Supplementary Information (SI) for Green Chemistry.

Sustainable Water Purification: Life Cycle Trade-Offs in Carbon-Based Catalyst Design

A. Sofia G. G. Santos [1], Victor F. Ferreira [2] *, Carla A. Orge [1], M. Fernando R. Pereira [1], O. Salomé G. P. Soares [1] *

[1] *LSRE-LCM, ALiCE, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal.*

[2] *Energy Systems Analytics, Catalonia Institute for Energy Research (IREC), Sant Adrià de Besòs, 08930 Barcelona, Spain*

* Corresponding author: salome.soares@fe.up.pt; vjferreira@irec.cat

Supplementary information

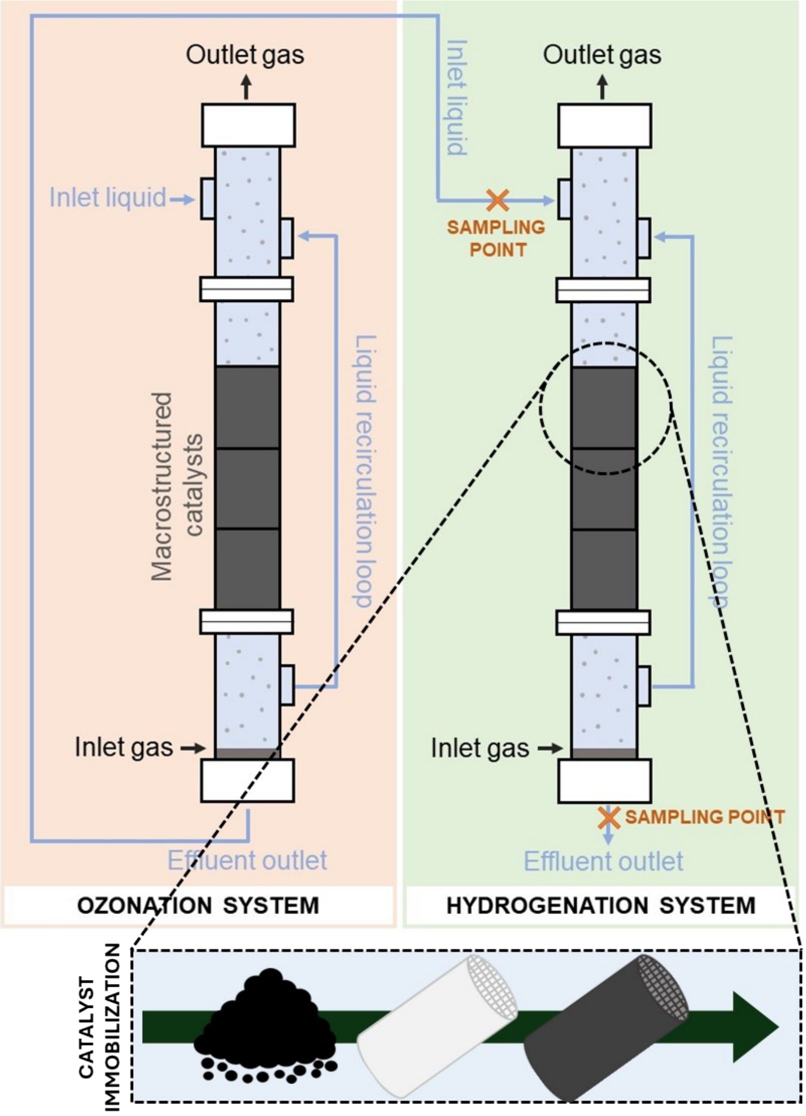


Figure SI 1 – Schematic representation of the integrated catalytic system developed for the simultaneous treatment of organic and inorganic species present in water

Table SI 1 – Inventory for all the process related with Scenario 1 (WCP_550 + O_3 | WCP(CNT:TiO_2)_550_Pd_200_Cu).

Scenario 1 WCP_550 + O_3 | WCP(CNT:TiO_2)_550_Pd_200_Cu							
Stage of the process		**Parameters**	**Inlet**		**Outlet**		**Category**
			Unit	**Value**	**Unit**	**Value**	
Ozonation catalysts **WCP_550**	**Washcoating solution preparation (WSP)**	**Deionized water**	mL	40	mL	10	*Raw materials*
		CNT	g	0.75	g	0.15	
		Triton X-100™	mL	0.75	mL	0.188	
		NaOH	mL	0.5	mL	0.125	
		CNT(BM 4h)	kWh	0.8	--	--	
		Ultra-sonic probe	kWh	0.8	--	--	*Electrical equipments*
	Washcoating procedure (WP)	**Cordierite structure**	g	21	--	--	*Raw materials*
		Dip-coater	kWh	0.1	--	--	*Electrical equipments*
		Drying between coatings	kWh	6.25	--	--	
		Solution stirring	kWh	0.31	--	--	
	Thermal treatment (TTSD)	**Thermal treatment**	kWh	129.6	--	--	
		Nitrogen gas for thermal treatment	L	162.0	--	--	*Gas*
Hydrogenation catalysts **WCP(CNT:TiO_2)_550_Pd_200_Cu**	**Washcoating solution preparation (WSP)**	**Nyacol:H_2O (1:1) solution**	mL	20	mL	10	*Raw materials*
		CNT	g	0.45	g	75	
		TiO_2	g	0.45	g	75	
		Triton X-100™	mL	0.75	mL	0.188	
		NaOH	mL	0.5	mL	0.125	
		CNT(BM 4h)	kWh	0.4	--	--	*Electrical equipments*
		CNT:TiO_2	kWh	0.05	--	--	
		CNT:TiO_2	kWh	0.05	--	--	
		Ultra-sonic probe	kWh	0.8	--	--	
	Washcoating procedure (WP)	**Cordierite structure**	g	21	--	--	*Raw materials*
		Dip-coater	kWh	0.1	--	--	*Electrical equipments*

		Drying between coatings	kWh	0.21	--	--	
		Solution stirring	kWh	0.31	--	--	
	Thermal treatment (TTSD)	**Thermal treatment**	kWh	129.6	--	--	
		Nitrogen gas for thermal treatment	L	162.0	--	--	*Gas*
	Metal impregnation (MI)	**Palladium (II) chloride**	g	0.2127	g	0.18345	*Raw materials*
		Pure HCl	mL	2	--	--	
		Shaker bath	kWh	6.4	--	--	*Electrical equipments*
		Drying between coatings	kWh	0.21	--	--	
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*
		Hydrogen for thermal treatment	L	54.0	--	--	
		Cooper nitrate	g	0.0585	g	0.03177	*Raw materials*
		Shaker bath	kWh	6.4	--	--	*Electrical equipments*
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*
		Hydrogen for thermal treatment	L	54.0	--	--	
Tretament system	**Building materials (BM)**	**Acrylic columns**	g	500	--	--	*Raw materials*
		PFA tubes	g	278	--	--	
		Staineless steel parts and joints	g	500	--	--	
		Glass diffusers	g	5	--	--	
		Washing bottles	g	1000	--	--	
	Reaction experiments (RE)	**Mass controlers**	KWh	0.03	--	--	*Electrical equipments*
		Ozone analyser	KWh	0.015	--	--	
		Controller box	KWh	0.09	--	--	
		Pump	kWh	0.023	--	--	
		Ozone generator	kWh	0.96	--	--	
		Oxygen for ozone generation	L	60	--	--	*Gas*
		Ozone			--	--	

Comment [VF]: I see that the inventory for the treatment system values are the same in all cases. It is quite repetitive. Maybe, you could move them to a alone table and leave a note that the parameter and flows for all tests are the same. You could save space in the suplementary section. What do you think?

		Hydrogen (hydrogenation system)	L	30	--	--	
		Carbon dioxide (hydrogenation system)	L	30	--	--	

Table SI 2 - Inventory for all processes related with Scenario 2 (WCP_550 + O_3 | CVD_Pd_200_Cu).

Scenario 2 WCP_550 + O_3 | CVD_Pd_200_Cu							
Stage of the process		**Parameters**	**Inlet**		**Outlet**		**Category**
			Unit	**Value**	**Unit**	**Value**	
Ozonation catalysts WCP_550	**Washcoating solution preparation (WSP)**	**Deionized water**	mL	40	mL	10	*Raw materials*
		CNT	g	0.75	g	0.15	
		Triton X-100™	mL	0.75	mL	0.188	
		NaOH	mL	0.5	mL	0.125	
		CNT(BM 4h)	kWh	0.8	--	--	*Electrical equipment*
		Ultra-sonic probe	kWh	0.8	--	--	
	Washcoating procedure (WP)	**Cordierite structure**	g	21	--	--	*Raw materials*
		Dip-coater	kWh	0.1	--	--	*Electrical equipment*
		Drying between coatings	kWh	6.25	--	--	
		Solution stirring	kWh	0.31	--	--	
	Thermal treatment (TTSD)	**Thermal treatment for surfactant decomposition**	kWh	129.6	--	--	
		Nitrogen gas for thermal treatment	L	162.0	--	--	*Gas*
Hydrogenation catalyst CVD_Pd_200_Cu	**Cordierite (CORD)**	**Cordierite structure**	g	21	--	--	*Raw materials*
	Nyacol coating (NC)	**Nyacol:H_2O (1:4) solution**	mL	10	mL	10	
		Dip-coater	kWh	0.024	--	--	*Electrical equipment*
		Drying between coatings	kWh	0.21	--	--	
		Thermal treatment for Al_2O_3 modification	kWh	172.8	--	--	
		Nitrogen gas for thermal treatment	L	216.0			*Gas*

	Nickel coating (NicC)	**Nickel solution**	mL	50	mL	10	*Raw materials*
		Dip-coater	kWh	0.048	--	--	*Electrical equipment*
		Drying between coatings (*)	kWh	0.21	--	--	
		Thermal treatment for nickel transformation	kWh	172.8	--	--	
		Nitrogen gas for thermal treatment	L	198			*Gas*
	Growth step (GS)	**Thermal treatment for carbon growth**	kWh	142.8	--	--	*Electrical equipment*
		Nitrogen gas for thermal treatment (heating)	L	43.5	--	--	*Gas*
		Nitrogen for thermal treatment (first treatment)	L	6.75	--	--	
		Hydrogen for thermal treatment (first treatment)	L	6.75	--	--	
		Hydrogen for thermal treatment (second treatment)	L	5.4	--	--	
		Ethane thermal treatment (second treatment)	L	5.4	--	--	
		Nitrogen (cool down)	L	90	--	--	
	Metal impregnation (MI)	**Palladium (II) chloride**	g	0.2127	g	0.18345	*Raw materials*
		Pure HCl	mL	2	--	--	
		Shaker bath	kWh	6.4	--	--	*Electrical equipment*
		Drying between coatings (*)	kWh	0.21	--	--	
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*
		Hydrogen for thermal treatment	L	54.0	--	--	
		Cooper nitrate	g	0.2364	g	0.20967	*Raw materials*
		Shaker bath	kWh	6.4	--	--	*Electrical equipment*
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*
		Hydrogen for thermal treatment	L	54.0	--	--	
Tretament system	**Building materials (BM)**	**Acrylic columns**	g	500	--	--	*Raw materials*
		PFA tubes	g	278	--	--	
		Staineless steel parts and joints	g	500	--	--	
		Glass difusers (2)	g	5	--	--	

		Washing bottles	g	1000	--	--	
	Reaction experiments (RE)	**Mass controlers**	KWh	0.03	--	--	*Electrical equipment*
		Ozone analyser	KWh	0.015	--	--	
		Controller box	KWh	0.09	--	--	
		Pump	kWh	0.023	--	--	
		Ozone generator	kWh	0.96	--	--	
		Oxygen for ozone generation	L	60	--	--	*Gas*
		Ozone			--	--	
		Hydrogen (hydrogenation system)	L	30	--	--	
		Carbon dioxide (hydrogenation system)	L	30	--	--	
		Hydrogen for thermal treatment	L	54.0	--	--	

Table SI 3 - Inventory for all the process related with Scenario 3 (WCP_{SA}_550 + O_3 | WCP(CNT:TiO_2)$_{SA}$_550_Pd_200_Cu).

Scenario 3 **WCP_{SA}_550 + O_3 | WCP(CNT:TiO_2)$_{SA}$_Pd_200_Cu**							
Stage of the process		**Parameters**	**Inlet**		**Outlet**		**Category**
			Unit	**Value**	**Unit**	**Value**	
Ozonation catalysts **WCP_{SA}_550**	**Cordierite preparation (CORD)**	**Pure Nyacol**	mL	40.0	mL	10	*Raw materials*
		Thermal treatment for Al_2O_3 modification	kWh	48.0	--	--	*Electrical equipment*
		Nitrogen gas for thermal treatment	L	60.0	--	--	*Gas*
	Washcoating solution preparation (WSP)	**Cordierite structure**	g	21	--	--	*Raw materials*
		Deionized water	mL	40	mL	10	
		CNT	g	0.7	g	0.1	
		Sodium Alginate	g	0.687	g	0.097	
		CNT(BM 4h)	kWh	0.4	--	--	*Electrical equipment*
		Mechanical stirring	kWh	0.1	--	--	
		Ultra-sonic probe	kWh	0.8	--	--	
		Solution stirring	kWh	0.31	--	--	

	Thermal treatment (TTSD)	**Thermal treatment for surfactant decomposition**	kWh	144	--	--	
		Nitrogen gas for thermal treatment	L	180	--	--	*Gas*
<u>Hydrogenation catalyst</u> **WCP(CNT:TiO$_2$)$_{SA}$_550_Pd_200_Cu**	**Cordierite preparation (CP)**	**Pure Nyacol**	mL	40.0	mL	10	*Raw materials*
		Thermal treatment for Al$_2$O$_3$ modification	kWh	48.0	--	--	*Electrical equipment*
		Nitrogen gas for thermal treatment	L	60.0	--	--	*Gas*
	Washcoating solution preparation (WSP)	**Cordierite structure**	g	21	--	--	*Raw materials*
		Deionized water	mL	40	mL	10	
		CNT	g	0.45	g	0.05	
		TiO$_2$	g	0.45	g	0.05	
		Sodium Alginate	g	0.87	g	0.097	
		CNT(BM 4h)	kWh	0.4	--	--	*Electrical equipment*
		CNT:TiO$_2$	kWh	0.05	--	--	
		Mechanical stirring	kWh	0.1	--	--	
		Ultra-sonic probe	kWh	0.8	--	--	
		Solution stirring	kWh	0.31	--	--	
	Thermal treatment (TTSD)	**Thermal treatment for surfactant decomposition**	kWh	144	--	--	
		Nitrogen gas for thermal treatment	L	180	--	--	*Gas*
	Metal impregnation (MI)	**Palladium (II) chloride**	g	0.2127	g	0.18345	*Raw materials*
		Pure HCl	mL	2	--	--	
		Shaker bath	kWh	6.4	--	--	*Electrical equipment*
		Drying between coatings	kWh	0.21	--	--	
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*
		Hydrogen for thermal treatment	L	54.0	--	--	
		Cooper nitrate	g	0.0585	g	0.03177	*Raw materials*
		Shaker bath	kWh	6.4	--	--	*Electrical equipment*
		Reductive thermal treatment	kWh	108	--	--	
		Nitrogen for thermal treatment	L	81.0	--	--	*Gas*

		Hydrogen for thermal treatment	L	54.0	--	--	
Tretament system	**Building materials (BM)**	**Acrylic columns**	g	500	--	--	*Raw materials*
		PFA tubes	g	278	--	--	
		Staineless steel parts and joints	g	500	--	--	
		Glass difusers	g	5	--	--	
		Washing bottles	g	1000	--	--	
	Reaction experiments (RE)	**Mass controlers**	KWh	0.03	--	--	*Electrical equipment*
		Ozone analyser	KWh	0.015	--	--	
		Controller box	KWh	0.09	--	--	
		Pump	kWh	0.023	--	--	
		Ozone generator	kWh	0.96	--	--	
		Oxygen for ozone generation	L	60	--	--	*Gas*
		Ozone			--	--	
		Hydrogen (hydrogenation system)	L	30	--	--	
		Carbon dioxide (hydrogenation system)	L	30	--	--	

Table SI 4 – Mid points impact categories considered for the life cycle analysis.

Impact Category	Units	Description
Environmental Footprint		
EF 3.1 Acidification	Mole of H+ eq.	Measures the release of acidifying substances, such as SO_2 and NO_x, into the environment, which can harm ecosystems. Unlike eutrophication, it focuses on pH changes rather than nutrient overload.
EF 3.1 Climate Change total	kg CO2 eq.	Quantifies all greenhouse gas emissions, expressed as CO_2 equivalents. It differs from the subcategories by encompassing biogenic, fossil, and land-use changes.
EF 3.1 Climate Change, biogenic	kg CO2 eq.	Assesses CO_2 emissions/removals from biological sources, such as plant growth or decay, distinguishing it from fossil or land-use sources.
EF 3.1 Climate Change, fossil	kg CO2 eq.	Focuses on greenhouse gases from fossil fuel combustion, excluding biogenic and land-use impacts.
EF 3.1 Climate Change, land use and land use change	kg CO2 eq.	Evaluates CO_2 emissions resulting from changes in land use, such as deforestation, making it distinct from fossil or biogenic sources.
EF 3.1 Ecotoxicity, freshwater total	CTUe	Measures toxic effects on freshwater ecosystems from chemical exposure. Includes both inorganic and organic pollutants.
EF 3.1 Ecotoxicity, freshwater inorganics	CTUe	Focuses on the impact of inorganic substances, like heavy metals, on aquatic life, differing from organic pollutants.
EF 3.1 Ecotoxicity, freshwater organics	CTUe	Measures the toxicity of organic chemicals, such as pesticides, in freshwater environments, distinct from inorganics.
EF 3.1 Eutrophication, freshwater	kg P eq.	Evaluates nutrient enrichment in freshwater systems, primarily driven by phosphorus, leading to algal blooms.
EF 3.1 Eutrophication, marine	kg N eq.	Similar to freshwater eutrophication but specific to marine environments, focusing on nitrogen.
EF 3.1 Eutrophication, terrestrial	Mole of N eq.	Assesses nutrient enrichment on land ecosystems, expressed in nitrogen equivalents.
EF 3.1 Human toxicity, cancer total	CTUh	Quantifies the risk of cancer in humans due to chemical exposure. Includes both organic and inorganic contributors.
EF 3.1 Human toxicity, cancer inorganics	CTUh	Focuses on the cancer risks from inorganic substances, such as heavy metals, distinct from organic sources.
EF 3.1 Human toxicity, cancer organics	CTUh	Evaluates cancer risks from organic pollutants, such as solvents, distinguishing it from inorganics.
EF 3.1 Human toxicity, non-cancer total	CTUh	Measures non-cancer health risks from chemical exposure, both organic and inorganic.
EF 3.1 Human toxicity, non-cancer inorganics	CTUh	Focuses on non-cancer risks from inorganic pollutants, differing from organic substances.
EF 3.1 Human toxicity, non-cancer organics	CTUh	Evaluates non-cancer risks from organic chemicals, such as pesticides, separate from inorganic risks.
EF 3.1 Ionising radiation, human health	kBq U235 eq.	Assesses human health impacts from radioactive emissions, such as those from nuclear energy production.
EF 3.1 Land Use	Pt	Measures the impact of land occupation and transformation on ecosystem services.
EF 3.1 Ozone depletion	kg CFC-11 eq.	Quantifies substances that deplete the ozone layer, such as chlorofluorocarbons (CFCs).
EF 3.1 Particulate matter	Disease incidences	Assesses health impacts due to inhalable particulate matter, linked to respiratory diseases.
EF 3.1 Photochemical ozone formation, human health	kg NMVOC eq.	Evaluates the creation of ground-level ozone, a harmful pollutant caused by volatile organic compounds.
EF 3.1 Resource use, fossils	MJ	Quantifies fossil energy resource depletion, distinct from minerals and metals.

EF 3.1 Resource use, mineral and metals	kg Sb eq.	Measures the depletion of non-renewable minerals and metals, expressed in antimony equivalents.
EF 3.1 Water use	m³ world equiv.	Assesses the environmental impact of water consumption, accounting for scarcity.
Energy demand		
Primary energy demand from ren. and non-ren. resources (gross cal. value)	MJ	Total energy demand, including renewable and non-renewable resources. Net excludes losses during transformation.
Primary energy demand from ren. and non-ren. resources (net cal. value)	MJ	
Primary energy from non-renewable resources (gross cal. value)	MJ	Focuses solely on non-renewable energy consumption, differentiating from renewable resources.
Primary energy from non-renewable resources (net cal. value)	MJ	
Primary energy from renewable resources (gross cal. value)	MJ	Assesses energy derived from renewable sources, excluding non-renewable components
Primary energy from renewable resources (net cal. value)	MJ	

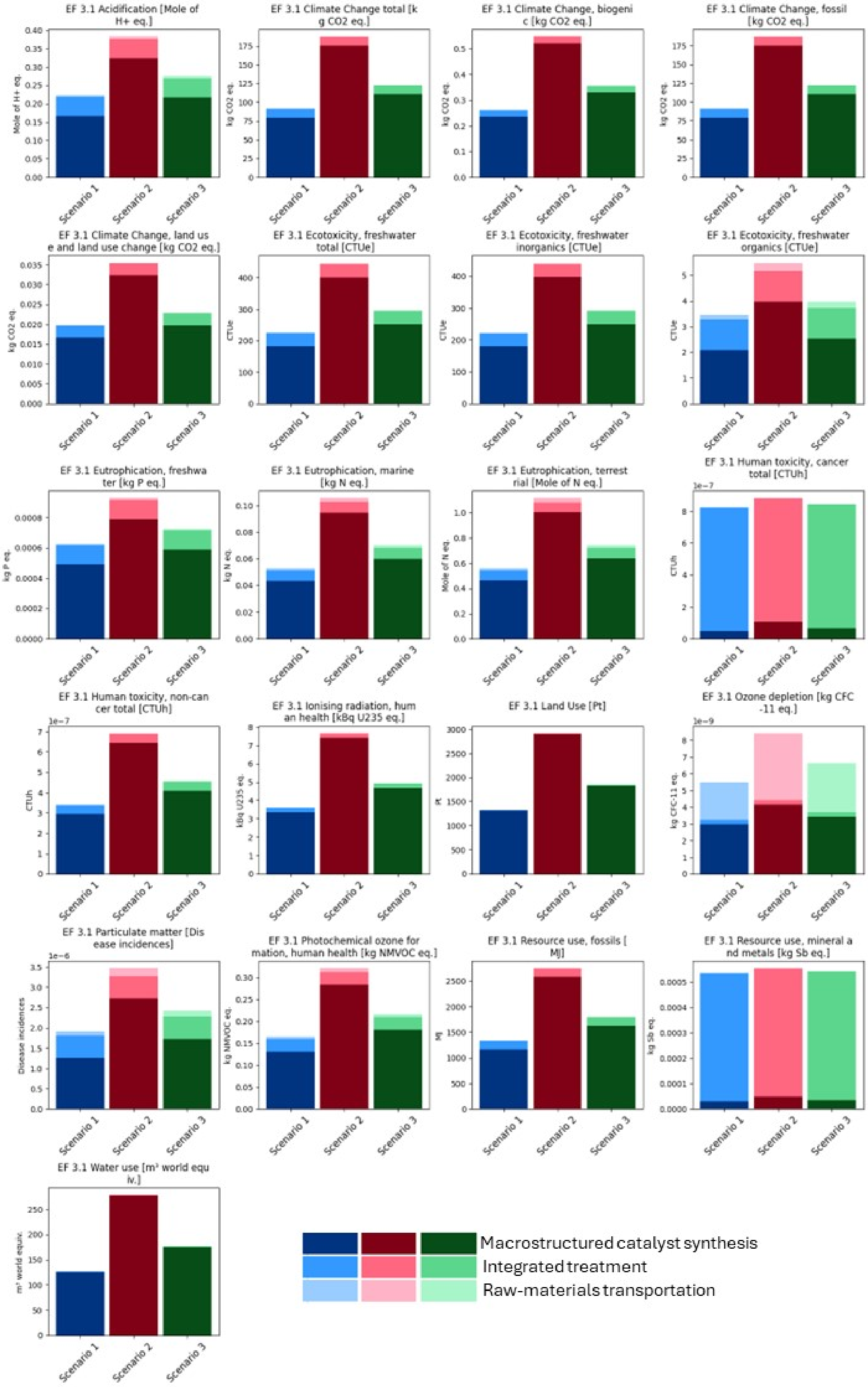
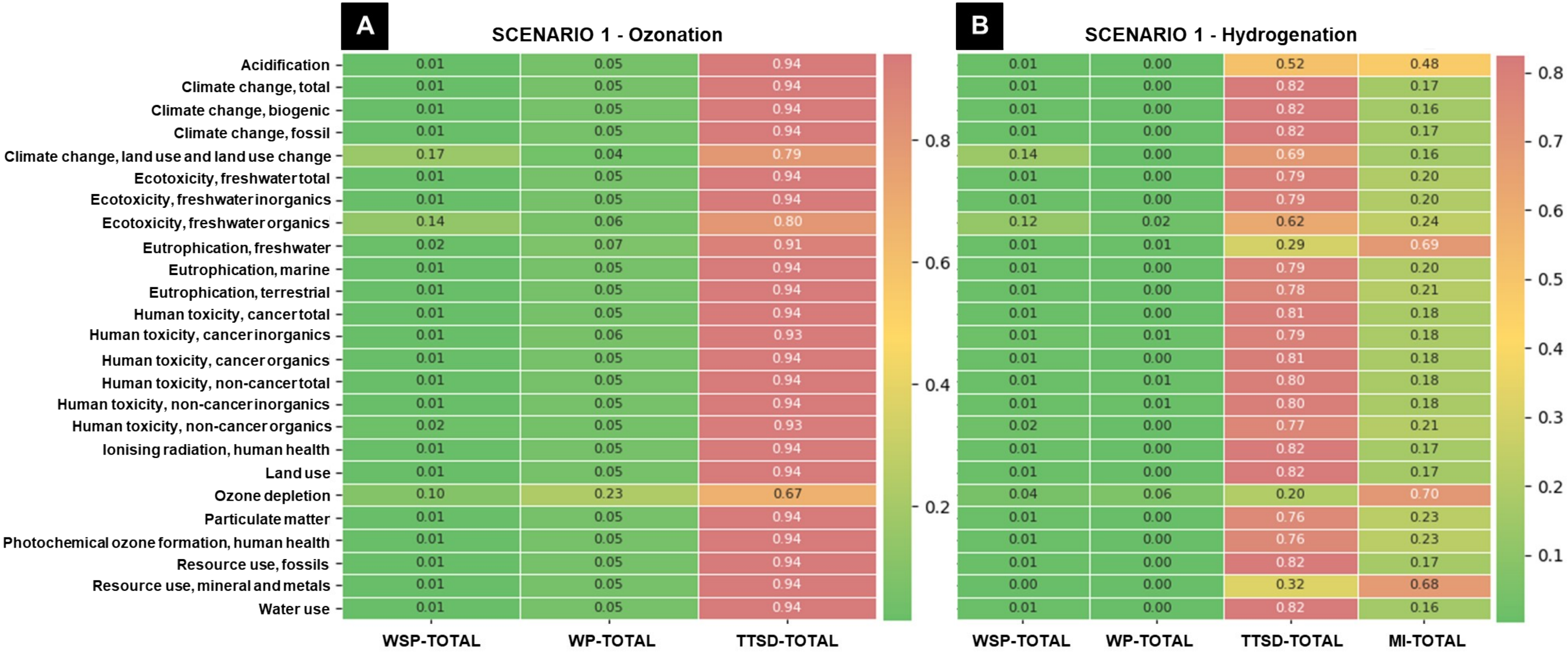


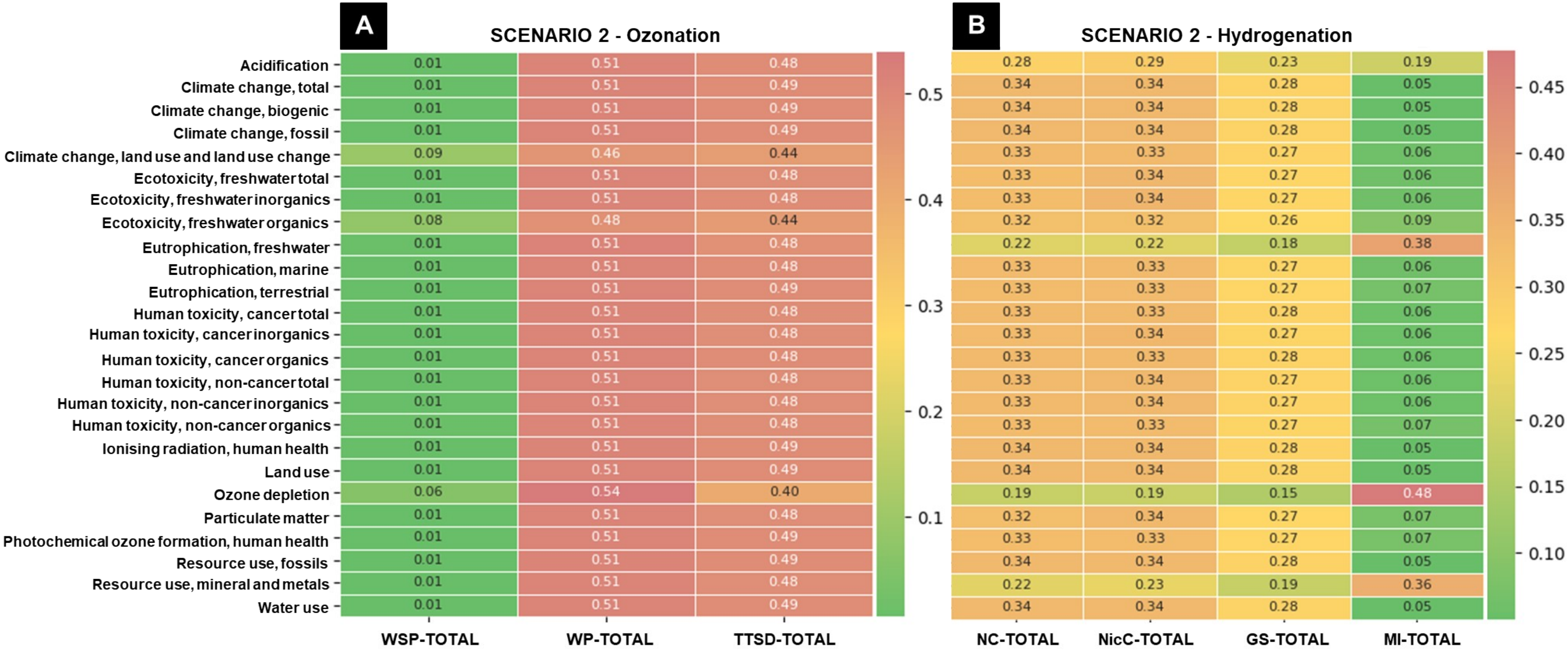
Figure SI 2 - Results of environmental impact categories of scenarios, accounting for the three main phases of the system life cycle: macrostructured catalysts synthesis, integrated treatment application/construction, raw-materials transportation.



	WSP-TOTAL	WP-TOTAL	TTSD-TOTAL
Acidification	0.01	0.05	0.94
Climate change, total	0.01	0.05	0.94
Climate change, biogenic	0.01	0.05	0.94
Climate change, fossil	0.01	0.05	0.94
Climate change, land use and land use change	0.17	0.04	0.79
Ecotoxicity, freshwater total	0.01	0.05	0.94
Ecotoxicity, freshwater inorganics	0.01	0.05	0.94
Ecotoxicity, freshwater organics	0.14	0.06	0.80
Eutrophication, freshwater	0.02	0.07	0.91
Eutrophication, marine	0.01	0.05	0.94
Eutrophication, terrestrial	0.01	0.05	0.94
Human toxicity, cancer total	0.01	0.05	0.94
Human toxicity, cancer inorganics	0.01	0.06	0.93
Human toxicity, cancer organics	0.01	0.05	0.94
Human toxicity, non-cancer total	0.01	0.05	0.94
Human toxicity, non-cancer inorganics	0.01	0.05	0.94
Human toxicity, non-cancer organics	0.02	0.05	0.93
Ionising radiation, human health	0.01	0.05	0.94
Land use	0.01	0.05	0.94
Ozone depletion	0.10	0.23	0.67
Particulate matter	0.01	0.05	0.94
Photochemical ozone formation, human health	0.01	0.05	0.94
Resource use, fossils	0.01	0.05	0.94
Resource use, mineral and metals	0.01	0.05	0.94
Water use	0.01	0.05	0.94

	WSP-TOTAL	WP-TOTAL	TTSD-TOTAL	MI-TOTAL
Acidification	0.01	0.00	0.52	0.48
Climate change, total	0.01	0.00	0.82	0.17
Climate change, biogenic	0.01	0.00	0.82	0.16
Climate change, fossil	0.01	0.00	0.82	0.17
Climate change, land use and land use change	0.14	0.00	0.69	0.16
Ecotoxicity, freshwater total	0.01	0.00	0.79	0.20
Ecotoxicity, freshwater inorganics	0.01	0.00	0.79	0.20
Ecotoxicity, freshwater organics	0.12	0.02	0.62	0.24
Eutrophication, freshwater	0.01	0.01	0.29	0.69
Eutrophication, marine	0.01	0.00	0.79	0.20
Eutrophication, terrestrial	0.01	0.00	0.78	0.21
Human toxicity, cancer total	0.01	0.00	0.81	0.18
Human toxicity, cancer inorganics	0.01	0.01	0.79	0.18
Human toxicity, cancer organics	0.01	0.00	0.81	0.18
Human toxicity, non-cancer total	0.01	0.01	0.80	0.18
Human toxicity, non-cancer inorganics	0.01	0.01	0.80	0.18
Human toxicity, non-cancer organics	0.02	0.00	0.77	0.21
Ionising radiation, human health	0.01	0.00	0.82	0.17
Land use	0.01	0.00	0.82	0.17
Ozone depletion	0.04	0.06	0.20	0.70
Particulate matter	0.01	0.00	0.76	0.23
Photochemical ozone formation, human health	0.01	0.00	0.76	0.23
Resource use, fossils	0.01	0.00	0.82	0.17
Resource use, mineral and metals	0.00	0.00	0.32	0.68
Water use	0.01	0.00	0.82	0.16

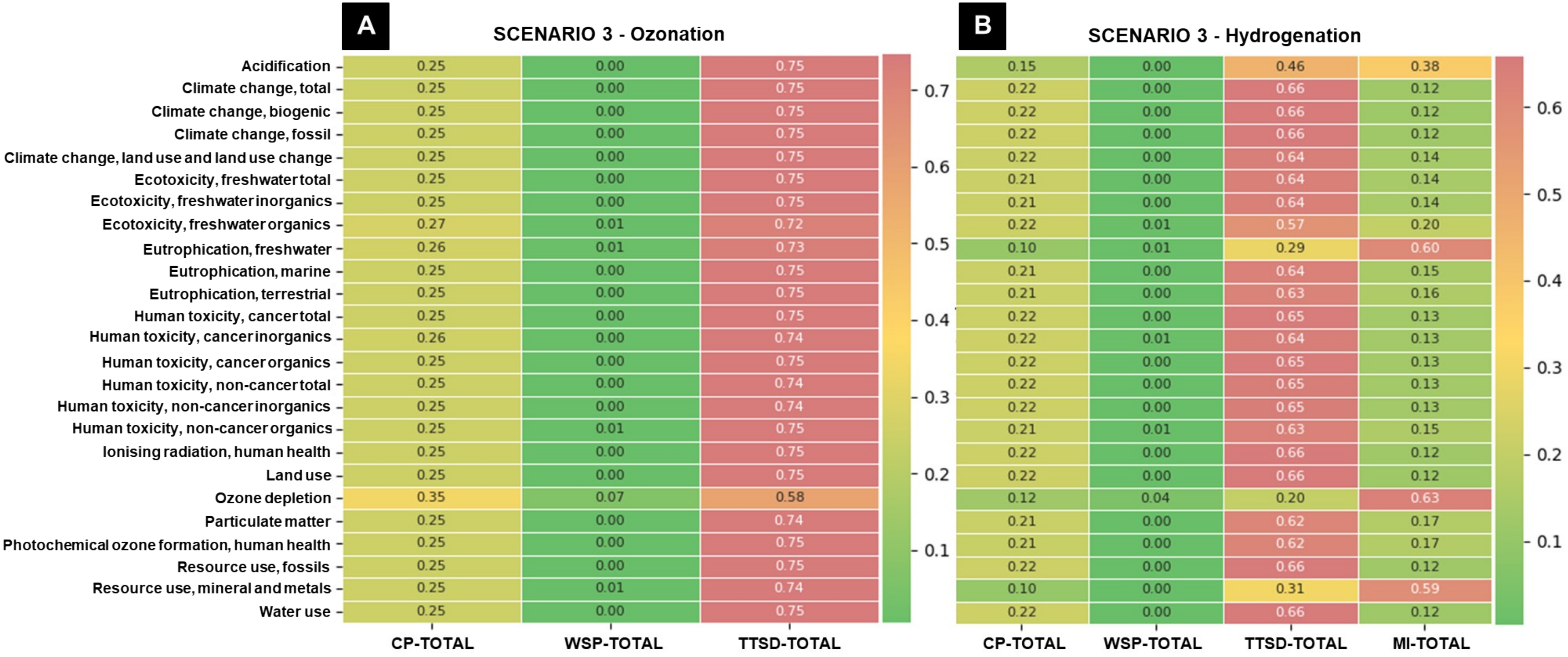
Figure SI 3 - Heat map across impact categories of the stages involved in the synthesis of macrostructured catalysts. Scenario 1 (WCP_550 and WCP(CNT:TiO_2)_550_Pd_200_Cu): Ozonation (A) and Hydrogenation (B).



	WSP-TOTAL	WP-TOTAL	TTSD-TOTAL
Acidification	0.01	0.51	0.48
Climate change, total	0.01	0.51	0.49
Climate change, biogenic	0.01	0.51	0.49
Climate change, fossil	0.01	0.51	0.49
Climate change, land use and land use change	0.09	0.46	0.44
Ecotoxicity, freshwater total	0.01	0.51	0.48
Ecotoxicity, freshwater inorganics	0.01	0.51	0.48
Ecotoxicity, freshwater organics	0.08	0.48	0.44
Eutrophication, freshwater	0.01	0.51	0.48
Eutrophication, marine	0.01	0.51	0.48
Eutrophication, terrestrial	0.01	0.51	0.49
Human toxicity, cancer total	0.01	0.51	0.48
Human toxicity, cancer inorganics	0.01	0.51	0.48
Human toxicity, cancer organics	0.01	0.51	0.48
Human toxicity, non-cancer total	0.01	0.51	0.48
Human toxicity, non-cancer inorganics	0.01	0.51	0.48
Human toxicity, non-cancer organics	0.01	0.51	0.48
Ionising radiation, human health	0.01	0.51	0.49
Land use	0.01	0.51	0.49
Ozone depletion	0.06	0.54	0.40
Particulate matter	0.01	0.51	0.48
Photochemical ozone formation, human health	0.01	0.51	0.49
Resource use, fossils	0.01	0.51	0.49
Resource use, mineral and metals	0.01	0.51	0.48
Water use	0.01	0.51	0.49

	NC-TOTAL	NicC-TOTAL	GS-TOTAL	MI-TOTAL
Acidification	0.28	0.29	0.23	0.19
Climate change, total	0.34	0.34	0.28	0.05
Climate change, biogenic	0.34	0.34	0.28	0.05
Climate change, fossil	0.34	0.34	0.28	0.05
Climate change, land use and land use change	0.33	0.33	0.27	0.06
Ecotoxicity, freshwater total	0.33	0.34	0.27	0.06
Ecotoxicity, freshwater inorganics	0.33	0.34	0.27	0.06
Ecotoxicity, freshwater organics	0.32	0.32	0.26	0.09
Eutrophication, freshwater	0.22	0.22	0.18	0.38
Eutrophication, marine	0.33	0.33	0.27	0.06
Eutrophication, terrestrial	0.33	0.33	0.27	0.07
Human toxicity, cancer total	0.33	0.33	0.28	0.06
Human toxicity, cancer inorganics	0.33	0.34	0.27	0.06
Human toxicity, cancer organics	0.33	0.33	0.28	0.06
Human toxicity, non-cancer total	0.33	0.34	0.27	0.06
Human toxicity, non-cancer inorganics	0.33	0.34	0.27	0.06
Human toxicity, non-cancer organics	0.33	0.33	0.27	0.07
Ionising radiation, human health	0.34	0.34	0.28	0.05
Land use	0.34	0.34	0.28	0.05
Ozone depletion	0.19	0.19	0.15	0.48
Particulate matter	0.32	0.34	0.27	0.07
Photochemical ozone formation, human health	0.33	0.33	0.27	0.07
Resource use, fossils	0.34	0.34	0.28	0.05
Resource use, mineral and metals	0.22	0.23	0.19	0.36
Water use	0.34	0.34	0.28	0.05

Figure SI 4 - Heat map across impact categories of the stages involved in the synthesis of macrostructured catalysts. Scenario 1 (WCP_550 and CVD_Pd_200_Cu): Ozonation (A) and Hydrogenation (B).



	CP-TOTAL	WSP-TOTAL	TTSD-TOTAL
Acidification	0.25	0.00	0.75
Climate change, total	0.25	0.00	0.75
Climate change, biogenic	0.25	0.00	0.75
Climate change, fossil	0.25	0.00	0.75
Climate change, land use and land use change	0.25	0.00	0.75
Ecotoxicity, freshwater total	0.25	0.00	0.75
Ecotoxicity, freshwater inorganics	0.25	0.00	0.75
Ecotoxicity, freshwater organics	0.27	0.01	0.72
Eutrophication, freshwater	0.26	0.01	0.73
Eutrophication, marine	0.25	0.00	0.75
Eutrophication, terrestrial	0.25	0.00	0.75
Human toxicity, cancer total	0.25	0.00	0.75
Human toxicity, cancer inorganics	0.26	0.00	0.74
Human toxicity, cancer organics	0.25	0.00	0.75
Human toxicity, non-cancer total	0.25	0.00	0.74
Human toxicity, non-cancer inorganics	0.25	0.00	0.74
Human toxicity, non-cancer organics	0.25	0.01	0.75
Ionising radiation, human health	0.25	0.00	0.75
Land use	0.25	0.00	0.75
Ozone depletion	0.35	0.07	0.58
Particulate matter	0.25	0.00	0.74
Photochemical ozone formation, human health	0.25	0.00	0.75
Resource use, fossils	0.25	0.00	0.75
Resource use, mineral and metals	0.25	0.01	0.74
Water use	0.25	0.00	0.75

	CP-TOTAL	WSP-TOTAL	TTSD-TOTAL	MI-TOTAL
Acidification	0.15	0.00	0.46	0.38
Climate change, total	0.22	0.00	0.66	0.12
Climate change, biogenic	0.22	0.00	0.66	0.12
Climate change, fossil	0.22	0.00	0.66	0.12
Climate change, land use and land use change	0.22	0.00	0.64	0.14
Ecotoxicity, freshwater total	0.21	0.00	0.64	0.14
Ecotoxicity, freshwater inorganics	0.21	0.00	0.64	0.14
Ecotoxicity, freshwater organics	0.22	0.01	0.57	0.20
Eutrophication, freshwater	0.10	0.01	0.29	0.60
Eutrophication, marine	0.21	0.00	0.64	0.15
Eutrophication, terrestrial	0.21	0.00	0.63	0.16
Human toxicity, cancer total	0.22	0.00	0.65	0.13
Human toxicity, cancer inorganics	0.22	0.01	0.64	0.13
Human toxicity, cancer organics	0.22	0.00	0.65	0.13
Human toxicity, non-cancer total	0.22	0.00	0.65	0.13
Human toxicity, non-cancer inorganics	0.22	0.00	0.65	0.13
Human toxicity, non-cancer organics	0.21	0.01	0.63	0.15
Ionising radiation, human health	0.22	0.00	0.66	0.12
Land use	0.22	0.00	0.66	0.12
Ozone depletion	0.12	0.04	0.20	0.63
Particulate matter	0.21	0.00	0.62	0.17
Photochemical ozone formation, human health	0.21	0.00	0.62	0.17
Resource use, fossils	0.22	0.00	0.66	0.12
Resource use, mineral and metals	0.10	0.00	0.31	0.59
Water use	0.22	0.00	0.66	0.12

Figure SI 5 - Heat map across impact categories of the stages involved in the synthesis of macrostructured catalysts. Scenario 1 (WCP$_{SA}$_550 and WCP(CNT:TiO$_2$)$_{SA}$_550_Pd_200_Cu): Ozonation (A) and Hydrogenation (B).

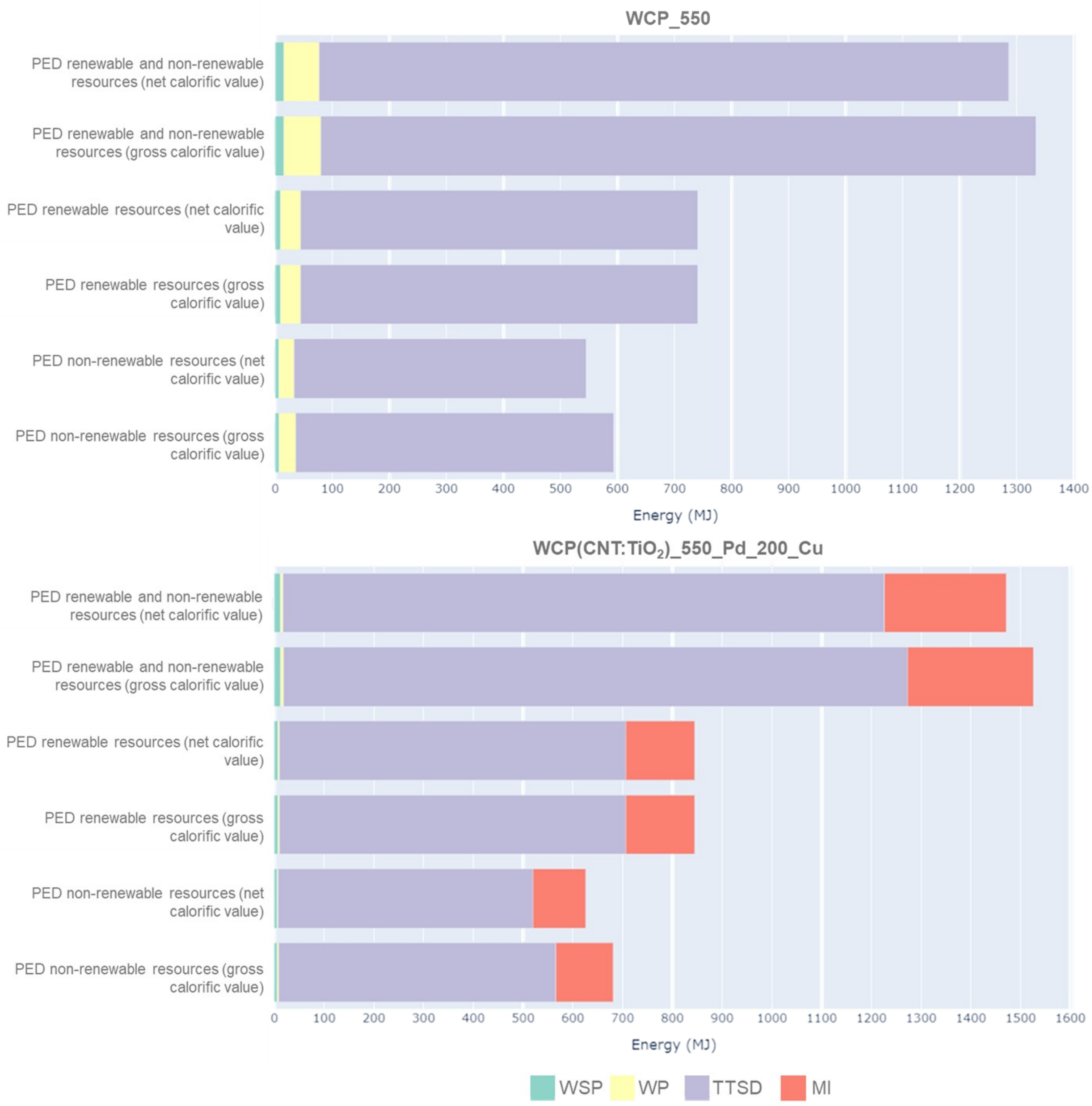


Figure SI 6 - Primary energy demand impacts of WCP_550 and WCP(CNT:TiO_2)_550_Pd_200_Cu synthesis for each stage WS, WP, TTSD and MI

Figure SI 7 - Primary energy demand impacts of WCP_550 synthesis for each stage (WSP, WP and TTSD.

Figure SI 8 - Primary energy demand impacts of WCP(CNT:TiO_2)_550_Pd_200_Cu synthesis for each stage WSP, WP, TTSD and MI

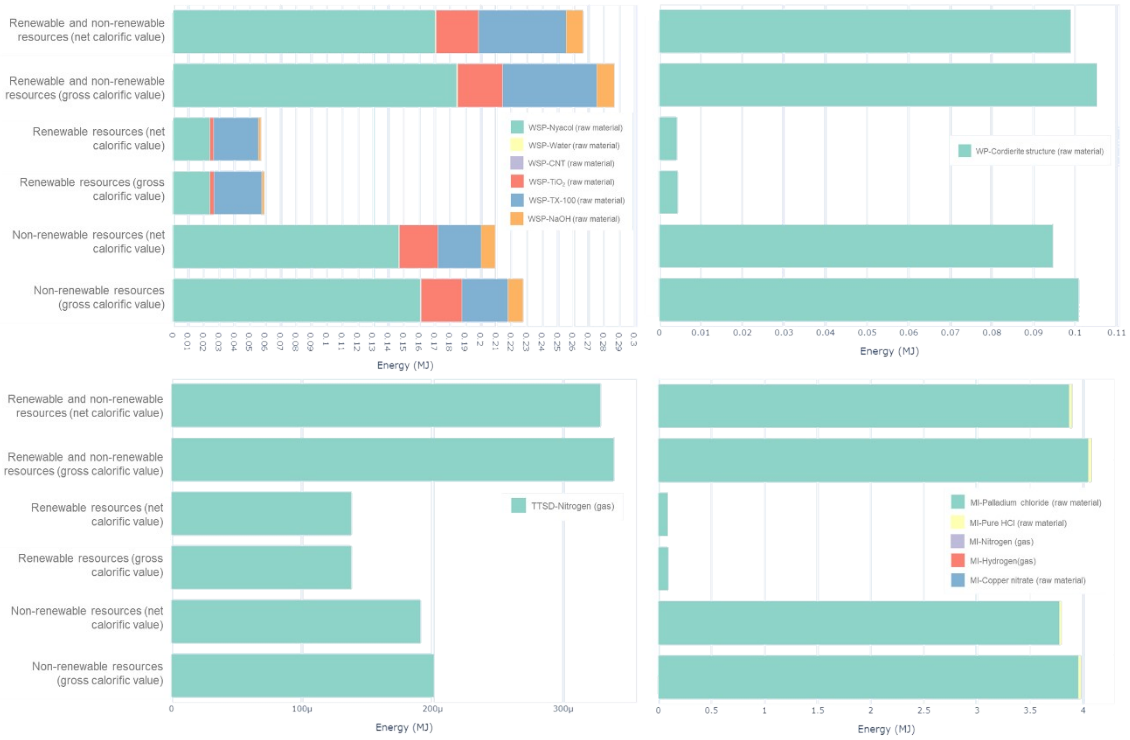


Figure SI 9 - Primary energy demand impacts of WCP(CNT:TiO_2)_550_Pd_200_Cu synthesis for each stage WSP, WP, TTSD and MI) excluding inputs related to energy consumption.

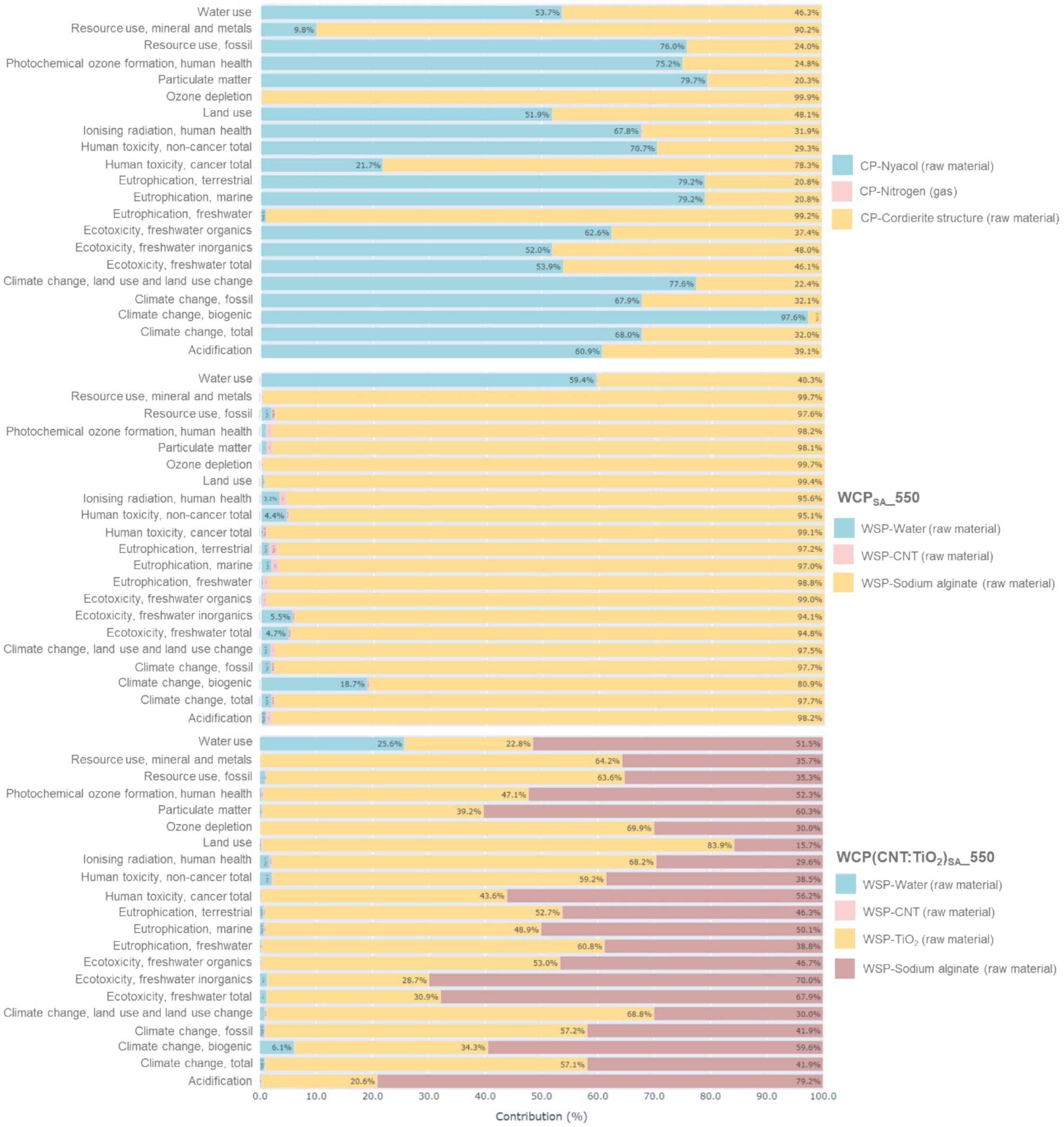


Figure SI 10 - Percentage results of WCP$_{SA}$_550 and WCP(CNT:TiO$_2$)$_{SA}$_550 catalysts synthesis of CP and WSP stages across impact categories, excluding the inputs related to energy consumption, .

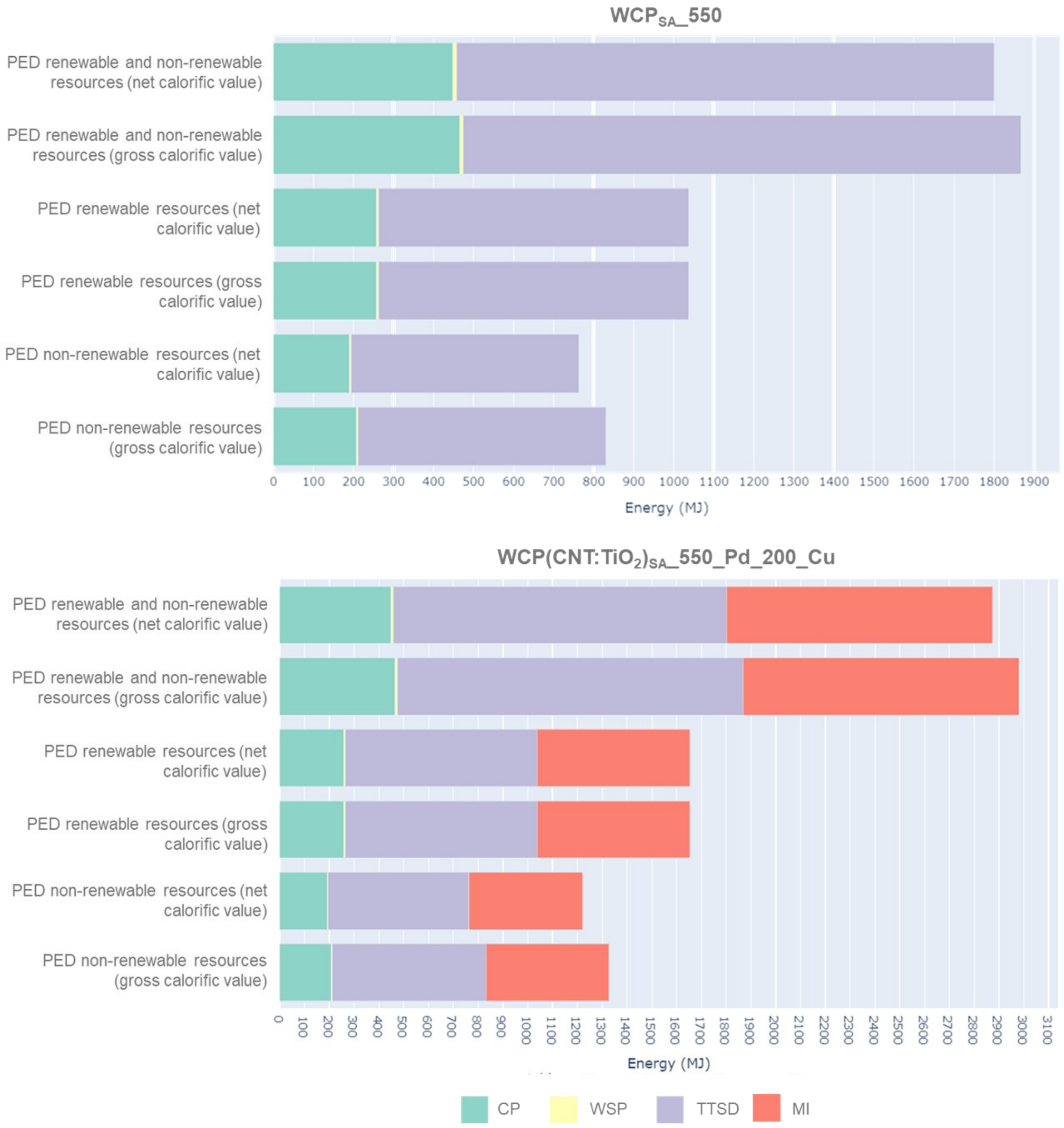


Figure SI 11 - Primary energy demand results for each stage related to WCP_{SA}_550 and $WCP(CNT:TiO_2)_{SA}\_550\_Pd\_200\_Cu$ synthesis.

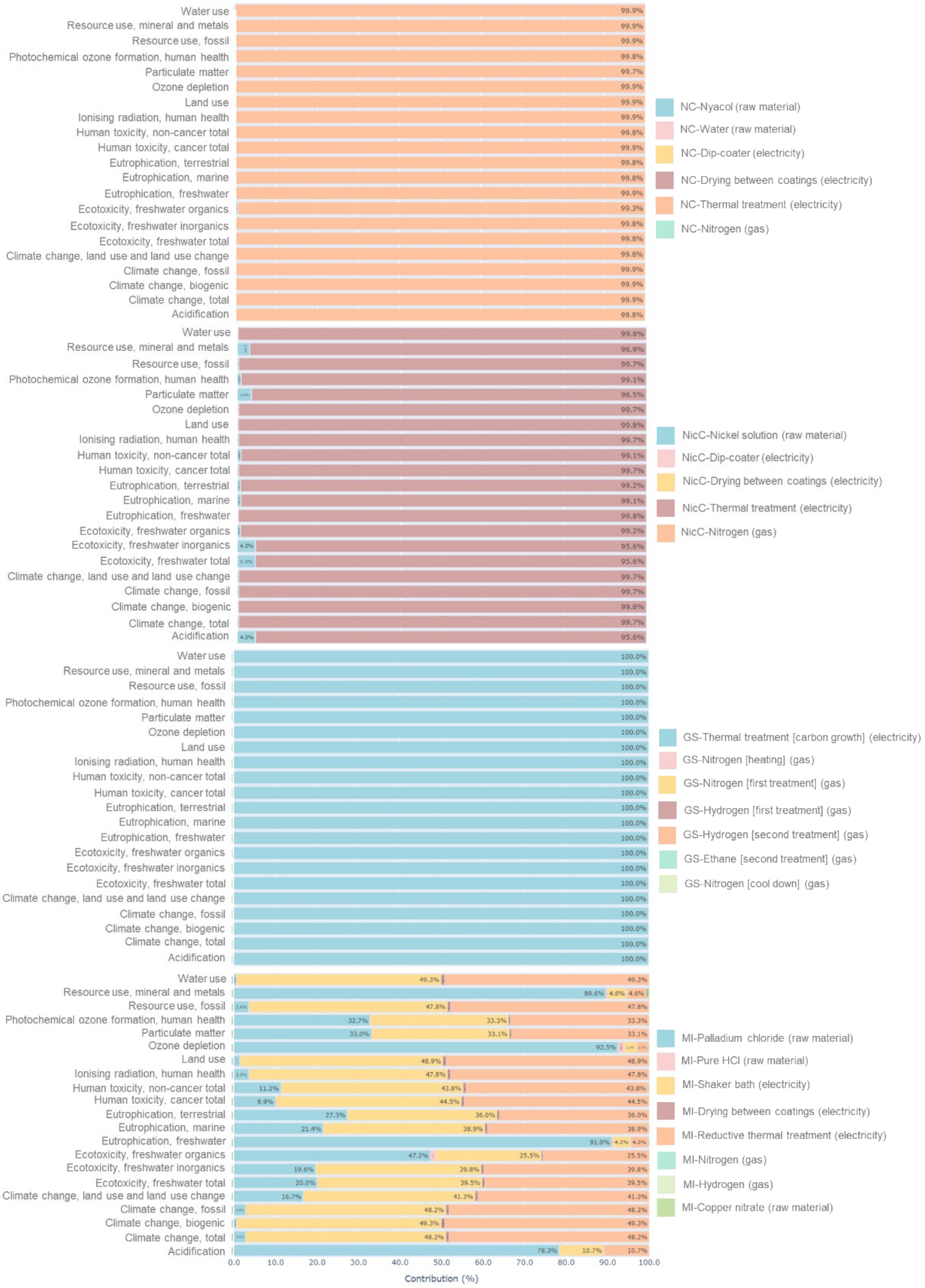


Figure SI 12 - Environmental impacts by material and energy inputs in terms of percentage of NC, NicC and GS stages for the synthesis of CVD_Pd_200_Cu.

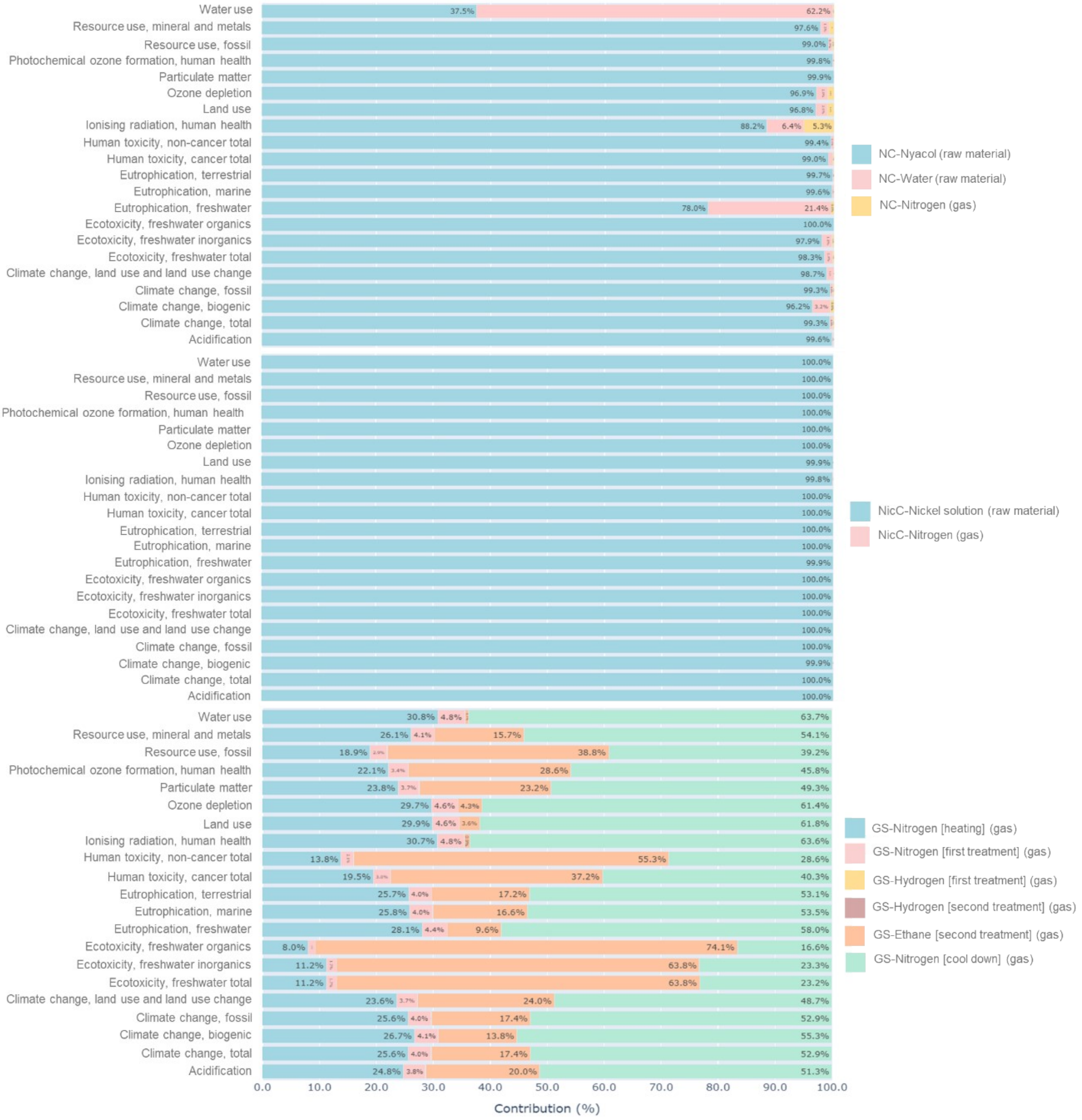


Figure SI 13 – Environmental impacts by material and energy inputs, in terms of percentage, for NC, NicC and GS stages for the synthesis of CVD_Pd_200_Cu, except inputs related to energy consumption.

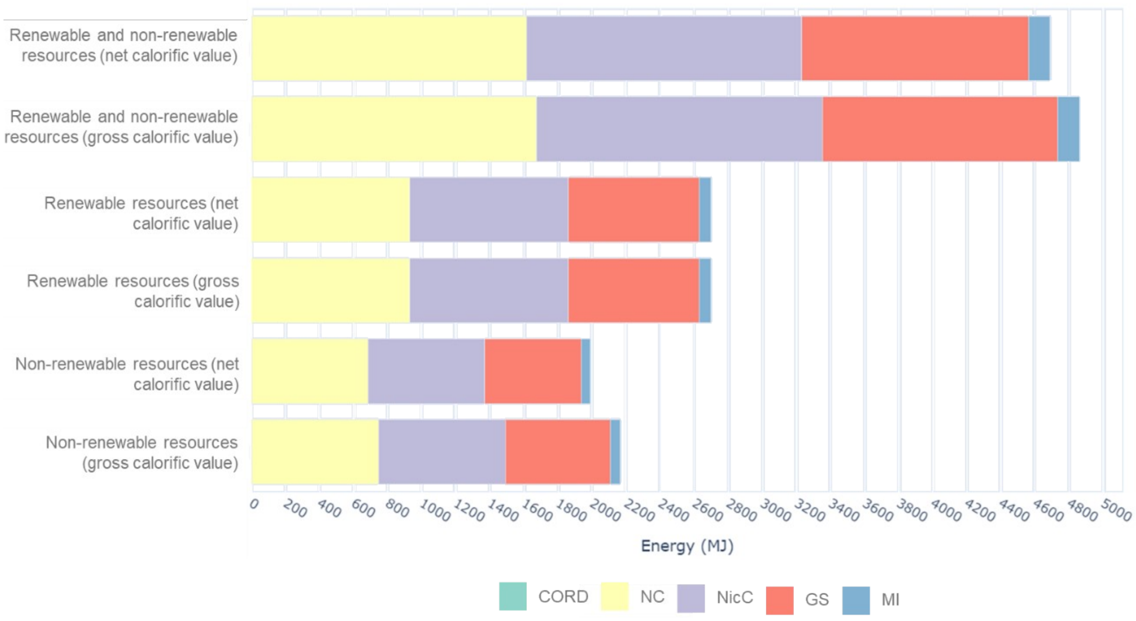


Figure SI 14 - Primary energy demand results for each stage related to CVD_Pd_200_Cu synthesis (CORD, NC, NicC, GS and MI).

Figure SI 15 - Primary energy demand results for each stage related to CVD_Pd_200_Cu synthesis (NC, NicC, GS and MI.

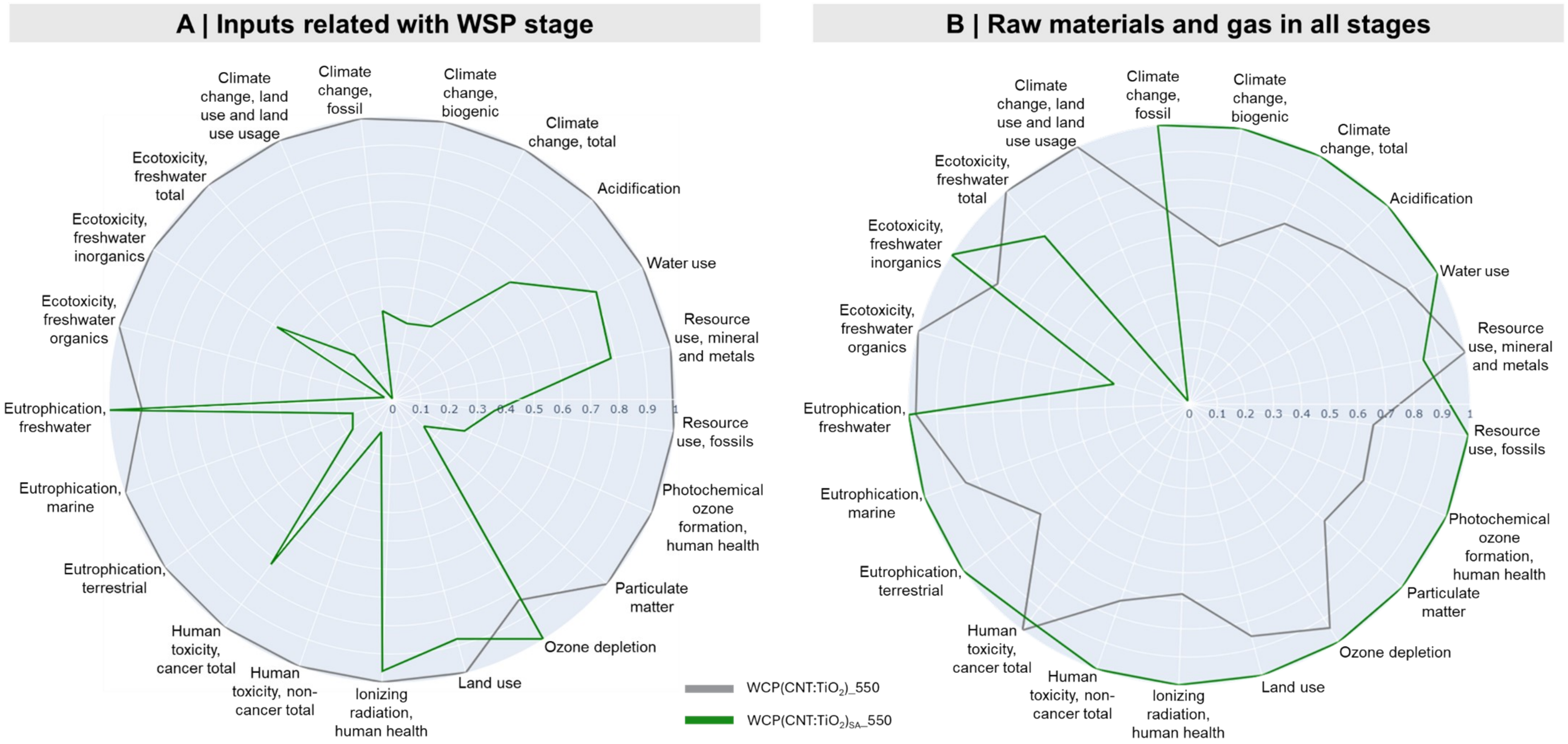


Figure SI 16 - Normalised radar chart comparing impact categories for the macrostructured catalysts synthesised through washcoating (WCP(CNT:TiO_2)_550 and WCP(CNT:TiO_2)$_{SA}$_550) : considering only the inputs related to WSP stage (A), considering only inputs related to raw materials and gas used in the different preparation stages (B).

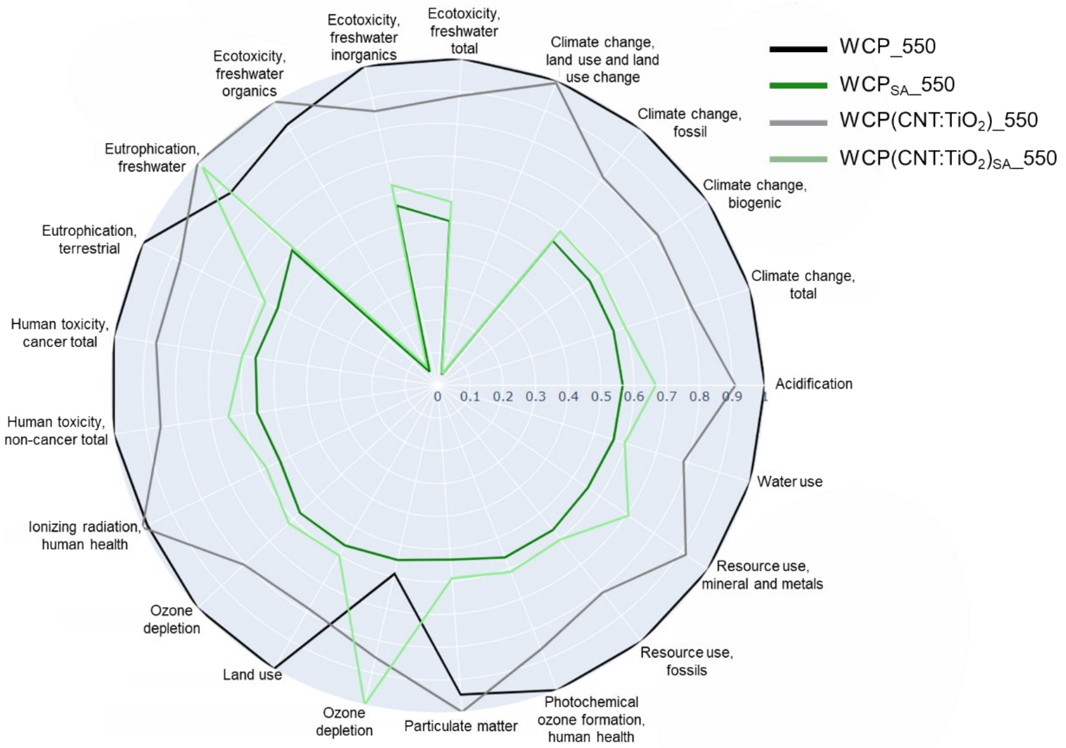


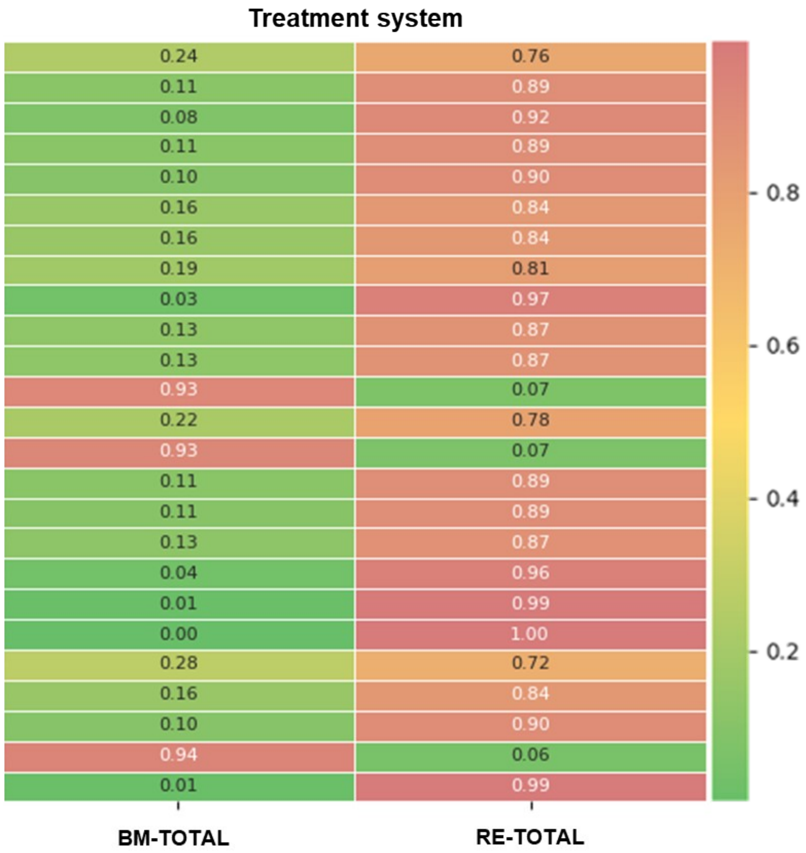
Figure SI 17 - Normalised radar chart across different impact categories for WSP stage of TX-100 and SA based catalysts.

Life cycle analysis of the integrated treatment system

Regarding the applied treatment system, the impacts can be divided into two major groups: the construction of the integrated system (BM phase – Building Materials) and the operation of the integrated system (RE phase – Reaction Experiments). The operation phase involves all the processes related to the reaction for water treatment during 30 h. The inputs of each stage can be found in supplementary information associated with each one of the studied scenarios (Tables SI 1 to 3 for the treatment system).

An important factor to consider is that the impacts from the building materials stage occur only once during the construction of the integrated catalytic system. Structural replacements are rarely required, as the components are made of highly durable materials with excellent longevity. In contrast, the RE stage, which involves the repeated application of the reaction process for water treatment, has the highest frequency of occurrence and impact.

To properly analyse the results for this stage, it is essential to consider the contribution of each stage (BM and RE) over the entire lifetime of the treatment system. To address this, parameters were calculated based on the scalability of each stage. It was assumed that approximately 300 experiments, each lasting 5 h, were conducted over a 5-year period using the same system without any modifications. The updated heatmap, reflecting these scalability adjustments, is presented in Figure SI 18.



BM-TOTAL	RE-TOTAL
0.24	0.76
0.11	0.89
0.08	0.92
0.11	0.89
0.10	0.90
0.16	0.84
0.16	0.84
0.19	0.81
0.03	0.97
0.13	0.87
0.13	0.87
0.93	0.07
0.22	0.78
0.93	0.07
0.11	0.89
0.11	0.89
0.13	0.87
0.04	0.96
0.01	0.99
0.00	1.00
0.28	0.72
0.16	0.84
0.10	0.90
0.94	0.06
0.01	0.99

Figure SI 18 – Heat map relating to impact categories involving the integrated treatment system considering the repeatability of RE stage regarding BM stage.

In this vein, considering the scalability process, the impact distribution shifts significantly, with the majority of impacts linked to the reaction system operation for water treatment for the majority of the considered categories (around 80-90 % of the total impact). Figure SI 19 presents the results on the impact distribution related to the integrated system application and construction.

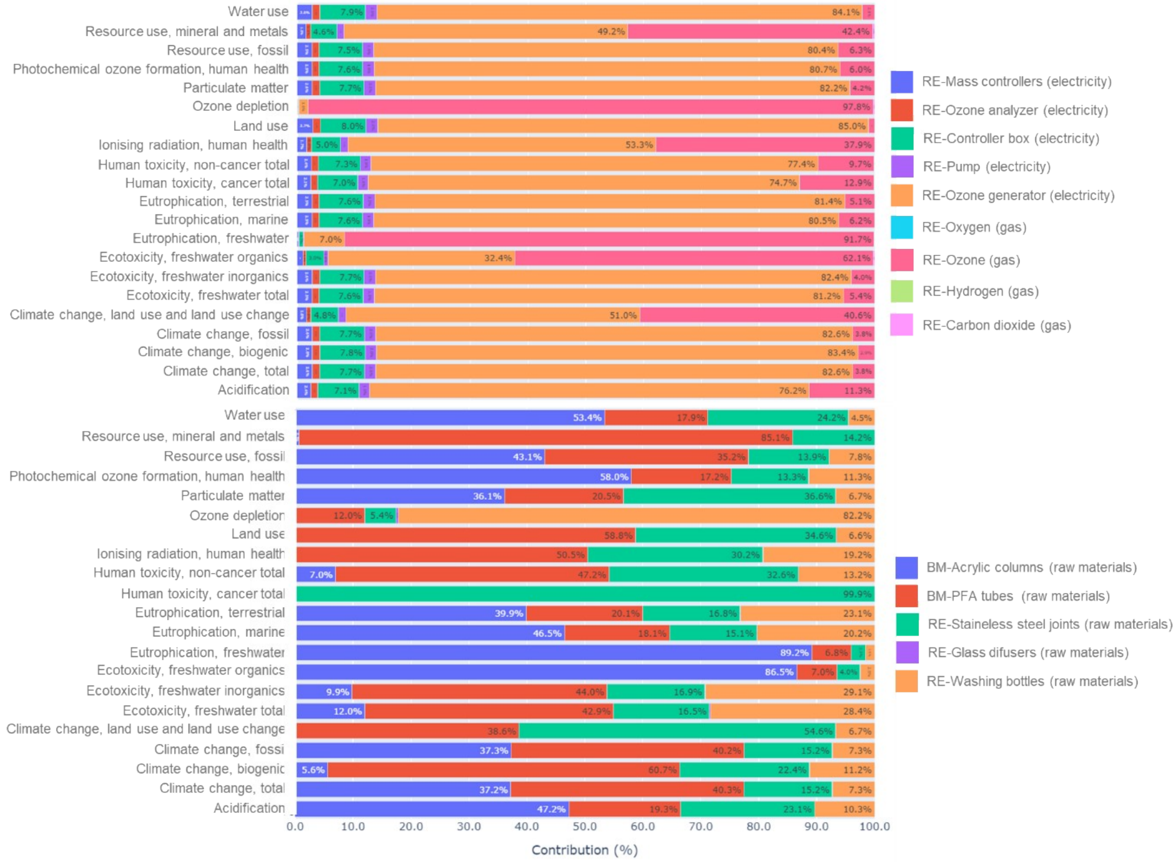


Figure SI 19 - Environmental impact category results in terms of percentage for RE and BM stages of integrated system application and construction.

Focusing on the distribution of the impacts associated with the system implementation during reaction, it is evident that the great contribution is related to electricity consumption, with particular emphasis on the use of the ozone generator and the controller box connected to the system (namely for the impacts associated with water use, land use and ionizing radiation). Generally, these contributions are due to the composition of the electricity source used. The use of non-renewable energy sources, particularly fossil fuels, is associated with significant environmental impacts. These include contributions to climate change through greenhouse gas emissions, as well as higher impacts on water and land use. Fossil fuel extraction and use, often require large quantities of water, which can deplete water resources in water-scarce regions and involve mining or drilling processes that lead to land disturbance and habitat loss. Therefore, it is crucial to assess the energy sources used during the system implementation phase to address these combined impacts and explore strategies for their mitigation. Figure SI 20, present in supplementary information, presents the primary energy demand results obtained for each phase related with the integrated treatment system application and construction.

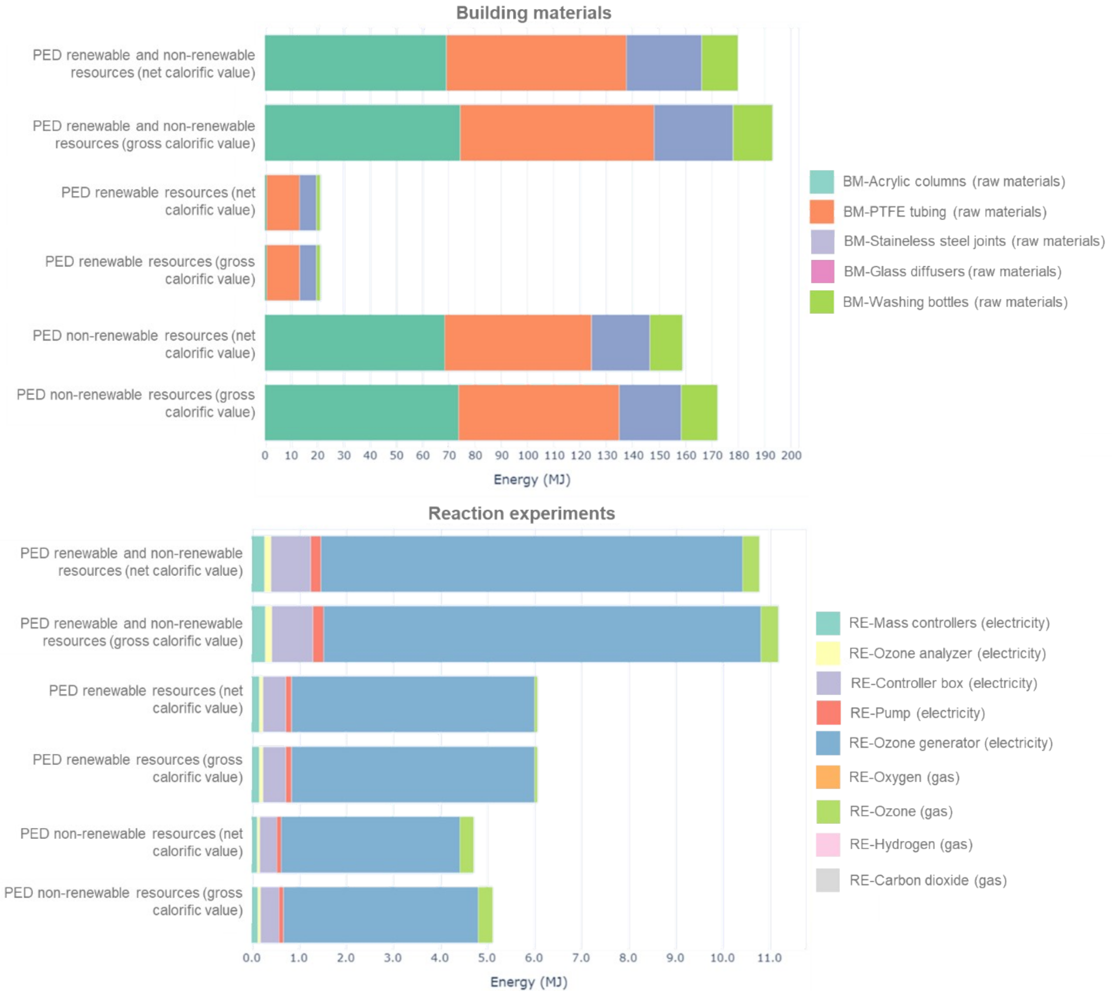


Figure SI 20 – Primary energy demand results for each stage of the integrated treatment system by materials and components: Building materials (BM) and reaction experiments (RE) phase.

Starting from the BM stage, there is a significant difference between the energy recorded between renewable resources (around 20 MJ, gross cal. value) and non-renewable resources (around 170 MJ, gross cal. value). This great difference indicates that almost all the energy used in this phase comes from non-renewable sources. This suggests that the materials and processes used for system construction heavily rely on fossil fuels such as oil, coal and natural gas. Additionally, the value obtained for renewable and non-renewable resources was very similar to that obtained for non-renewable resources (around 194 MJ, gross cal. value). This fact reinforces that renewable sources minimally contribute to this stage of the process (only around 12.3 %), so the processes related to the acquisition and transformation of raw materials hardly incorporate any renewable energy. This pattern confirms that the construction phase is highly dependent on fossil energy use, reflecting typical industrial practices that have yet to widely incorporate renewable sources.

For the specific case of the integrated system implementation, for this stage, renewable resources and non-renewable resources present very close values (around 6 MJ Vs 5.3 MJ). This indicates an almost equal balance between the use of renewable and non-renewable energies at this stage, showing that there is a significant integration of renewable sources for the application of treatment processes.

During BM phase, there was an overwhelming dependence on non-renewable sources (~194 MJ against 20 MJ renewable). In the RE phase, the difference has been drastically reduced, showing that the treatment uses more sustainable practices that are less dependent on fossil fuels.

Total energy consumption in the RE phase (around 3.6 MJ) is also considerably lower than in the BM phase (194 MJ), which reinforces the relative sustainability of this stage. The integration of renewable sources indicates more favourable conditions for implementing sustainable practices in energy use. Less dependence on fossil energy reduces the carbon footprint of this stage, contributing less to greenhouse gas emissions.

In RE stage, the greatest contribution is associated with the ozone generator operation, contributing to around 86 % of the total energy used to produce 1 L of clean water.

Regarding the difference between net and gross values, for the non-renewable sources and mix for renewable and non-renewable sources, a small difference was registered, indicating inevitable energy losses during the process, reflecting that not all the potential energy from this source can be used due to thermodynamic and operational limitations and so the use of the energy is not fully efficient.

This difference is non-existent or insignificant when the primary energy demand is related to the use of renewable sources, since these types of energies are less susceptible to heat loss (unlike fossil-fuels-dependent sources).

Given that the system operates under laboratory-scale conditions, where energy consumption is not yet optimized, electricity emerges as a major contributor to the overall environmental impacts (as it was reported for the macrostructured catalysts synthesis stage). This setup represents a conservative or "worst-case" scenario compared to industrial-scale implementations, which typically benefit from higher energy efficiency.

Additionally, the environmental impacts associated with O_3 production and use during treatment are noteworthy. O_3 use significantly affects impact categories such as ozone depletion, freshwater ecotoxicity, and freshwater eutrophication. Although ozone itself is not a long-lived atmospheric pollutant, its release into the troposphere can be harmful due to its high reactivity, potentially causing respiratory issues even at low concentrations and degrading materials and surfaces through oxidation (1,2).

Beyond direct effects, O_3 use can also indirectly contribute to freshwater eutrophication. These impacts rely from the life cycle of the treatment process rather than ozone itself, particularly from the energy required to generate O_3. If fossil-based electricity is used, associated emissions may include nutrients that contribute to eutrophication (3–5). Moreover, emissions from the production and transport of ozone generators, as well as the supply of pure oxygen used in O_3 formation, can also introduce nutrient-related pollutants.

Additionally, the effluent treatment by-products formed during the oxidative treatment (namely phosphorous) and the quality of the treatment (if all organic compounds are completely degraded during treatment and if the system is capable of mitigating nutrients formation) play a key role in contributing to this impact (6,7). This last point is the only one that can be overcome by the know-how that exists in the applied process.

One important aspect of the plant's operation is the way the unreacted O_3 is handled before being released. After going through the oxidation column, the O_3 that does not react is sent to a hood at the top of the column, where it is mixed with an aqueous KI solution. This reaction turns the O_3 into O_2. O_2 is then released into the environment through the hood's extraction system. Since the whole system is sealed and there is no O_3 leakage from its formation to its disposal, and no O_3 is emitted into the environment, making the process impact-free in what concerns O_3 released directly into the atmosphere.

Considering the system's high energy dependency, it was analysed based on the main energy source associated with each process input. Primary energy demand is a sustainability indicator that quantifies the total energy extracted from nature before any conversion or transformation, including all energy sources used directly in a system or a product production chain (from resource extraction until the final delivery).

This way, for the construction phase (BM), where most of the used energy is prevenient from non-renewable sources, in addition to the heavy dependence on fossil fuels, there is a problem related to energy use, since there are inevitable energy losses throughout the process, making this stage one of the main areas of study for reducing the impact associated with the water treatment process.

Regarding the impacts associated with the BM phase, the most significant contributions are primarily linked to the reliance on fossil resources and the high energy demand during their production (see Figure SI 20) (8,9). The greatest contribution to the overall impact of the BM phase is mainly attributed to the use of acrylic (to construct the two columns where the reaction will take place), the use of PTFE tubing and stainless-steel joints to connect all the stages of the treatment process. In this last case, the use of PTFE-based materials is mandatory, so they are resistant to the ozone used during the oxidation process conducted in the system.

Acrylic production is related to the polymerization of methyl methacrylate, which requires fossil-fuel-based processes that can lead to greenhouse gas emissions. Additionally, acrylic synthesis involves energy-intensive processes and the use of chemical reagents that will contribute to categories such as climate change, acidification and photochemical ozone formation (10).

The use of PTFE can be especially impactful on the production stage due to the use of fluorinated compounds, more specifically perfluorooctanoic acid (PFOA) or its alternatives, that are highly resistant in the environment and can conduct to ecotoxicity in freshwater ecosystems, at this stage, and, also, contribute to human toxicity related to cancer and non-cancer diseases (11–

14). Additionally, polymerization is an energy-intensive process due to the high temperatures applied, which can further contribute to climate change impacts.

Stainless steel production requires extensive mining and processing of iron ore, nickel, and chromium, all of which have high resource use (fossil and mineral) impacts. The smelting and refining stages are energy-intensive, contributing significantly to climate change, acidification, and particulate matter emissions. Additionally, stainless steel can influence toxicity categories due to the release of heavy metals during extraction and manufacturing processes (15).

The less impactful phase is attributed to the production/use of the glass parts of the system (glass diffusers and washing bottles), except for the impact category related to ozone depletion (around 92 % of the total impact). Generally, glass manufacturing involves high-temperature processes, requiring substantial energy that is usually obtained from fossil fuels. However, the primary contributor to ozone depletion at this phase may be related to the use of substances like halogenated compounds during the production and/or cleaning phases of the process (some refrigerants or insulation materials are used in glass production and may include ozone-depleting substances).

Table SI 5 – Environmental impact results of the treatment system per 1 L of treated water of all categories across the scenarios studied by each life cycle phase (catalysts synthesis, treatment system and transportation).

Catalyst scenario		**Acidification [mol H^+ eq.]**	**Climate change, total [kg CO_2 eq.]**	**Climate change, biogenic [kg CO_2 eq.]**	**Climate change, fossil [kg CO_2 eq.]**	**Climate change, land use and land use change [kg CO_2 eq.]**	**Ecotoxicity, freshwater total [CTUe]**	**Ecotoxicity freshwater inorganics [CTUe]**
Scenario 1	Catalysts synthesis*	0.254	134.118	0.399	133.693	0.026	304.084	300.858
	Treatment system**	0.003	1.912	0.006	1.906	0.001	4.402	4.298
	Transportation***	0.004	0.327	0.000	0.326	0.000	2.551	2.351
	TOTAL****	0.015	7.575	0.022	7.551	0.001	17.280	17.084
Scenario 2	Catalysts synthesis	0.410	230.221	0.684	229.495	0.042	523.455	518.342
	Treatment system	0.003	1.912	0.006	1.906	0.001	4.402	4.298
	Transportation	0.007	0.547	0.000	0.547	0.000	4.271	3.937
	TOTAL	0.023	12.927	0.038	12.886	0.002	29.563	29.254
Scenario 3	Catalysts synthesis	0.325	178.375	0.530	177.813	0.032	402.974	399.027
	Treatment system	0.003	1.841	0.006	1.835	0.001	4.172	4.130
	Transportation	0.006	0.426	0.000	0.425	0.000	3.324	3.063
	TOTAL	0.019	10.036	0.030	10.004	0.002	22.804	22.568

Catalyst scenario		**Ecotoxicity, freshwater organics [CTUe]**	**Eutrophication, freshwater [kg P eq.]**	**Eutrophication, marine [kg N eq.]**	**Eutrophication, terrestrial [mol N eq.]**	**Human toxicity, cancer total [CTUh]**	**Human toxicity, non-cancer total [CTUh]**	**Ionizing radiation, human health [kBq U325 eq]**
Scenario 1	Catalysts synthesis	3.226	6.61E-04	7.23E-02	0.769	8.14E-08	4.93E-07	5.659
	Treatment system	0.104	6.93E-05	1.05E-03	0.011	3.83E-09	7.44E-09	0.123
	Transportation	0.200	8.17E-06	1.84E-03	0.020	7.77E-10	1.88E-09	0.002
	TOTAL	0.196	4.10E-05	4.17E-03	0.044	4.78E-09	2.79E-08	0.321
Scenario 2	Catalysts synthesis	5.113	9.59E-04	1.23E-01	1.311	1.39E-07	8.44E-07	9.713
	Treatment system	0.104	6.93E-05	1.05E-03	0.011	3.83E-09	7.44E-09	0.123

	Transportation	0.334	1.37E-05	3.08E-03	0.034	1.30E-09	3.15E-09	0.004
	TOTAL	0.308	5.79E-05	7.09E-03	0.075	8.03E-09	4.75E-08	0.547
Scenario 3	Catalysts synthesis	3.947	7.99E-04	9.58E-02	1.018	1.08E-07	6.55E-07	7.525
	Treatment system	0.042	3.72E-04	1.35E-03	0.011	3.66E-04	3.66E-04	0.077
	Transportation	0.260	1.06E-05	2.39E-03	0.026	1.01E-09	2.46E-09	0.003
	TOTAL	0.236	6.56E-05	5.53E-03	0.059	2.03E-05	2.04E-05	0.423

Catalyst scenario		**Land Use [Pt]**	**Ozone depletion [kg CFC-11 eq.]**	**Particulate matter [Disease incidences]**	**Photochemical ozone formation, human health [KG nmvoc eq.]**	**Resource use, fossil [MJ]**	**Resource use, mineral and metals [kg Sb eq.]**	**Water use [m^3 world eq.]**
Scenario 1	Catalysts synthesis	2216.545	3.69E-09	2.08E-06	2.18E-01	1974.723	4.02E-05	211.747
	Treatment system	30.169	1.25E-09	3.03E-08	3.14E-03	28.854	2.31E-06	2.915
	Transportation	1.747	2.40E-09	1.13E-07	5.28E-03	4.263	3.32E-07	0.012
	TOTAL	124.915	4.08E-10	1.23E-07	1.26E-02	111.547	2.38E-06	11.926
Scenario 2	Catalysts synthesis	3805.436	4.88E-09	3.55E-06	3.71E-01	3389.245	5.96E-05	363.609
	Treatment system	30.169	1.25E-09	3.03E-08	3.14E-03	28.854	2.31E-06	2.915
	Transportation	2.924	4.01E-09	1.90E-07	8.84E-03	7.138	5.56E-07	0.019
	TOTAL	213.252	5.63E-10	2.10E-07	2.13E-02	190.291	3.47E-06	20.364
Scenario 3	Catalysts synthesis	2948.227	4.29E-09	2.75E-06	2.88E-01	2626.136	4.90E-05	281.675
	Treatment system	29.864	3.66E-04	3.66E-04	3.32E-03	27.058	3.68E-04	2.854
	Transportation	2.276	3.12E-09	1.48E-07	6.88E-03	5.555	4.33E-07	0.015
	TOTAL	165.576	2.03E-05	2.05E-05	1.66E-02	147.708	2.32E-05	15.808

Catalyst scenario		**Primary energy demand from renewable and non-renewable resources (net cal. value) [MJ]**	**Primary energy demand from renewable and non-renewable resources (gross cal. value) [MJ]**	**Primary energy demand from renewable resources (net cal. value) [MJ]**	**Primary energy demand from renewable resources (gross cal. value) [MJ]**	**Primary energy demand from non-renewable resources (net cal. value) [MJ]**	**Primary energy demand from non-renewable resources (gross cal. value) [MJ]**

Scenario 1	Catalysts synthesis	4826.583	4652.933	2148.410	1974.767	2678.173	2678.166
	Treatment system	67.826	65.367	31.309	28.854	36.518	36.513
	Transportation	4.598	4.304	4.557	4.263	0.041	0.041
	TOTAL	272.167	262.367	121.349	111.549	150.818	150.818
Scenario 2	Catalysts synthesis	8286.952	7988.807	3687.467	3389.326	4599.485	4599.480
	Treatment system	67.826	65.367	31.309	28.854	36.518	36.513
	Transportation	7.698	7.206	7.629	7.138	0.069	0.068
	TOTAL	464.582	447.854	207.022	190.295	257.560	257.559
Scenario 3	Catalysts synthesis	6420.073	6189.088	2857.175	2626.194	3562.899	3562.894
	Treatment system	65.561	63.182	29.437	27.058	36.124	36.124
	Transportation	5.991	5.608	5.938	5.555	0.054	0.053
	TOTAL	360.646	347.660	160.697	147.712	199.949	199.948

*Calculated total impact for the synthesis of 6 macrostructured catalysts (3 catalysts for ozonation system and 3 catalysts for hydrogenation system) considering the preparations used for each scenario.

**Treatment system application and construction considering the ‘repeatability indexes’ attributed to the impacts related to the building materials. Calculated impacts corresponding to the application of the treatment system for a 30 h reaction.

***Calculated total impacts of transportation for the inputs related to each scenario.

****Total impact of the system (considering catalyst synthesis, treatment system application and raw materials/gas transportation) calculated for L of treated water.

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