Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary material: Environmental Assessment of the Near-net-shape Electrochemical Metallisation Process and the Kroll – Electron Beam Melting Process for Titanium Manufacture

Aleksei Dolganov[a], Matthew T. Bishop[a,b], Marco Tomatis[c], George Z. Chen[a, b, d*], Di Hu[a, b, e*]

1. LCI for the Kroll Process

	Item	Unit	Chlorination and refining	Reduction and distillation	Electrolysis of MgCl2	Total
Input	Synthetic rutile	kg	3.53E+04			3.53E+04
	Fresh water	kg	4.40E+02			4.40E+02
	Petroleum coke	kg	6.51E+02			6.51E+02
	Sodium hydroxide	kg	4.52E+03			4.52E+03
	Magnesium (make up)	kg		4.10E+01		4.10E+01
	Chlorine (make up)	kg	1.62E+03			1.62E+03
	Sulfuric acid	kg			6.98E+01	6.98E+01
	Raw coal	kg	3.53E+03			3.53E+03
	Crude oil	kg	8.51E+02			8.51E+02
	Natural gas	m3	9.16E+01			9.16E+01
	Electric power	kWh	2.55E+03	4.85E+03	1.45E+04	2.19E+04
Output	CO_2	kg	8.42E+03	4.00E+03	1.19E+04	2.43E+04
	SO_2	kg	5.17E+01	2.71E+01	8.11E+01	1.60E+02
	NO_x	kg	4.60E+01	1.84E+01	5.51E+01	1.20E+02
	CO	kg	6.15E+02	5.62E+00	1.68E+01	6.37E+02
	CH_4	kg	1.66E+01	5.31E-02	1.59E-01	1.68E+01
	N_2O	kg	3.96E-02	7.33E-02	2.19E-01	3.32E-01
	NMVOC	kg	1.60E+01	1.47E-01	4.40E-01	1.66E+01
	HCl	kg			3.92E+00	3.92E+00
	HF	kg			6.36E-01	6.36E-01
	As	kg	4.03E-03	7.56E-03	2.26E-02	3.42E-02
	Cd	kg	2.75E-05	4.81E-05	1.44E-04	2.20E-04
	Cr	kg	3.40E-04	6.38E-04	1.91E-03	2.89E-03
	Hg	kg	1.77E-04	3.32E-04	9.92E-04	1.50E-03
	Ni	kg	5.29E-04	9.47E-04	2.83E-03	4.31E-03
	Pb	kg	3.61E-03	6.63E-03	1.98E-02	3.00E-02
	V	kg	5.82E-03	1.09E-02	3.26E-02	4.93E-02
	Zn	kg	4.84E-03	9.08E-03	2.71E-02	4.10E-02
	Particulates	kg	7.95E-01	1.51E+00	4.52E+00	6.83E+00
	COD	kg	1.53E-01	2.81E-01	8.41E-01	1.28E+00

	Spent alkali liquor	kg	4.60E+03			4.60E+03
	Other residue	kg		9.30E+01	1.62E-01	9.32E+01
	Hydrochloric acid (concentration: 20%) byproduct	kg	5.13E+02			5.13E+02

2. Calculated data for Figure 7

Impact category	Unit	Total	Molten salt electrolysis	DIW
Global warming	kg CO_2 eq	10.069	6.306316903	3.76263
Stratospheric ozone depletion	kg CFC11 eq	2E-06	1.33303E-06	1.16E-06
Ionizing radiation	kBq Co-60 eq	0.3337	0.186851108	0.146876
Ozone formation, Human health	kg NO_x eq	0.0223	0.014205071	0.00806
Fine particulate matter formation	kg PM2.5 eq	0.0191	0.012373489	0.006706
Ozone formation, Terrestrial ecosystems	kg NO_x eq	0.0224	0.014241437	0.008151
Terrestrial acidification	kg SO_2 eq	0.0452	0.030588044	0.014632
Freshwater eutrophication	kg P eq	0.0027	0.001353089	0.001388
Marine eutrophication	kg N eq	0.0002	8.24852E-05	0.000131
Terrestrial ecotoxicity	kg 1,4-DCB	10.087	5.427960923	4.659518
Freshwater ecotoxicity	kg 1,4-DCB	0.3003	0.186646057	0.113676
Marine ecotoxicity	kg 1,4-DCB	0.3974	0.241109474	0.156335
Human carcinogenic toxicity	kg 1,4-DCB	0.281	0.172558564	0.108455
Human non-carcinogenic toxicity	kg 1,4-DCB	4.8067	2.467593234	2.339102
Land use	m2a crop eq	0.14	0.068711602	0.071244
Mineral resource scarcity	kg Cu eq	0.0082	0.003043756	0.005131
Fossil resource scarcity	kg oil eq	2.0019	1.168175347	0.833714
Water consumption	m^3	0.0613	0.030037679	0.031283

3. Calculated data for Figure 9.

	Unit	Titanium dioxide	Water	Polyethylene glycol	Electricity
Global warming	kg CO_2 eq	3.208838	1.03E-05	0.196406	0.357376
Stratospheric ozone depletion	kg CFC11 eq	1.06E-06	3.21E-12	3.66E-08	6.41E-08
Ionizing radiation	kBq Co-60 eq	0.130263	3.77E-07	0.011412	0.005201
Ozone formation, Human health	kg NO_x eq	0.006884	2.48E-08	0.000366	0.00081
Fine particulate matter formation	kg PM2.5 eq	0.005871	1.69E-08	0.000269	0.000566
Ozone formation, Terrestrial ecosystems	kg NO_x eq	0.006952	2.55E-08	0.000388	0.000812
Terrestrial acidification	kg SO_2 eq	0.012703	3.12E-08	0.000548	0.001382
Freshwater eutrophication	kg P eq	0.001278	3.31E-09	5.69E-05	5.38E-05
Marine eutrophication	kg N eq	0.000124	4.18E-10	3.63E-06	3.36E-06
Terrestrial ecotoxicity	kg 1,4-DCB	4.024702	4.95E-05	0.358989	0.275778
Freshwater ecotoxicity	kg 1,4-DCB	0.099516	4.65E-07	0.004252	0.009907
Marine ecotoxicity	kg 1,4-DCB	0.137777	6.56E-07	0.005986	0.012572
Human carcinogenic toxicity	kg 1,4-DCB	0.093562	1.31E-06	0.005866	0.009025
Human non-carcinogenic toxicity	kg 1,4-DCB	2.119865	1.21E-05	0.126141	0.093085
Land use	m2a crop eq	0.065461	3.09E-07	0.00216	0.003622
Mineral resource scarcity	kg Cu eq	0.004574	1.94E-07	0.000403	0.000154
Fossil resource scarcity	kg oil eq	0.665465	2.21E-06	0.104903	0.063345
Water consumption	m^3	0.027915	0.000377	0.002477	0.000514

4. **Calculated data for Figure 10 A.**

	Initial	Electricity + 5%	Electricity - 5%
Global warming	10.04894689	10.3154381	9.782455672
Stratospheric ozone depletion	2.49018E-06	2.53796E-06	2.4424E-06
Ionizing radiation	0.333727564	0.337605986	0.329849141
Ozone formation, Human health	0.022265299	0.022869593	0.021661006
Fine particulate matter formation	0.019079632	0.019501988	0.018657276
Ozone formation, Terrestrial ecosystems	0.022392904	0.02299819	0.021787617
Terrestrial acidification	0.045219923	0.046250197	0.044189648
Freshwater eutrophication	0.002741233	0.00278134	0.002701125
Marine eutrophication	0.000213411	0.000215919	0.000210903
Terrestrial ecotoxicity	10.08747872	10.29312328	9.881834152
Freshwater ecotoxicity	0.30032247	0.307710277	0.292934663
Marine ecotoxicity	0.397444269	0.406818777	0.38806976
Human carcinogenic toxicity	0.281013273	0.287743143	0.274283403
Human non-carcinogenic toxicity	4.806695461	4.876107643	4.73728328
Land use	0.139955334	0.142656395	0.137254274
Mineral resource scarcity	0.008175106	0.008290254	0.008059958
Fossil resource scarcity	2.001889745	2.049125384	1.954654105
Water consumption	0.061520991	0.061904209	0.061137774

5. Calculated data for Figure 10 B.

	Initial	Synthetic Rutile + 5%	Synthetic Rutile - 5%
Global warming	10.04894689	10.23707839	9.860815388
Stratospheric ozone depletion	2.49018E-06	2.54804E-06	2.43232E-06
Ionizing radiation	0.333727564	0.341071387	0.326383741
Ozone formation, Human health	0.022265299	0.022668311	0.021862288
Fine particulate matter formation	0.019079632	0.01941494	0.018744325
Ozone formation, Terrestrial ecosystems	0.022392904	0.022800477	0.02198533
Terrestrial acidification	0.045219923	0.045951517	0.044488329
Freshwater eutrophication	0.002741233	0.00281064	0.002671826
Marine eutrophication	0.000213411	0.000219957	0.000206864
Terrestrial ecotoxicity	10.08747872	10.32045461	9.854502827
Freshwater ecotoxicity	0.30032247	0.30600629	0.294638649
Marine ecotoxicity	0.397444269	0.405261009	0.389627529
Human carcinogenic toxicity	0.281013273	0.286436008	0.275590537
Human non-carcinogenic toxicity	4.806695461	4.923650573	4.68974035
Land use	0.139955334	0.143517521	0.136393148
Mineral resource scarcity	0.008175106	0.008431673	0.007918538
Fossil resource scarcity	2.001889745	2.043575464	1.960204025
Water consumption	0.061520991	0.063085157	0.059956826

6. Calculated data for Figure 10 C.

Damage category	Unit	Stainless Steel 316	Titanium	Nickel	Molybdenum	Tantalum
Human health	DALY	2.37E-05	8.12E-05	0.000526	0.008236	0.000995
Ecosystems	species.yr	2.53E-08	1.45E-07	6.08E-07	4.70E-06	2.04E-06
Resources	USD2013	0.366226	1.45093	1.426282	20.15339	45.95617

7. **Calculated data for Figure 10 D.**

		Initial	Reusable
Human health	DALY	0.000111	0.000104
Ecosystems	species.yr	2.12E-07	2.05E-07
Recourses	USD2013	1.5	1.47

8. Calculated data for Figure 10 E.

		Initial	Argon - 50%	Smart consumption
Human health	DALY	0.000111	0.000106	0.000104
Ecosystems	species.yr	2.12E-07	2.04E-07	2.01E-07
Recourses	USD2013	1.5	1.42	1.39

9. Calculated data for Figure 11.

	Human health	Ecosystems	Resources
	DALY	species.yr	USD2013
Titanium turbine by the Kroll - EBM Process	0.000484	9.57761E-07	4.85741
Titanium turbine by the NEM Process	0.000147	2.83912E-07	1.78657

10. Calculated data for Figure 12.

Impact category	Unit	Titanium by FFC-Cambridge Process	Titanium by Kroll Process
Global warming	kg CO_2 eq	0.000249193	0.000365
Stratospheric ozone depletion	kg CFC11 eq	9.67325E-09	2.55E-08
Ionizing radiation	kBq Co-60 eq	1.14709E-08	6.4E-08
Ozone formation, Human health	kg NO_x eq	4.76384E-08	6.22E-08
Fine particulate matter formation	kg PM2.5 eq	2.68507E-05	4.34E-05
Ozone formation, Terrestrial ecosystems	kg NO_x eq	6.78941E-09	8.97E-09
Terrestrial acidification	kg SO_2 eq	2.39894E-08	2.56E-08
Freshwater eutrophication	kg P eq	4.27419E-09	1.08E-08
Marine eutrophication	kg N eq	7.96649E-13	1.89E-12
Terrestrial ecotoxicity	kg 1,4-DCB	3.64509E-10	3.87E-10
Freshwater ecotoxicity	kg 1,4-DCB	2.74434E-10	4.81E-10
Marine ecotoxicity	kg 1,4-DCB	4.16624E-07	6.97E-07
Human carcinogenic toxicity	kg 1,4-DCB	0.000151664	0.00027
Human non-carcinogenic toxicity	kg 1,4-DCB	0.000689372	0.001137
Land use	m2a crop eq	3.66029E-09	4.79E-09
Mineral resource scarcity	kg Cu eq	0.007959828	0.00782
Fossil resource scarcity	kg oil eq	0.598929728	1.592102
Water consumption	m^3	3.61356E-07	6.44E-07

11. Calculated data for Figure 13.

Impact category	Unit	Titanium turbine Kroll-EBM Process	Titanium turbine by the NEM Process
Global warming	kg CO_2 eq	0.000213747	5.93E-05
Stratospheric ozone depletion	kg CFC11 eq	2.60727E-08	7.77E-09
Ionizing radiation	kBq Co-60 eq	5.16005E-08	1.52E-08
Ozone formation, Human health	kg NO_x eq	4.67919E-07	1.29E-07
Fine particulate matter formation	kg PM2.5 eq	0.000238981	7.36E-05
Ozone formation, Terrestrial ecosystems	kg NO_x eq	6.6579E-08	1.84E-08
Terrestrial acidification	kg SO_2 eq	1.85157E-07	6.06E-08
Freshwater eutrophication	kg P eq	2.9572E-08	1.07E-08
Marine eutrophication	kg N eq	4.88704E-12	2E-12
Terrestrial ecotoxicity	kg 1,4-DCB	1.27012E-09	8.11E-10
Freshwater ecotoxicity	kg 1,4-DCB	1.49033E-09	1.33E-09
Marine ecotoxicity	kg 1,4-DCB	3.15619E-10	2.65E-10
Human carcinogenic toxicity	kg 1,4-DCB	1.8302E-05	5.96E-06
Human non-carcinogenic toxicity	kg 1,4-DCB	1.13769E-05	6.82E-06
Land use	m2a crop eq	2.20893E-08	8.19E-09
Mineral resource scarcity	kg Cu eq	0.017250917	0.013647
Fossil resource scarcity	kg oil eq	4.840159394	1.772923
Water consumption	m^3	1.32595E-06	8.43E-07