

New Sustainable Multilayered Membranes Based on ZrVTi for Hydrogen Purification

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Supplementary Materials

The complete Life cycle assessment inventory is listed in the following tables (tables S1-S14).

Table S1: Life cycle inventory for vanadium bearing magnetite (adapted from Da Silva et al 2021 [35]).

Dataset	Amount	Unit
Inputs		
Occupation, mineral extraction site	0.00249	m ² a
TiO ₂ , 54% in ilmenite, 18% in crude ore	0.25	kg
Iron ore	1.08	kg
Transformation, from forest, unspecified	0.000083	m ²
Transformation, to mineral extraction site	0.000083	m ²
Vanadium ore	0.034	kg
Water, well, GLO	0.000059	m ³
Blasting {GLO} market for Cut-off, U	0.00015	kg
Conveyor belt {GLO} market for Cut-off, U	5.6E-08	m
Diesel, burned in diesel-electric generating set, 10MW {GLO} market for Cut-off, U	0.0238	MJ
Electricity, medium voltage {CN} market group for Cut-off, U	0.0144	kWh
Heat, central or small-scale, natural gas {GLO} market group for Cut-off, U	0.0154	MJ
industrial machine, heavy, unspecified {RoW} market for industrial machine, heavy, unspecified Cut-off, U	0.000012	kg
Mine infrastructure, open cast, ilmenite from hard-rock ore {GLO} market for Cut-off, U	3.1E-11	p
Petrol, unleaded {RoW} market for Cut-off, U	0.0627	kg
Recultivation, ilmenite mine {GLO} market for Cut-off, U	0.000083	m ²
Outputs		
Vanadium bearing magnetite (Magnetite 72% Fe, 2.2% V ₂ O ₅)	1.53	kg
Ilmenite, 54% titanium dioxide	0.46	kg

Particulates, < 2.5 um to air	0.000018	kg
Particulates, < 10 um to air	0.00024	kg
Particulates, > 2.5 um, and < 10um to air	0.000096	kg
Water to air	0.00879	kg
Water, GLO to water	0.00005	m ³

Table S2: Life cycle inventory for Vanadium pentaoxide V₂O₅ bearing cast iron (adapted from Da Silva et al 2021 [35]).

Dataset	Amount	Unit
Inputs		
Water, cooling, unspecified natural origin, RoW	0.005216	m ³
Anode, for metal electrolysis {GLO} market for Cut-off, U	0.003	kg
Electric arc furnace converter {GLO} market for Cut-off, U	4E-11	p
Hard coal {CN} market for Cut-off, U	0.014	kg
Natural gas, high pressure {RoW} market for Cut-off, U	0.025	m ³
Oxygen, liquid {RoW} market for Cut-off, U	0.05073	kg
Quicklime, in pieces, loose {RoW} market for quicklime, in pieces, loose Cut-off, U	0.055	kg
Refractory, basic, packed {GLO} market for Cut-off, U	0.0135	kg
Pre-reduced V ₂ O ₅ magnetite adapted from Iron pellet {RoW} production Cut-off, U	1.46	kg
Electricity, medium voltage {GLO} market group for Cut-off, U	0.42	kWh
Outputs		
Vanadium pentaoxide V ₂ O ₅ bearing cast iron	1.320	kg
Benzene to air	2.31E-06	kg
Cadmium to air	3.65E-08	kg
Carbon monoxide, fossil to air	0.00232	kg
Chromium to air	1.25E-06	kg
Copper to air	2.31E-07	kg
Dioxins (TEQ) to air	4.54E-12	kg
Hydrocarbons, aromatic to air	7.7E-05	kg
Hydrogen chloride to air	5.2E-06	kg
Hydrogen fluoride to air	2.35E-06	kg
Lead to air	1.81E-06	kg
Mercury to air	2.22E-06	kg
Nickel to air	7.01E-07	kg
Nitrogen oxides to air	0.00018	kg
PAH, polycyclic aromatic hydrocarbons to air	3.73E-08	kg
Particulates, < 2.5 um to air	0.000166	kg
Particulates, > 10 um to air	5.86E-05	kg
Particulates, > 2.5 um, and < 10um to air	1.6596	kg
Polybrominated biphenyls to air	2.33E-08	kg
Sulfur dioxide to air	0.000077	kg

Water to air	0.002021	kg
Zinc to air	2.29E-05	kg
Inert waste, for final disposal {RoW} market for inert waste, for final disposal Cut-off, U	0.005	kg
electric arc furnace dust {RoW} market for electric arc furnace dust Cut-off, U	0.0096	kg
electric arc furnace slag {RoW} market for electric arc furnace slag Cut-off, U	0.928	kg

Table S3: Life cycle inventory for Vanadium Slag (25% V₂O₅) (adapted from Da Silva et al 2021 [35]).

Dataset	Amount	Unit
Inputs		
Water, cooling, unspecified natural origin, RoW	0.005216	m ³
Anode, for metal electrolysis {GLO} market for Cut-off, U	0.003	kg
Electric arc furnace converter {GLO} market for Cut-off, U	4E-11	p
Hard coal {CN} market for Cut-off, U	0.014	kg
Natural gas, high pressure {RoW} market for Cut-off, U	0.025	m ³
Oxygen, liquid {RoW} market for Cut-off, U	0.05073	kg
Quicklime, in pieces, loose {RoW} market for quicklime, in pieces, loose Cut-off, U	0.055	kg
Refractory, basic, packed {GLO} market for Cut-off, U	0.0135	kg
Pre-reduced V ₂ O ₅ magnetite adapted from Iron pellet {RoW} production Cut-off, U	1.46	kg
Vanadium pentaoxide V ₂ O ₅ bearing cast iron Fe	1.32	kg
Aluminium, wrought alloy {GLO} market for Cut-off, U	0.000015	kg
Argon, liquid {RoW} market for argon, liquid Cut-off, U	0.00329	kg
Cast iron {GLO} market for Cut-off, U	0.000052	kg
Diesel, burned in building machine {GLO} market for Cut-off, U	0.00346	MJ
Ethylene glycol {GLO} market for Cut-off, U	3.3E-08	kg
Ferrochromium, high-carbon, 68% Cr {GLO} market for Cut-off, U	0.00011	kg
Ferromanganese, high-coal, 74.5% Mn {GLO} market for Cut-off, U	0.000045	kg
Ferrosilicon {GLO} market for Cut-off, U	0.0037	kg
Molybdenum trioxide {GLO} market for Cut-off, U	0.000014	kg
nickel, class 1 {GLO} market for nickel, class 1 Cut-off, U	0.000033	kg
Propane, burned in building machine {GLO} market for Cut-off, U	0.00273	MJ
Electricity, medium voltage {CN} market group for Cut-off, U	0.54	kWh
Electricity, low voltage {CN} market group for Cut-off, U	0.0346	kWh
Heat, district or industrial, natural gas {RoW} market for heat, district or industrial, natural gas Cut-off, U	1.23	MJ
Outputs		
Vanadium Slag (25% V ₂ O ₅)	0.0613	kg
Steel, low alloyed	1.2	kg
Benzene to air	2.31E-06	kg

Cadmium to air	3.65E-08	kg
Carbon monoxide, fossil to air	0.00232	kg
Chromium to air	1.25E-06	kg
Copper to air	2.31E-07	kg
Dioxins (TEQ) to air	4.54E-12	kg
Hydrocarbons, aromatic to air	7.7E-05	kg
Hydrogen chloride to air	5.2E-06	kg
Hydrogen fluoride to air	2.35E-06	kg
Lead to air	1.81E-06	kg
Mercury to air	2.22E-06	kg
Nickel to air	7.01E-07	kg
Nitrogen oxides to air	0.00018	kg
PAH, polycyclic aromatic hydrocarbons to air	3.73E-08	kg
Particulates, < 2.5 um to air	0.000166	kg
Particulates, > 10 um to air	5.86E-05	kg
Particulates, > 2.5 um, and < 10um to air	1.6596	kg
Polybrominated biphenyls to air	2.33E-08	kg
Sulfur dioxide to air	0.000077	kg
Water to air	0.002021	kg
Zinc to air	2.29E-05	kg
Argon-40/kg to air	0.00329	kg
Benzene, hexachloro- to air	2E-08	kg
Water to water	0.003195	kg
Chloride to water	1.8E-06	kg
Chromium VI to water	1.9E-09	kg
Inert waste, for final disposal {RoW} market for inert waste, for final disposal Cut-off, U	0.005	kg
electric arc furnace dust {RoW} market for electric arc furnace dust Cut-off, U	0.0096	kg
electric arc furnace slag {RoW} market for electric arc furnace slag Cut-off, U	0.0498	kg
Scrap steel {RoW} market for scrap steel Cut-off, U	0.000052	kg
Spent solvent mixture {Europe without Switzerland} market for spent solvent mixture Cut-off, U	3.3E-08	kg
Blast furnace slag {GLO} market for Cut-off, U	0.0928	kg

Table S4: Life cycle inventory for Vanadium Pentaoxide V₂O₅ (adapted from Da Silva et al 2021 [35]).

Dataset	Amount	Unit
Inputs		
Vanadium Slag (25% V ₂ O ₅)	1.35	kg
ammonium sulfate {RoW} market for ammonium sulfate Cut-off, U	0.31	kg
Soda ash, dense {GLO} market for Cut-off, U	0.37	kg
Sodium sulfate, anhydrite {RoW} market for Cut-off, U	0.5	kg

Sulfuric acid {RoW} market for sulfuric acid Cut-off, U	0.46	kg
Transport, freight train {CN} market for Cut-off, U	0.46	tkm
Transport, freight, lorry 16-32 metric ton, EURO6 {RER} transport, freight, lorry 16-32 metric ton, EURO6 Cut-off, U	0.0771	tkm
water, deionised {RoW} market for water, deionised Cut-off, U	3.16	kg
Electricity, medium voltage {CN} market group for Cut-off, U	0.2	kWh
Heat, district or industrial, natural gas {RoW} market for heat, district or industrial, natural gas Cut-off, U	0.93	MJ
Outputs		
Vanadium Pentaoxide V ₂ O ₅	1.00	kg
Sodium sulfate, anhydrite	1.00	kg
Carbon dioxide to air	0.16	kg
Oxygen to air	0.0564	kg
Sulfur dioxide to air	0.23	kg
Water to air	0.0845	kg
Scrap steel {RoW} market for scrap steel Cut-off, U	0.065	kg
Spent solvent mixture {Europe without Switzerland} market for spent solvent mixture Cut-off, U	0.0632	kg
Slag from metallurgical grade silicon production {GLO} market for Cut-off, U	0.47	kg

Table S5: Life cycle inventory for Vanadium Chloride VCl₃ (adapted from Da Silva et al 2021 [35]).

Dataset	Amount	Unit
Inputs		
Vanadium Pentaoxide V ₂ O ₅	0.57813	kg
Hydrochloric acid, without water, in 30% solution state {RoW} market for Cut-off, U	0.69536	kg
Hydrogen, liquid {RoW} market for Cut-off, U	0.00641	kg
Electricity, medium voltage {CN} market group for Cut-off, U	0.33	kWh
Outputs		
Vanadium Chloride VCl ₃	1.0000	kg
Water to air	0.2632	kg

Table S6: Life cycle inventory for Vanadium (adapted from Titanium primary, triple-melt {GLO}| titanium production, primary, triple melt | Cut-off, U).

Dataset	Amount	Unit
Inputs		
Vanadium Chloride VCl ₃	3.087	kg
Argon, liquid {RER} market for argon, liquid Cut-off, U	0.030972	kg
Argon, liquid {RoW} market for argon, liquid Cut-off, U	0.147028	kg
Magnesium {GLO} market for Cut-off, U	0.01145	kg
Electricity, high voltage {GLO} market group for Cut-off, U	27.84	kWh

Heat, district or industrial, natural gas {GLO} market group for Cut-off, U	9	MJ
Outputs		
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	1.000	kg

Table S7: Life cycle inventory for Zirconium tetrachloride (adapted from Titanium tetrachloride {GLO}| production | Cut-off, U).

Dataset	Amount	Unit
Inputs		
Zirconium oxide {GLO} market for Cut-off, U	1.192	kg
Chlorine, liquid {RER} market for chlorine, liquid Cut-off, U	0.030972	kg
Chlorine, liquid {RoW} market for chlorine, liquid Cut-off, U	0.147028	kg
Coke {GLO} market for Cut-off, U	0.016	kg
Electricity, high voltage {GLO} market group for Cut-off, U	014	kWh
Heat, district or industrial, natural gas {GLO} market group for Cut-off, U	2.1	MJ
Outputs		
Zirconium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	1.000	kg

Table S8: Life cycle inventory for Zirconium (adapted from Titanium primary, triple-melt {GLO}| titanium production, primary, triple melt | Cut-off, U).

Dataset	Amount	Unit
Inputs		
Zirconium tetrachloride (adapted from Titanium tetrachloride {GLO} production Cut-off, U)	4.000	kg
Argon, liquid {RER} market for argon, liquid Cut-off, U	0.030972	kg
Argon, liquid {RoW} market for argon, liquid Cut-off, U	0.147028	kg
Magnesium {GLO} market for Cut-off, U	0.016	kg
Electricity, high voltage {GLO} market group for Cut-off, U	27.84	kWh
Heat, district or industrial, natural gas {GLO} market group for Cut-off, U	9	MJ
Outputs		
Zirconium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	1.000	kg

Table S9: Life cycle inventory for Pd₇₇Ag₂₃ membrane.

Dataset	Amount	Unit
Inputs		
Palladium {GLO} market for Cut-off, U	0.77	kg

Silver {GLO} market for Cut-off, U	0.23	kg
Outputs		
Pd ₇₇ Ag ₂₃ membrane	1.00	kg

Table S10: Life cycle inventory for V₉₃Pd₇ membrane with Pd coatings.

Dataset	Amount	Unit
Inputs		
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	0.86	kg
Palladium {GLO} market for Cut-off, U	0.37	kg
Outputs		
V ₉₃ Pd ₇ membrane with Pd coatings	1.00	kg

Table S11: Life cycle inventory for Ti₃₀Zr₉V₃₄Pd₂₇ membrane (ZrVTiPd2) with Pd coatings.

Dataset	Amount	Unit
Inputs		
Titanium primary, triple-melt {GLO} market for Cut-off, U	0.21	kg
Zirconium adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U	0.12	kg
Palladium {GLO} market for Cut-off, U	0.59	kg
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	0.25	kg
Outputs		
Ti ₃₀ Zr ₉ V ₃₄ Pd ₂₇ membrane ZrVTiPd2	1.00	kg

Table S12: Life cycle inventory for Ti₁₃Zr₅₂V₁₂Pd₂₃ membrane (ZrVTiPd3) with Pd coatings.

Dataset	Amount	Unit
Inputs		
Titanium primary, triple-melt {GLO} market for Cut-off, U	0.07	kg
Zirconium adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U	0.56	kg
Palladium {GLO} market for Cut-off, U	0.44	kg
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	0.07	kg
Outputs		
Ti ₁₃ Zr ₅₂ V ₁₂ Pd ₂₃ membrane (ZrVTiPd3)	1.00	kg

Table S13: Life cycle inventory for $\text{Ti}_{19}\text{Zr}_{39}\text{V}_{20}\text{Pd}_{22}$ membrane (ZrVTiPd4) with Pd coatings.

Dataset	Amount	Unit
Inputs		
Titanium primary, triple-melt {GLO} market for Cut-off, U	0.12	kg
Zirconium adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U	0.45	kg
Palladium {GLO} market for Cut-off, U	0.69	kg
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	0.13	kg
Outputs		
$\text{Ti}_{19}\text{Zr}_{39}\text{V}_{20}\text{Pd}_{22}$ membrane (ZrVTiPd4)	1.00	kg

Table S14: Life cycle inventory for $\text{Ti}_{23}\text{Zr}_{11}\text{V}_{27}\text{Pd}_{39}$ membrane (ZrVTiPd6) with Pd coatings.

Dataset	Amount	Unit
Inputs		
Titanium primary, triple-melt {GLO} market for Cut-off, U	0.14	kg
Zirconium adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U	0.13	kg
Palladium {GLO} market for Cut-off, U	0.74	kg
Vanadium (adapted from Titanium primary, triple-melt {GLO} titanium production, primary, triple melt Cut-off, U)	0.18	kg
Outputs		
$\text{Ti}_{23}\text{Zr}_{11}\text{V}_{27}\text{Pd}_{39}$ membrane (ZrVTiPd6)	1.00	kg