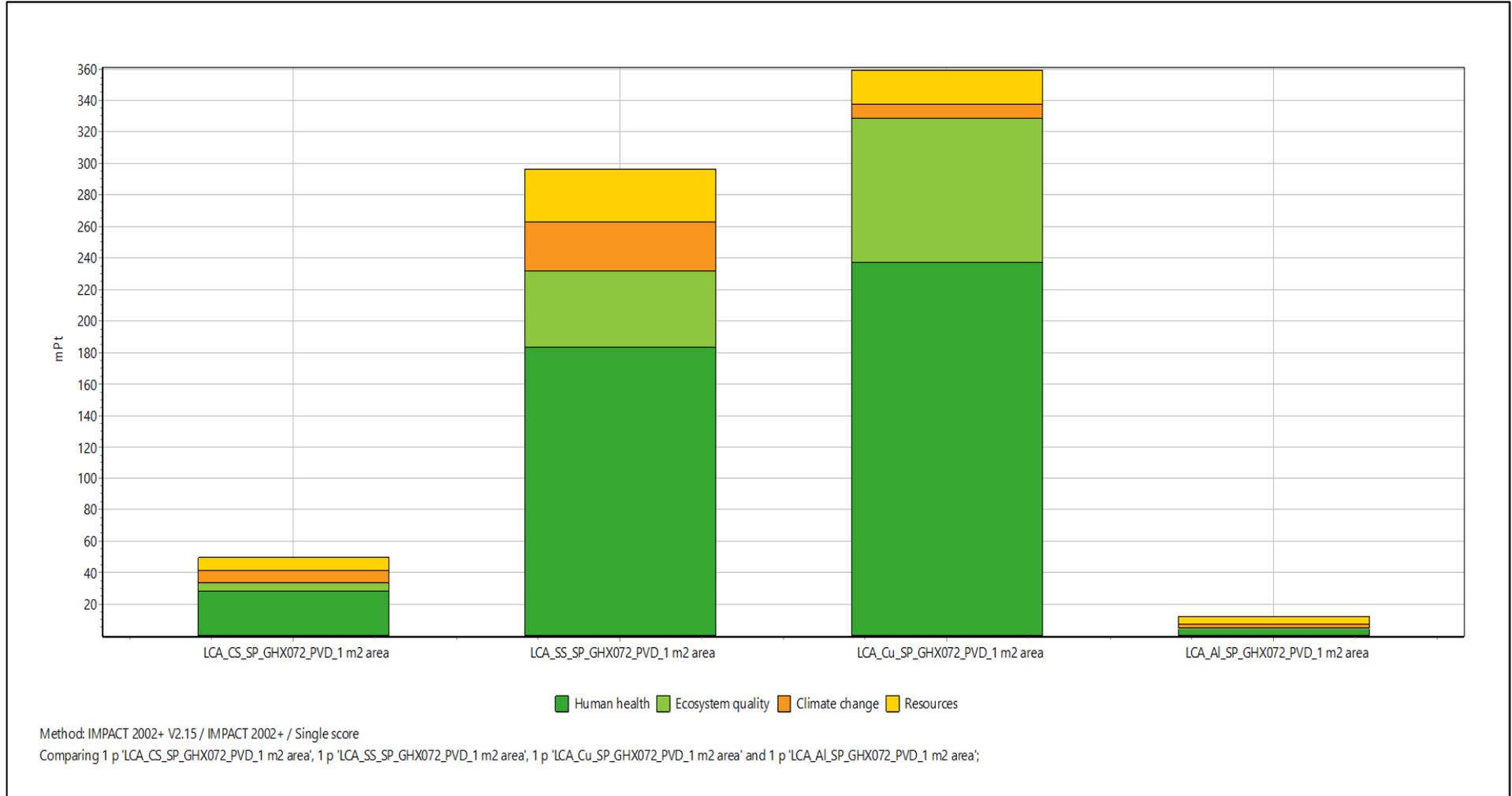
Using the data described in Tables 4.11, 4.12, 4.14, 4.19 and 4.20, LCA analyses of amorphous metal coating material GHX072 deposited onto carbon steel, stainless steel, aluminium and copper substrates using PVD method have been carried out. The comparative LCIA results of 4 endpoint damage categories (human health, ecosystem quality, climate change and resources) and the environmental impacts in terms of single score for these synthesised coatings GHX072 deposited over carbon steel, stainless steel, copper and aluminium substrates are presented in Figures 4.17 and 4.18, respectively. It is seen from Figure 4.17 that GHX072 synthesised coatings deposited over aluminium substrate showed the lower environmental footprints over 4 endpoint damage categories as compared with those of deposited over other substrates. The quantification of environmental footprints of over 4 endpoint damage categories for these synthesised coatings and is listed in Table 4.24.

**Table – 4.24** Quantification of environmental footprints over 4 endpoint damage categories for amorphous metal synthesised coatings over 1 m<sup>2</sup> area of substrates.

Endpoint Damage categories	Unit	Coating types			
		CS_GHX072	SS_GHX072	Cu_GHX072	Al_GHX072
Human health	DALY	0.00020	0.00130	0.00168	0.00003
Ecosystem quality	PDF*m2*yr	75.19	670.97	1250.76	9.49
Climate change	kg CO2 eq	74.32	304.91	94.68	28.19
Resources	MJ primary	1213.58	5165.79	3217.16	596.98



**Figure 4.17** – The percentage contribution of environmental footprints of GHX072 materials deposited onto carbon steel, stainless steel, copper and aluminium substrates materials each of 1 m<sup>2</sup> area for four endpoint damage categories.



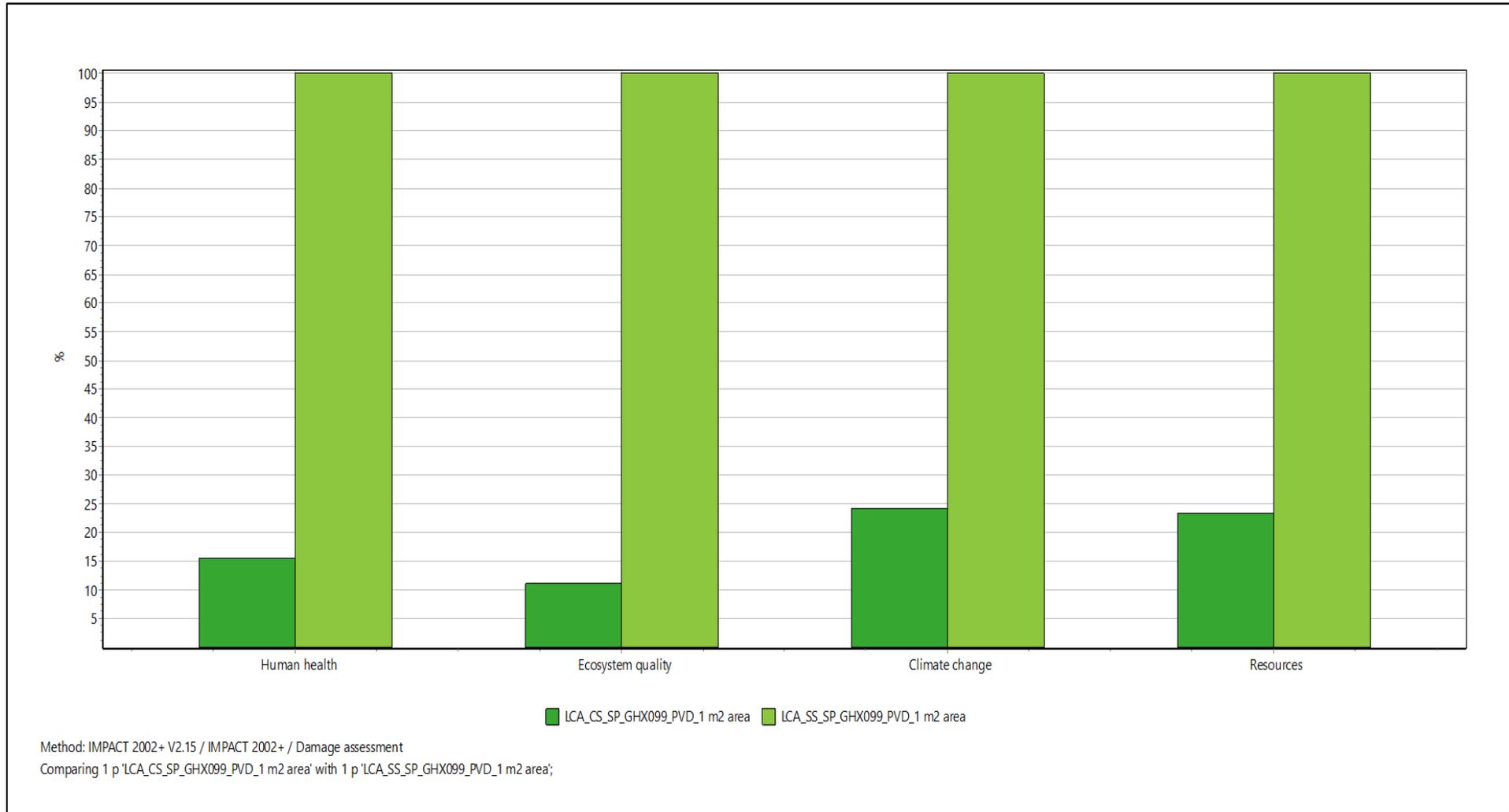
**Figure 4.18** – Single score results of environmental footprints of GHX072 materials deposited onto carbon steel, stainless steel, copper and aluminium substrates each of 1 m<sup>2</sup> area in units of mPt for four endpoint damage categories.

**Amorphous metal coating materials using PVD method for evaporators**

Using the data described in Tables 4.14, 4.19 and 4.20, LCA analyses of amorphous metal coating material GHX099 deposited onto carbon steel and stainless steel substrates using PVD method 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 GHX099 deposited over carbon steel and stainless steel substrates are presented in Figures 4.19 and 4.20, respectively. It is seen from Figure 4.19 that GHX099 synthesised coatings deposited over carbon steel substrate showed the lower environmental footprints over 4 endpoint damage categories as compared with that of deposited over stainless steel substrate. The quantification of environmental footprints of over 4 endpoint damage categories for these synthesised coatings and is listed in Table 4.25.

**Table – 4.25** Quantification of environmental footprints over 4 endpoint damage categories for amorphous metal synthesised coatings GHX099 over 1 m<sup>2</sup> area of substrates.

Endpoint Damage categories	Unit	Coating types	
		CS_GHX099	SS_GHX099
Human health	DALY	0.00020	0.00130
Ecosystem quality	PDF*m2*yr	75.10	670.89
Climate change	kg CO2 eq	74.13	304.71
Resources	MJ primary	1210.19	5162.41



**Figure 4.19-** The percentage contribution of environmental footprints of GHX099 materials deposited onto carbon steel and stainless steel substrates materials each of 1 m<sup>2</sup> area for four endpoint damage categories.

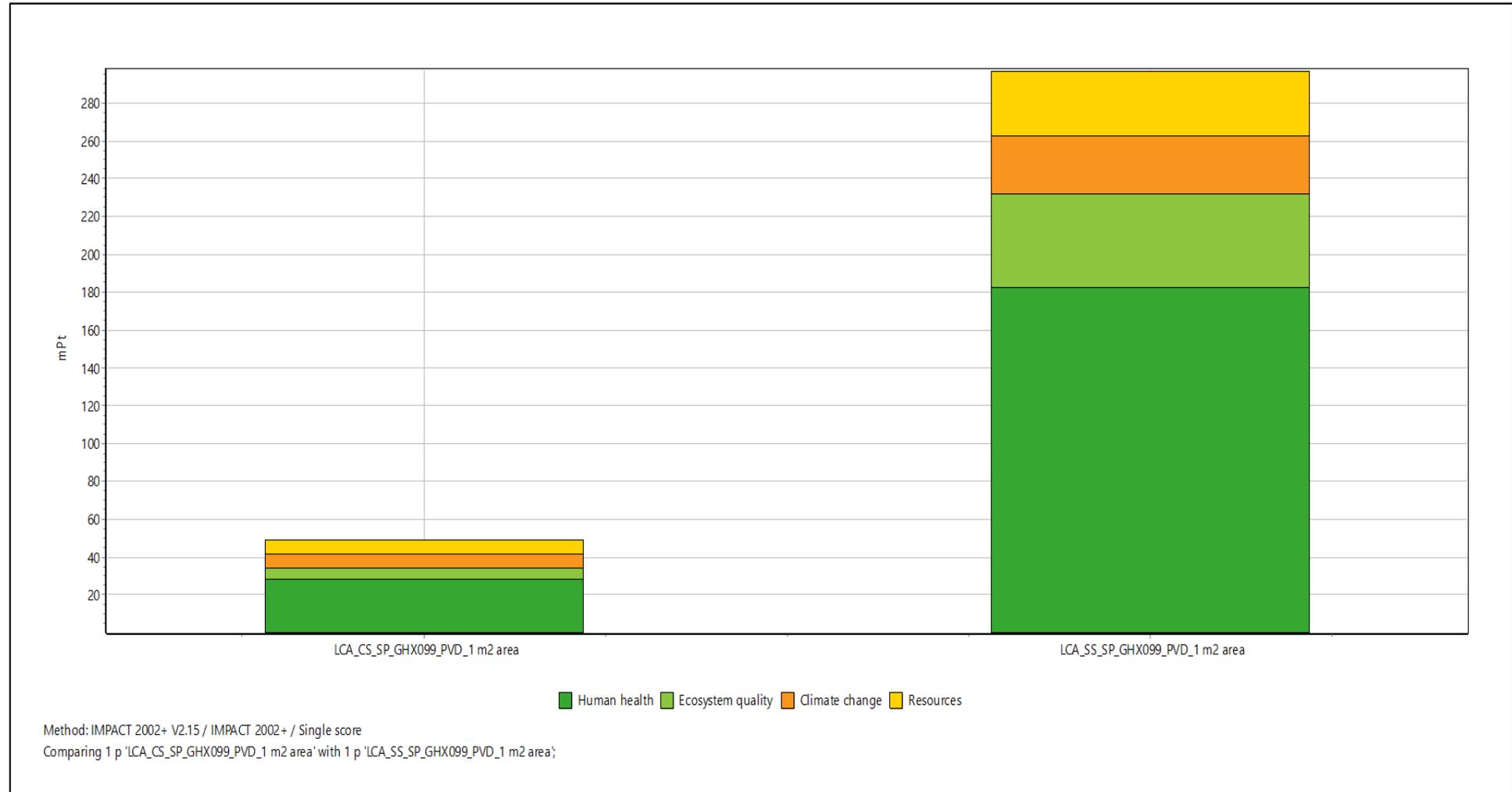


Figure 4.20 - Single score results of environmental footprints of GHX099 materials deposited onto carbon steel and stainless steel substrates each of 1 m<sup>2</sup> area in units of mPt for four endpoint damage categories.

### 4.3 Discussions

The sustainability assessment of phase change heat exchanger materials has been investigated by combining the costing and environmental performance of silica based hydrophobic coating (ShS-SMS35 & ShS-Gelest), functionalised hi-mesh coated (Tutoprom), robust hydrophobic and hydrophilic amorphous metal (GHX072 and GHX099) and undoped & doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coating ( HSP-0 and HSP-3.6) materials deposited onto various substrates developed for phase change heat exchangers alternative to the state of art materials SOA 316L and 254SMO. ShS-SMS35 & ShS-Gelest, Tutoprom, GHX072 coating systems are being developed for improving the heat transfer efficiency on the ORC liquid or vapour side of the plates and tubes of condenser. GHX099 and HSP-0 & HSP-3.6 coating systems are also being developed for improving the heat transfer efficiency on the ORC liquid or vapour side of the plates and tubes of evaporator. Using the total costing results from Tables 4.6-4.10 for phase change GeoHex materials and from Table A1 of Appendix for SOA materials, the relative costs of these GeoHex materials deposited onto various substrates along with the relative costs of SOA materials 316L and 254SMO have been evaluated and are shown in Figures 4.21 and 4.22, respectively. From the cost comparison results shown in Figure 4.21, all the GeoHex materials deposited onto the substrates showed higher costs ranging from 1.1-4.6 times as compared with SOA material 316L cost.

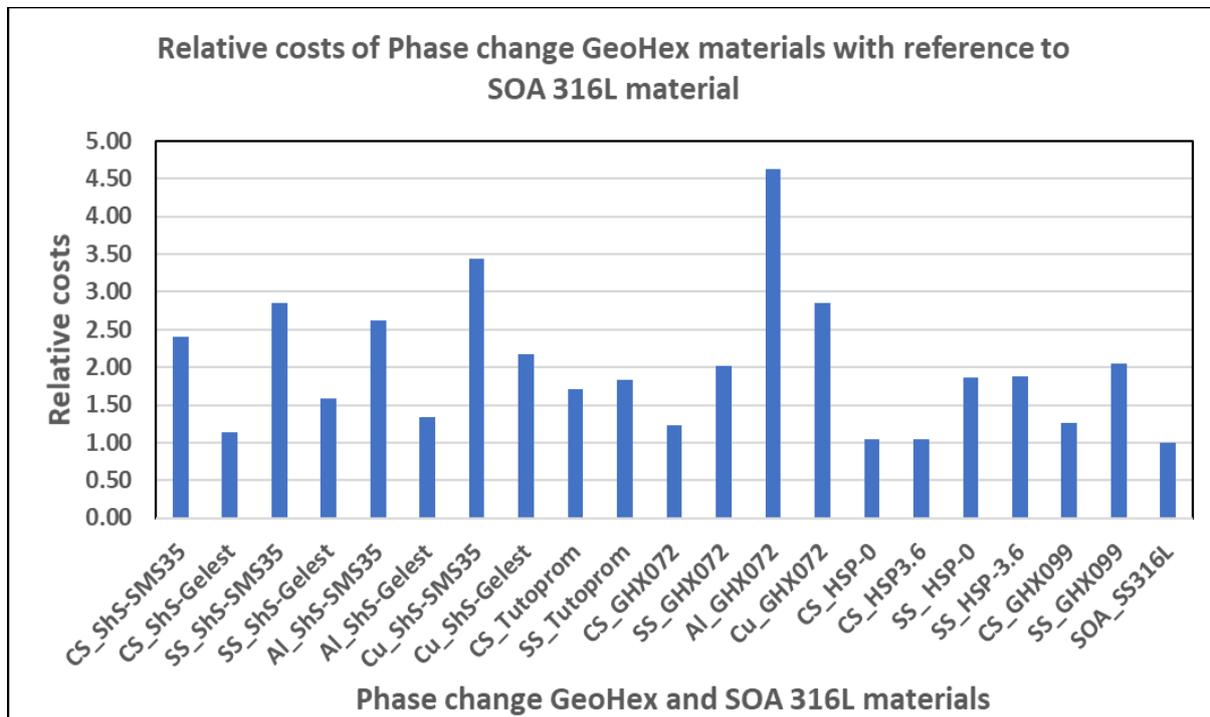
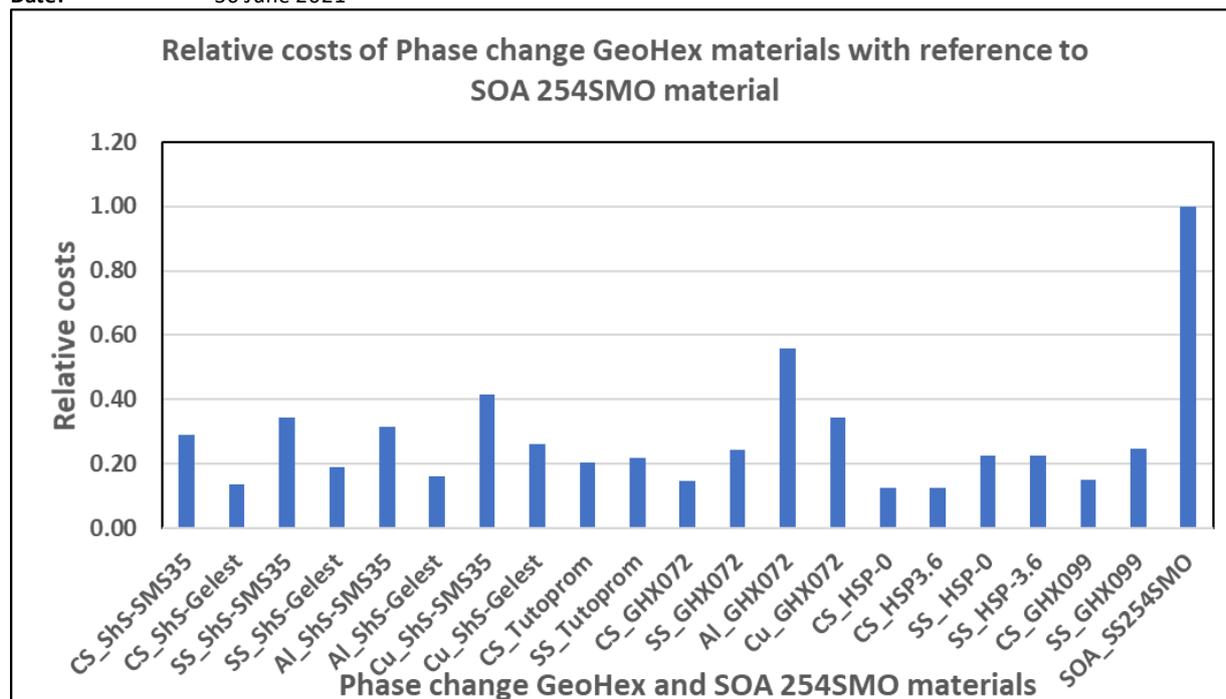


Figure 4.21 - Relative costs of phase change GeoHex materials deposited onto the substrates and SOA material 316L.



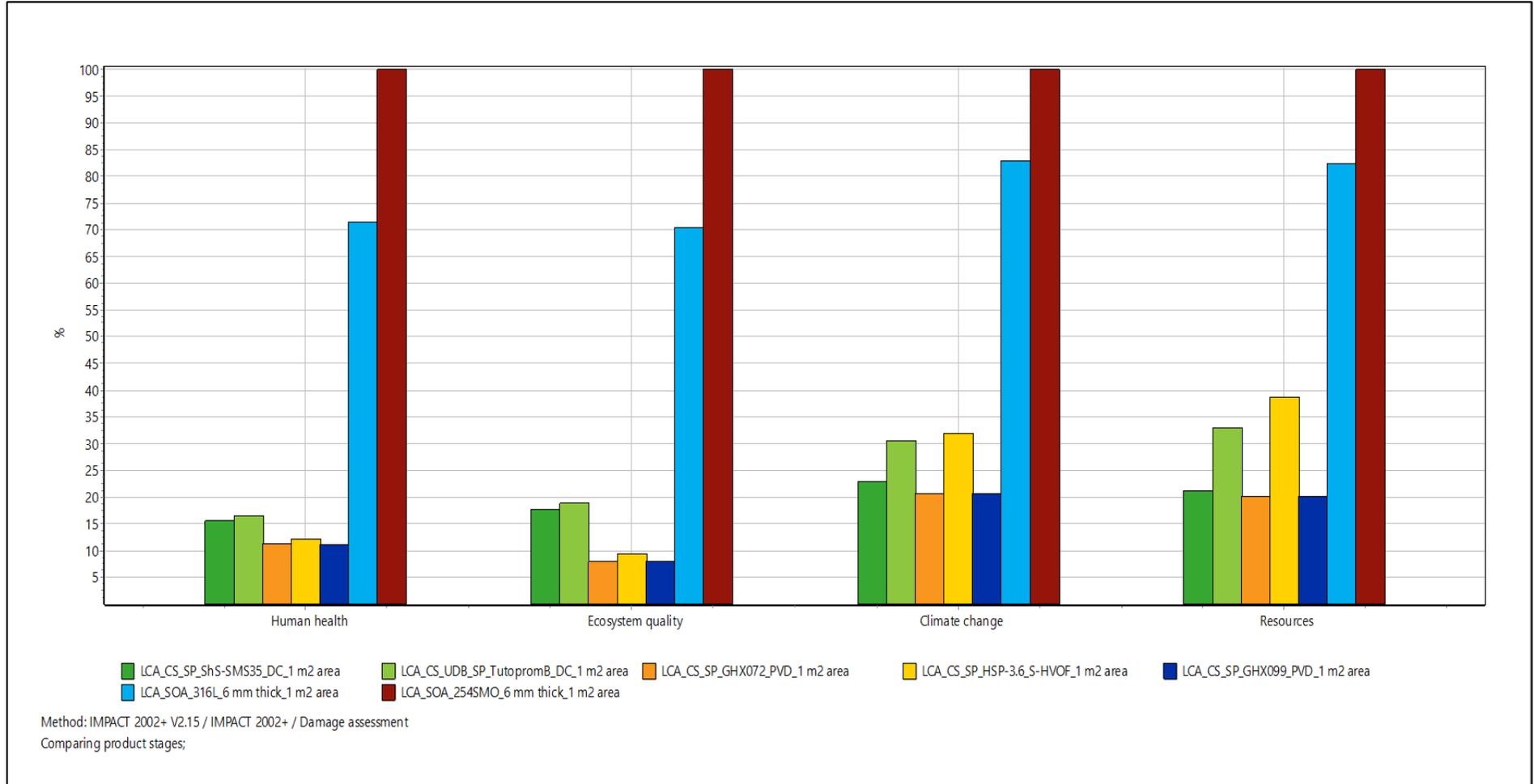
**Figure 4.22** - Relative costs of phase change GeoHex materials deposited onto the substrates and SOA material 254SMO.

It is evident from Figure 4.22 that all GeoHex materials deposited onto the substrates alternative to SOA material 254SMO showed cost savings ranging from 44% to 87%.

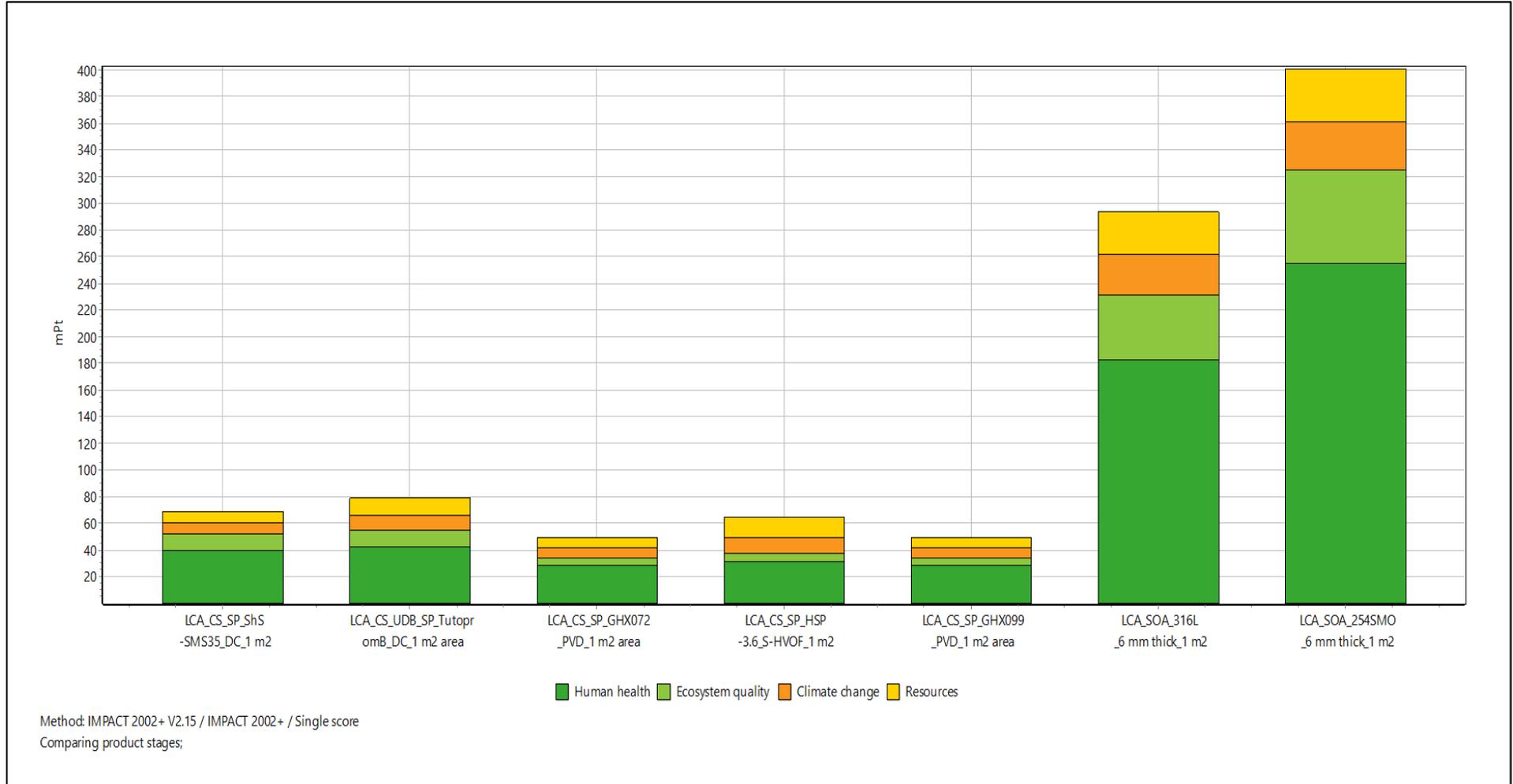
The percentage contribution of environmental footprints of phase change GeoHex materials (ShS-SMS35, Tutoprom, GHX072, GHX099 and HSP-3.6) deposited onto carbon steel substrates of 1 m<sup>2</sup> area and SOA material 316L for four endpoint damage categories have been evaluated with reference to the worst environmental footprint contribution of SOA 254SMO material of 1 m<sup>2</sup> area (considered as 100%) and presented in Figure 4.23. The single score results of environmental footprints in units of mPt of these GeoHex and SOA materials are also shown in Figure 4.24. The quantification of environmental footprints over 4 endpoint damage categories for these GeoHex materials deposited onto carbon steel and compared with SOA 316L and 254 SMO materials and are listed in Table 4.26.

**Table 4.26** – Quantification of environmental footprints over 4 endpoint damage categories for these GeoHex materials deposited onto carbon steel substrates and SOA 316L and 254SMO materials each of 1 m<sup>2</sup> area.

Environmental footprints	Unit	GeoHex and SOA materials						
		CS_ShS-SMS35	CS_Tutoprom	CS_GHX072	CS_HSP-3.6	CS_GHX099	SOA_316L	SOA_254SMO
Human health	DALY	0.0003	0.0003	0.0002	0.0002	0.0002	0.0013	0.0018
Ecosystem quality	PDF*m <sup>2</sup> *yr	169.23	178.95	75.19	89.48	75.10	669.93	950.18
Climate change	kg CO <sub>2</sub> eq	82.21	109.79	74.32	114.92	74.13	297.78	359.13
Resources	MJ primary	1279.64	1991.60	1213.58	2328.80	1210.19	4957.70	6014.16



**Figure 4.23** - The percentage contribution of environmental footprints of phase change GeoHex materials (ShS-SMS35, Tutoprom, GHX072, GHX099 and HSP-3.6) deposited onto carbon steel substrates of 1 m<sup>2</sup> area and SOA materials for four endpoint damage categories.



**Figure 4.24** - Single score results of environmental footprints in units of mPt for GeoHex materials (ShS-SMS35, Tutoprom, GHX072, GHX099 and HSP-3.6) deposited onto carbon steel substrates of 1 m<sup>2</sup> area and SOA materials.

**Date:** 30 June 2021

It has been calculated from the results of Table 4.26 and Figure 4.23 that the carbon footprint (climate change) savings of about 72%, 63%, 75%, 61% and 75% for using CS\_ShS-SMS35. CS\_Tutoprom, CS\_GHX072, CS\_HSP-3.6 and CS\_GHX099 materials deposited onto carbon steel, respectively instead of using SOA 316L material and the carbon footprint savings of about 77%, 69%, 79%, 68% and 79% for using CS\_ShS-SMS35. CS\_Tutoprom, CS\_GHX072, CS\_HSP-3.6 and CS\_GHX099 materials deposited on to carbon steel, respectively alternative to SOA 254SMO material.

It is evident from the single score results shown in Figure 4.24 that the total environmental footprints of CS\_ShS-SMS35. CS\_Tutoprom, CS\_GHX072, CS\_HSP-3.6 and CS\_GHX099 materials deposited onto carbon steel and SOA 316L & 254SMO materials are about 69, 79, 50, 65, 49, 294 and 400 mPt, respectively. Hence, the overall environmental footprint savings of about 77%, 73%, 83%, 78% and 83% for using CS\_ShS-SMS35. CS\_Tutoprom, CS\_GHX072, CS\_HSP-3.6 and CS\_GHX099 materials deposited onto carbon steel, respectively instead of using SOA 316L material and the environmental footprint savings of about 83%, 80%, 88%, 84% and 88% for using CS\_ShS-SMS35. CS\_Tutoprom, CS\_GHX072, CS\_HSP-3.6 and CS\_GHX099 materials deposited on to carbon steel, respectively instead of using 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 silica based hydrophobic coating (ShS-SMS35 & ShS-Gelest), functionalised hi-mesh coated (Tutoprom), robust hydrophobic and hydrophilic amorphous metal (GHX072 and GHX099) and undoped & doped  $\text{Al}_2\text{O}_3\text{-TiO}_2$  composite coating (HSP-0 and HSP-3.6) materials deposited onto various substrates developed for phase change heat exchangers alternative to the state of art materials SOA 316L and 254SMO. The research question was to determine which synthesised coating system was the best alternative to SOA material from an environmental and economic points of view. The relative costs of these GeoHex materials deposited onto various substrates along with the relative costs of SOA materials 316L and 254SMO have been demonstrated in Figures 4.21 and 4.22, respectively. The single score results of environmental footprints in units of mPt of phase change GeoHex materials (ShS-SMS35, Tutoprom, GHX072, GHX099 and HSP-3.6) deposited onto carbon steel substrates and SOA materials are also shown in Figure 4.24. 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 of phase change GeoHex materials with respect to SOA materials

GeoHex and SOA materials	Relative costs of GeoHex materials with respect to SOA material		Relative environmental footprints with respect to SOA material	
	316L	254SMO	316L	254SMO
CS_ShS-SMS35	2.41	0.29	0.23	0.17
CS_TutopromB	1.70	0.21	0.27	0.20
CS_GHX072	1.23	0.15	0.17	0.12
CS_HSP-3.6	1.05	0.13	0.22	0.16
CS_GHX099	1.26	0.15	0.17	0.12
SOA_316L	1.00	-	1.00	-
SOA_254SMO	-	1.00	-	1.00

It is demonstrated that the costs of phase change GeoHex materials (ShS-SMS35, Tutoprom, GHX072, GHX099 and HSP-3.6) deposited onto carbon steel is in the range of 1.05-2.41 times higher and the overall environmental footprint savings of these materials is in the range of 73% - 83% as compared with SOA 316L material; whereas the respective cost and overall environmental footprint savings are in the ranges of 71%-87% and 80%-88%, respectively as compared with SOA 254SMO material. Finally, it is concluded that phase change GeoHex materials alternative to SOA 254SMO material are more sustainable than when compared those with the alternative to SOA 316L material.

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 decisions.

- Water footprint impact category can be included from an environmental point of view.
- The economical evaluation with costing analyses can be improved by conducting a complete life cycle costing analysis.
- The cost and environmental impact weightings should be considered if there is a trade-off between the environmental and economic aspects for the GeoHex heat exchanger materials.

## Appendix A: Inventory data and calculations

**Table A1** - Substrate and SOA materials inventory data from the tasks 3.2, 3.4, 3.5 and 4.2

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

Material name	Material type	Grade of the materials	Substrate dimension used	Density of the material	Mass of 1 m <sup>2</sup> area substrate of 6 mm thick	Cost of purchased cold rolled substrate material	Cost of purchased cold rolled substrate material	Unit cost of purchased cold rolled substrate material	Cost of substrate material for 1 m <sup>2</sup> area	Hardware power for cutting	Machining time for cutting	Electrical energy used for cutting	Unit cost of electricity	Electrical energy (calculated) cost for cutting	Labour time	Unit labour cost	labour cost (calculated)	Total cost of final substrate dimension of 1 m <sup>2</sup> area and 6 mm thick
			[mm x mm x mm]	[kg/m <sup>3</sup> ]	[kg]	[€]	[€]	[€/kg]	[€]	[kW]	[min]	[kWh]	[€/kWh]	[€]	[min]	[€/h]	[€]	[€]
Substrate	Aluminium	Q-panel	102 x 152 x 0.6	?		0.60	0.72	?	48.00	NA	NA				?			
Substrate	Copper	C103	1000 x 1000 x 6	8900	53.4	715	858.00	16.07	858.00	20	10	3.33	0.2	0.67	10	28.5	4.75	863.42
Substrate	stainless steel	304L	1000 x 1000 x 6	8734	52.404	500	600.00	11.45	600.00	20	10	3.33	0.2	0.67	10	28.5	4.75	605.42
Substrate	Carbon steel	P355NH	1000 x 1000 x 6	7800	46.8	350	420.00	8.97	420.00	20	10	3.33	0.2	0.67	10	28.5	4.75	425.42
Substrate	Aluminium	Q-panel	1000 x 1000 x 6	2730	16.38	387	464.40	28.35	464.40	NA	NA				10	28.5	4.75	469.15
Substrate/SOA	Stainless steel	316L	1000x1000x6	7899	47.39	400	480	10.13	480	20	10	3.33	0.20	0.67	10	28.5	4.75	485.42
Substrate	Aluminum (Al)	3003	1000x1000x6	2730	16.38	1400	1680	102.56	1680	20	10	3.33	0.20	0.67	10	28.5	4.75	1685.42
Substrate	Carbon Steel	S275JR	1000 x 1000 x 6	7850	47.1		83.84	1.78	83.84	20	10	3.33	0.2	0.67	10	28.5	4.75	89.26
SOA	stainless steel	254SMO	1000 x 1000 x 6	8050	48.3		4015.8	83.14	4015.8	20	10	3.33	0.2	0.67	10	28.5	4.75	4021.22

**Table A2** - Substrate surface preparation cost calculations (Grit blasting and chemical treatment)

AIM - to determine the substrate surface preparation cost for 1 m<sup>2</sup> area using consumables, labour and electrical energy

Grade of the materials	Substrate dimension	Grit blasting										Stage 3										Labour time	Labour cost	Total cost to prepare surface (calculated)
		Grit blasting machine power	Grit blasting time	Electrical energy consumption for grit blasting	Cost of electrical energy	Name of grit material	Grit flow rate	Amount of grit materials used	Unit cost of grit material	Reuse factor for grit material	Cost of grit materials (calculated)	Amount of alkaline solution used	Unit cost of purchased alkaline solution	Cost of alkaline solution	Amount of de-ionised water used	Unit cost of purchased de-ionised water	Cost of de-ionised water	Amount of phosphoric acid used	Unit cost of purchased phosphoric acid	Cost of phosphoric acid				
		[kW]	[min]	[kWh]	[€]		[g/min]	[g]	[€/kg]		[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]				
P355NH	1000 x 1000 x 6	1.6	60	1.6	0.32	aluminium oxide grit #100	500	30000	3	20	4.5	0.5	7	3.5	5	0.75	3.75	1	7.25	7.25	60	28.5	47.82	

Grade of the materials	Substrate dimension	Grit blasting										Stage 3										Labour time	Labour cost	Total cost to prepare surface (calculated)				
		Grit blasting machine power	Grit blasting time for 1 m <sup>2</sup> area substrate	Electrical energy consumption for grit blasting	Cost of electrical energy	Name of grit material	Grit flow rate	Amount of grit materials used	Unit cost of grit material	Reuse factor for grit material	Cost of grit materials (calculated)	Amount of alkaline solution used	Unit cost of purchased alkaline solution	Cost of alkaline solution	Amount of de-ionised water used	Unit cost of purchased de-ionised water	Cost of de-ionised water	Amount of oxalic acid used	Unit cost of purchased oxalic acid	Cost of oxalic acid	Hardware power for drying				Time for drying	Electrical energy used for drying	Unit cost of electricity	Electrical energy cost for drying (calculated)
		[kW]	[min]	[kWh]	[€]		[g/min]	[g]	[€/kg]		[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[kg]	[€/kg]	[€]	[kW]				[min]	[kWh]	[€/kWh]	[€]
304L	1000 x 1000 x 6	1.6	60	1.6	0.32	aluminium oxide grit #100	500	30000	3	20	4.5	0.5	7	3.5	5	0.75	3.75	1	62.5	62.5	2.65	15	0.6625	0.2	0.1325	35	16.625	91.33

Grade of the materials	Substrate dimension	Grit blasting										Stage 3										Labour time	Labour cost	Total cost to prepare surface (calculated)				
		Grit blasting machine power	Grit blasting time	Electrical energy consumption	Cost of electrical energy	Name of grit material	Grit flow rate	Amount of grit materials used for 1 m <sup>2</sup> area	Unit cost of grit material	Reuse factor for grit material	Cost of grit materials (calculated)	Amount of alkaline solution used	Unit cost of purchased alkaline solution	Cost of alkaline solution	Amount of de-ionised water used	Unit cost of purchased de-ionised water	Cost of de-ionised water	Amount of ammonium persulfate used	Unit cost of purchased ammonium persulfate	Cost of ammonium persulfate	Hardware power for drying				Time for drying	Electrical energy used for drying	Unit cost of electricity	Electrical energy cost for drying (calculated)
		[kW]	[min]	[kWh]	[€]		[g/min]	[g]	[€/kg]		[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[kg]	[€/kg]	[€]	[kW]				[min]	[kWh]	[€/kWh]	[€]
Cu-C103	1000 x 1000 x 6	1.6	60	1.6	0.32	aluminium oxide grit #100	500	30000	3	20	4.5	0.5	7	3.5	5	0.75	3.75	1	84	84	2.65	15	0.6625	0.2	0.1325	40	19	115.2025

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Grade of the materials	Substrate dimension	Grit blasting											Stage 3											Labour time	Labour cost	Total cost to prepare surface (calculated)											
		Grit blasting machine power	Grit blasting time	Electrical energy consumption	Cost of electrical energy	Name of grit material	Grit flow rate	Amount of grit materials used	Unit cost of grit material	Reuse factor for grit material	Cost of grit materials (calculated)	Amount of alkaline solution used	Unit cost of purchased alkaline solution	Cost of alkaline solution	Amount of deionised water used	Unit cost of purchased deionised water	Cost of deionised water	Amount of phosphoric acid used	Unit cost of purchased phosphoric acid	Cost of phosphoric acid	Amount of tetra sodium pyrophosphate	Unit cost of tetra sodium pyrophosphate	Cost of tetra sodium pyrophosphate				Amount of sodium hydroxide	Unit cost of sodium hydroxide	Cost of sodium hydroxide	Amount of sodium metasilicate	Unit cost of sodium metasilicate	Cost of sodium metasilicate	Hardware power for drying	Time for drying	Electrical energy used for drying	Unit cost of electricity	Electrical energy cost for drying (calculated)
		[kW]	[min]	[kWh]	[€]	[g/min]	[g]	[€/kg]		[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[kg]	[€/kg]	[€]	[litre]				[€/litre]	[€]	[kg]	[€/kg]	[€]	[min]	[kWh]	[€/kWh]	[€]		
P355&316L	1000 x 1000 x 6	1.6	60	1.6	0.32	aluminium oxide grit #100	500	30000	3	20	4.5	0.5	7	3.5	5	0.75	3.75	1	7.25	7.25	0.25	80	20	1	40	40	0.25	210	52.5	2.65	60	2.65	0.2	0.53	60	28.5	160.85

Table A3 - Substrate surface preparation cost calculations (Grit blasting, Degreasing, etching and anodising)

AIM - to determine the substrate surface preparation cost for 1 m<sup>2</sup> area using consumables, labour and electrical energy

Substrate type	Grade of the materials	Substrate dimension	Grit blasting										Degreasing							Total cost to prepare surface (calculated)
			Grit blasting machine power	Grit blasting time	Electrical energy consumption	Cost of electrical energy	Name of grit material	Grit flow rate	Amount of grit materials used	Unit cost of grit material	Reuse factor for grit material	Cost of grit materials (calculated)	Amount of METFIN AK 16 used	Unit cost of purchased METFIN AK 16	Cost of METFIN AK 16	Power of thermal bath	Time of thermal bath	Electrical energy consumption for thermal bath		
			[kW]	[min]	[kWh]	[€]	[g/min]	[g]	[€/kg]		[€]	[litre]	[€/litre]	[€]	[kW]	[min]	[kWh]			
Aluminium	Q-panel	1000 x 1000 x 6	1.6	60	1.6	0.32	aluminium oxide grit #100	500	30000	3	20	4.5	3	7	21	1.2	15	0.3	0.06	
Etching										Anodising							Total cost to prepare surface (calculated)			
Amount of sulphuric acid used	Unit cost of purchased sulphuric	Cost of sulphuric acid	Amount of sodium dichromate used	Unit cost of purchased sodium dichromate	Cost of sodium dichromate	Power of thermal bath	Time of thermal bath	Electrical energy consumption for thermal bath	Cost of electrical energy	Amount of orthophosphoric acid used	Unit cost of purchased orthophosphoric acid	Cost of orthophosphoric acid	Labour time	Labour cost						
[litre]	[€/litre]	[€]	[kg]	[€/kg]	[€]	[kW]	[min]	[kWh]	[€]	[litre]	[€/litre]	[€]	[min]	[€]						
0.95	25	23.75	0.25	72	18	1.2	30	0.6	0.12	0.36	67.4	24.264	35	16.625	108.639					

Table A4 - Substrate surface preparation cost calculations (Surface treatment)

AIM - to determine the substrate surface preparation cost for 1 m<sup>2</sup> area using consumables, labour and electrical energy

Material type	Substrate dimension	Amount of acetone used	Unit cost of purchased acetone	Cost of acetone	Amount of isopropanol used	Unit cost of isopropanol	Cost of isopropanol (calculated)	Name of the polishing materials (CarbiMet S)	Amount of polishing materials used	Unit cost of polishing material	Cost of polishing materials (calculated)	Amount of deionised water used	Unit cost of deionised water	Cost of deionised water (calculated)	Power of ultrasound bath	Duration of ultrasound bath used	Electrical energy used	Electrical cost to run ultrasound bath	Labour time	Labour cost	Cr layer deposition cost for adhesion	Total cost to prepare surface (calculated)
		[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]		# pcs	[€/100 pcs]	[€]	[litre]	[€/litre]	[€]	[kW]	[min]	[kWh]	[€]	[min]	[€]	[€]	[€]
		[mm x mm x mm]	[litre]	[€/litre]	[€]	[litre]	[€/litre]		[€]	[mm x mm x mm]	[litre]	[€/litre]	[€]	[litre]	[€/litre]	[€]	[kW]	[min]	[kWh]	[€]	[min]	[€]
Carbon Steel (S275JR)	1000 x 1000 x 6	1.6	6.75	10.8	1.6	21	33.6	P280/P1200/P2500	1/1/1/	215/203/203	6.21	1.6	0.6	0.96	1.00E-01	10	1.67E-02	3.33E-03	30	14.25	18.69	84.51
Stainless steel (316L)	1000x1000x6	1.1	6.75	7.425	1.1	21	23.1	P280/P1200/P2500	1/1/1/	215/203/203	6.21	1.1	0.6	0.66	1.00E-01	10	1.67E-02	3.33E-03	30	14.25	18.69	70.33
Aluminium (3003)	1000x1000x6	1.1	6.75	7.425	1.1	21	23.1	P280/P1200/P2500	1/1/1/	215/203/203	6.21	1.1	0.6	0.66	1.00E-01	10	1.67E-02	3.33E-03	30	14.25	18.69	135.22
Copper (C103)	1000x1000x6	1.1	6.75	7.425	1.1	21	23.1	P280/P1200/P2500	1/1/1/	215/203/203	6.21	1.1	0.6	0.66	1.00E-01	10	1.67E-02	3.33E-03	30	14.25	18.69	99.58

**Table A5 – Cr layer Deposition cost calculations**

Coating name	Area (cm2)	Coating Deposition cost components																		
		Vacuum pressure	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	Amount of inert gas used	Unit cost of inert gas	Cost of inert gas (calculated)	Area of the coating	Thickness of the coating	labour time	labour cost	Cr layer deposition cost
		[Pa]	[kW]	[min]	[kWh]	[€/kWh]	[€]	[kW]	[min]	[kWh]	[€]		[l]	[€/l]	[€]	[cm2]	[µm]	(min)/(%)	(€)	[€]
Cr Adhesion layer	10000	2.90e-3	6.00E-01	120	1.20E+00	0.2	0.24	5.50E-02	120	1.10E-01	0.0220	Ar(5N)	6	0.471	2.83	10000	0.2	30	14.25	18.69

**Table A6 – Surface bonding (UDB) cost calculations**

Materials	Substrate dimension	Power of the grinding linisher	Grinding time	Electrical energy	Cost of electrical energy	Name of grit material	Grit material type	number of abrasive papers used		Unit cost of 600 grit SiC material paper	Cost of 600 grit SiC materials (calculated)	Unit cost of 1200 SiC grit material paper	Cost of 1200 grit SiC materials (calculated)	Amount of acetone	Unit cost of purchased acetone/isopropanol	Cost of acetone/isopropanol	Labour time	Labour cost	Pre-UDB cost	UDB machine power	Machining time	Electrical energy for UDB instrument	Electrical energy cost (calculated)	Labour time	Labour cost	UDB cost	Total cost to surface bonding (calculated)	
	[mm x mm x mm]	[W]	[min]	[kWh]	[€]			600 grit	1200 grit	[€]	[€]	[€]	[€]	[litre]	[€/litre]	[€]	[min]	[€]	[€]	[kW]	[min]	[kWh]	[€]	[min]	[€]	[€]	[€]	
	CS and SS	1000x1000x6	750	50	0.625			0.13	SiC	600	1200	2	2	1	2	1	2	0.5	13	6.5	20	9.5	20.13	30	120	60	12	30

**Table A7 – Coating deposition cost calculations (silica based hydrophobic) using Dip coating method**

AIM - to determine the cost of coating material deposited over 1 m<sup>2</sup> area of substrate based on the data given

coating material	Stage 1: Immersion						Stage 2: Start-up			Stage 4: Drainage		Stage 5: Evaporation		Electrical energy						Labour time	Labour cost	Total deposition cost (calculated)
	Volume of coating material used for 1 m2 substrate	Density of coating material	Mass of coating material used	Unit cost of Coating material	total cost of coating material	Immersion speed	time elapsed of substrate submerged in coating material	Withdrawal speed	thickness of coating	time elapsed for draining excess liquid	time elapsed for evaporation stage	Power of equipment used for maintaining constant speed	Time required for maintaining constant speed	Power of equipment used for drainage or evaporation stages	Time required for drainage or evaporation stages	Electrical energy consumption	Cost of electrical energy					
	[m3]	[kg/m3]	[kg]	[€/kg]	[€]	[mm/min]	[min]	[mm/min]	[mm]	[min]	[min]	[kW]	[min]	[kW]	[min]	[kWh]	[€]					
Sharc Sapphire/SMS35 333HMDS (25:75)	0.0005	1635.25	0.817625	805.25	658.39	100	0.5	100	0.001	0.5	60	N/A	N/A	2.65	60	2.65	0.53	30	14.25	673.17		
Sharc Sapphire/Gelest (25:75)	0.0005	1727.5	0.86375	46.25	39.95	100	0.5	100	0.001	0.5	60	N/A	N/A	2.65	60	2.65	0.53	30	14.25	54.73		

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**Table A8** – Coating deposition cost calculations (Tutoprom bright) using Dip Coating method

AIM - to determine the cost of coating material deposited over 1 m<sup>2</sup> area of substrate based on the data given.

Coating material	Stage 1: Immersion					Stage 2: Start-up			Stage 4: Drainage		Stage 5: Evaporate		Electrical energy							
	Volume of coating material used	Density of coating material	Mass of coating material used	Unit cost of Coating material	total cost of coating material	Immersion speed	time elapsed of substrate submerged in coating material	Withdrawal speed	thickness of coating	time elapsed for draining excess liquid	time elapsed for evaporation stage	Power of equipment used for maintaining constant speed	Time required for maintaining constant speed	Power of equipment used for drainage or evaporation stages	Time required for drainage or evaporation stages	Electrical energy consumption	Cost of electrical energy	Labour time	Labour cost	Total deposition cost (calculated)
	[m <sup>3</sup> ]	[kg/m <sup>3</sup> ]	[kg]	[€/kg]	[€]	[mm/min]	[min]	[mm/min]	[mm]	[min]	[min]	[kW]	[min]	[kW]	[min]	[kWh]	[€]	[min]	[€]	[€]
Tutoprom Bright	0.0005	860	0.43	360	154.8	100	0.5	100	0.001	0.5	60	N/A	N/A	2.65	60	2.65	0.53	30	14.25	169.58

**Table A9** – Coating deposition cost calculations (Amorphous metal coatings) using PVD method

AIM - to determine the cost of coating deposited over 1 m<sup>2</sup> area of substrate based on the data given.

Coating ID	Coating composition	at. wt.	Coating deposition (Sputtering - PVD)																		Coating material cost	PVD target cost	Total deposition cost to coat 1μm thick over 1 m <sup>2</sup> area of substrate (calculated)
			Vacuum pressure	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 (if any)	Duration of cooling	Electrical energy used for cooling	Cost of electrical energy for cooling	Type of inert gas used	Amount of inert gas used	Unit cost of inert gas	Cost of inert gas (calculated)	Area of the coating	Thickness of the coating	Labour time	Labour cost			
			[Pa]	[kW]	[min]	[kWh]	[€/kWh]	[€]	[kW]	[min]	[kWh]	[€]		[litre]	[€/litre]	[€]	[cm <sup>2</sup> ]	[μm]	[min]	[€]			
GHX099	Zr:Si:La	60:20:20	2.90e-3	6.00e-01	300	3	0.2	0.6	5.50E-02	300	0.275	0.055	Ar(5N)	110	0.471	51.81	10000	1	300	142.5	31	129.243	355.208
GHX072	Zr:Si:Nd	17:57:26	2.90e-3	6.00e-01	300	3	0.2	0.6	5.50E-02	300	0.275	0.055	Ar(5N)	110	0.471	51.81	10000	1	300	142.5	30	118.0614	343.0264

**Table A10** – Coating deposition cost calculations (Fe doped Al<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> composite coatings) using S-HVOF method

AIM - to determine the cost of coating material deposited over 1 m<sup>2</sup> area of substrate based on the data given.

Coating ID	Fe doping (%)	Coating deposition																								Total deposition cost to coat (calculated)		
		Hardware power of HVOF thermal spraying equipment	HVOF machine time	Electrical energy used for HVOF machine	Unit cost of electricity	Cost of electrical energy	Type of fuel gas used	Fuel gas flow rate	Amount of fuel gas	Volume of fuel gas used	Unit cost of fuel gas	Cost of fuel gas (calculated)	Oxygen flow rate	Volume of oxygen used	Unit cost of oxygen	Cost of oxygen (calculated)	Precursor flow rate	Number of passes	Deposition time for 1 pass	Total deposition time	Amount of precursor used	Unit cost of precursor solution	Cost of precursor	Area of the coating	Thickness of the coating		Labour time	Labour cost
		[kW]	[min]	[kWh]	[€/kWh]	[€]		[litre/min]	[litre]	[m <sup>3</sup> ]	[€/m <sup>3</sup> ]	[€]	[litre/min]	[litre]	[€/m <sup>3</sup> ]	[€]	[ml/min]		[s]	[min]	[l]	[€/litre]	[€]	[cm <sup>2</sup> ]	[μm]		[min]	[€]
HSP-0	0	80	40	53.33	0.2	10.67	Hydrogen	788	31520	31.52	4.8	151.30	280	11200	1.3	14.56	30	50	2400	40	1.2	118.82	142.58	10000	6	120	57	376.11
HSP-3.6	3.6	80	40	53.33	0.2	10.67	Hydrogen	788	31520	31.52	4.8	151.30	280	11200	1.3	14.56	30	50	2400	40	1.2	118.96	142.75	10000	6	120	57	376.27