Supplementary Materials

Life cycle assessment of refractory alumina products: use of hotspot and scenario analysis as ecodesign tools

Sarah Badioli[1,2,*], Marielle Dargaud[2], Thibault Champion[2] and Angélique Léonard[1]

[1] University of Liège, Chemical Engineering research unit, 4000 Liège, Belgium
[2] Saint-Gobain Research Provence, Performance Ceramics and Refractories, 84300 Cavaillon, France
* Correspondence: : sarah.badioli@uliege.be.

Calcined alumina production

Table S1 presents the inventory of 1 ton calcined alumina (CA) production in China. The values are adapted from the primary data collected by the International Aluminium Institute in 2019 (IAI, 2022). Compared to the original inventory, the emissions to air attributed to fuel burning and electricity supply are removed in order to avoid double-counting. The choice lies in the use of ecoinvent as a commercial database, which includes the abovementioned emissions in the datasets describing energy supply.

Table S1 Life cycle inventory of calcined alumina production in China. Reference unit: 1 ton. Adapted from (IAI, 2022)

Input	**Unit**	**Value**
Bauxite	kg	2685
Caustic soda	kg	81
Calcined lime	kg	52
Water	m3	7
Heavy oil	MJ	610
Diesel oil	MJ	5
Natural gas	MJ	296
Coal	MJ	8875
Electricity	MJ	592
Factory	pcs	5E-08
Bulk bag	kg	1.3
Wooden pallet	n.	0.07
Transport (road)	tkm	22
Transport (rail)	tkm	566
Transport (sea)	tkm	4305
Output	**Unit**	**Value**
Particulates (to air)	kg	0.4
Water (to air)	m3	2.9
Water (to water)	m3	4.2
Mercury (to water)	kg	1.4E-07
Oil (to water)	kg	0.8
Suspended solids (to water)	kg	7.6E-02
Red mud	kg	1220
Inert waste	kg	17
Hazardous waste	kg	7.9

Scenario of calcined alumina production – Natural gas

Table S2 describes the impacts arising from calcined alumina production when natural gas replaces hard coal as the main energy source. Aside from the change in energy source, the inventory of CA production is described in Table S1. The results are shown as LCIA characterized impacts and the relative reduction compared to the benchmark production (using hard coal as the main energy source).

Table S2 LCIA characterized results and reduction over benchmark of CA production, Natural gas scenario. EF 3.1, reference unit 1 ton.

	Characterized results – Natural gas scenario		**Reduction over benchmark (hard coal)**
Acidification	3.9E+00	Mole of H^+ eq.	-72%
Climate Change - total	8.7E+02	kg CO_2 eq.	-50%
Ecotoxicity, freshwater - total	4.5E+03	CTUe	-33%
Eutrophication, freshwater	5.1E-01	kg P eq.	-41%
Eutrophication, marine	9.0E-01	kg N eq.	-54%
Eutrophication, terrestrial	9.9E+00	Mole of N eq.	-52%
Human toxicity, cancer - total	6.9E-06	CTUh	-2%
Human toxicity, non-cancer - total	9.5E-05	CTUh	-9%
Ionizing radiation, human health	2.5E+01	kBq U235 eq.	-14%
Land Use	3.2E+03	Pt	-34%
Ozone depletion	6.9E-05	kg CFC-11 eq.	8%
Particulate matter	5.1E-05	Disease incidences	-73%
Photochemical ozone formation, human health	3.3E+00	kg NMVOC eq.	-45%
Resource use, fossils	1.2E+04	MJ	-40%
Resource use, minerals and metals	1.7E-03	kg Sb eq.	2%
Water use	3.1E+02	m^3 world eq.	-5%

LCIA normalized and weighted results of alumina production

Table S3 LCIA normalized and weighted results of calcined (CA), tabular (TA), and white fused alumina (WFA) production. EF3.1, reference unit 1 ton.

	Normalized results (persons equivalent)			Weighted results (point)		
	CA	**TA**	**WFA**	**CA**	**TA**	**WFA**
Acidification	2.5E-01	3.0E-01	4.1E-01	1.5E-02	1.9E-02	2.6E-02
Climate Change, total	2.3E-01	2.8E-01	4.5E-01	4.9E-02	5.9E-02	9.5E-02
Ecotoxicity, freshwater, total	1.2E-01	1.4E-01	2.0E-01	2.3E-03	2.6E-03	3.9E-03
Eutrophication, freshwater	5.5E-01	6.2E-01	7.5E-01	1.5E-02	1.8E-02	2.1E-02
Eutrophication, marine	9.9E-02	1.2E-01	2.0E-01	2.9E-03	3.5E-03	5.8E-03
Eutrophication, terrestrial	1.2E-01	1.4E-01	2.3E-01	4.3E-03	5.1E-03	8.5E-03
Human toxicity, cancer, total	4.1E-01	4.4E-01	4.5E-01	8.8E-03	9.3E-03	9.7E-03
Human toxicity, non-cancer, total	8.1E-01	8.7E-01	9.6E-01	1.5E-02	1.6E-02	1.8E-02
Ionizing radiation, human health	7.0E-03	7.6E-03	2.3E-02	3.5E-04	3.8E-04	1.2E-03
Land Use	6.0E-03	6.7E-03	9.9E-03	4.7E-04	5.4E-04	7.9E-04
Ozone depletion	1.2E-03	1.3E-03	1.3E-03	7.7E-05	8.2E-05	8.5E-05
Particulate matter	3.2E-01	3.9E-01	5.3E-01	2.9E-02	3.5E-02	4.8E-02
Photochemical ozone formation, human health	1.5E-01	1.8E-01	2.8E-01	7.1E-03	8.4E-03	1.3E-02
Resource use, fossils	3.1E-01	3.8E-01	6.5E-01	2.6E-02	3.2E-02	5.4E-02
Resource use, minerals and metals	2.6E-02	2.8E-02	4.3E-02	1.9E-03	2.1E-03	3.3E-03
Water use	2.9E-02	3.1E-02	4.6E-02	2.5E-03	2.7E-03	3.9E-03

LCIA normalized and weighted results of alumina blocks production

Table S4 LCIA normalized and weighted results of fused cast high-alumina block production (benchmark). EF3.1, reference unit 1 ton

	Normalized results (persons equivalent)	Weighted results (point)
Acidification	9.8E-01	6.1E-02
Climate Change - total	1.0E+00	2.2E-01
Ecotoxicity, freshwater - total	5.3E-01	1.0E-02
Eutrophication, freshwater	1.7E+00	4.6E-02
Eutrophication, marine	4.5E-01	1.3E-02
Eutrophication, terrestrial	5.4E-01	2.0E-02
Human toxicity, cancer - total	1.0E+00	2.1E-02
Human toxicity, non-cancer - total	2.1E+00	3.9E-02
Ionising radiation, human health	5.2E-02	2.6E-03
Land Use	2.7E-02	2.2E-03
Ozone depletion	3.0E-03	1.9E-04
Particulate matter	1.3E+00	1.1E-01
Photochemical ozone formation, human health	6.8E-01	3.3E-02
Resource use, fossils	1.5E+00	1.3E-01
Resource use, mineral and metals	1.4E-01	1.0E-02
Water use	1.1E-01	9.0E-03

Identification of critical impact categories

Table S5 shows the hierarchy of the most relevant environmental categories deduced at the normalization and weighting stage for the three alumina forms and fused cast alumina blocks. The four categories showing the highest normalized impacts (top) are compared with those contributing to at least 80% of the global weighted impacts (bottom). Such a comparison is meant to highlight the influence of the LCIA method on results interpretation.

Table S5 Most relevant impact categories on normalized (top) and weighted (bottom) impacts for alumina products. EF3.1.

	CA	TA	WFA	High-alumina block
4 highest normalized impacts	Non-cancer human toxicity; Freshwater eutrophication; Cancer human toxicity; Particulate matter	Non-cancer human toxicity; Freshwater eutrophication; Cancer human toxicity; Particulate matter	Non-cancer human toxicity; Freshwater eutrophication; Fossil resource use; Particulate matter	Non-cancer human toxicity; Freshwater eutrophication; Fossil resource use; Particulate matter
80% weighted impacts	Climate change; Particulate matter; Fossil resource use; Acidification; Freshwater eutrophication; Non-cancer human toxicity	Climate change; Particulate matter; Fossil resource use; Acidification; Freshwater eutrophication; Non-cancer human toxicity	Climate change; Fossil resource use; Particulate matter; Acidification; Freshwater eutrophication; Non-cancer human toxicity	Climate change; Fossil resource use; Particulate matter; Acidification; Freshwater eutrophication; Non-cancer human toxicity

Scenario analysis of block production

Table S6 compares the environmental impacts of the six production scenarios applied to fused cast high-alumina block manufacturing. The scenarios are detailed in Table 4 in the main manuscript. Scenario 1 involves reducing virgin CA consumption by using 50% of internally recirculated scrap. Scenario 2, instead, consider using a low-impact virgin CA produced from natural gas (NG-CA) instead of coal. Scenarios 3 and 4 consider improved production efficiency by better design of blocks and lower rejection rate, respectively. Scenario 5 studies the effects of substituting the Chinese electricity grid mix with one having 87% of hydroelectricity. Lastly, scenario 6 aggregates the previous changes by considering improved production efficiency, the use of 30% of recycled scrap and 70% of natural-gas-based CA, and the consumption of hydroelectricity.

Table S6 LCIA characterized results of fused cast high-alumina block production scenarios. EF3.1, reference unit 1 ton.

	Unit	Scenario 1 (recycled)	Scenario 2 (NG-CA)	Scenario 3 (design)	Scenario 4 (rejection)	Scenario 5 (hydro)	Scenario 6 (best case)
Acidification	Mole of H^+ eq.	39.1	33.3	40.9	48.4	38.2	9.4
Climate Change, total	kg CO_2 eq.	5834	5973	5933	7007	4832	1494
Ecotoxicity, freshwater, total	CTUe	21682	25309	22751	26877	22427	9001
Eutrophication, freshwater	kg P eq.	1.7	1.9	2.0	2.4	2.1	0.7
Eutrophication, marine	kg N eq.	6.6	6.6	6.7	7.9	5.4	1.6
Eutrophication, terrestrial	Mole of N eq.	70.7	71.7	71.4	84.4	58.1	18
Human toxicity, cancer, total	CTUh	9.4E-06	1.7E-05	1.3E-05	1.5E-05	1.7E-05	7.8E-06
Human toxicity, non-cancer, total	CTUh	1.6E-04	2.5E-04	2.0E-04	2.4E-04	2.4E-04	1.1E-04
Ionizing radiation, human health	kBq U235 eq.	186.3	211.1	165.7	195.6	171.6	97.1
Land Use	Pt	15702	18695	17034.6	19913	16971	7137
Ozone depletion	kg CFC-11 eq.	8.6E-05	1.7E-04	1.2E-04	1.4E-04	1.6E-04	8.0E-05
Particulate matter	Disease incidences	5.3E-04	4.4E-04	5.6E-04	6.6E-04	5.2E-04	1.2E-04
Photochemical ozone formation, human health	kg NMVOC eq.	20.5	22	20.9	24.7	18.1	6.3
Resource use, fossils	MJ	74650	81163	74478	87949	59298	21272
Resource use, mineral and metals	kg Sb eq.	6.4E-03	8.7E-03	6.5E-03	7.7E-03	8.3E-03	4.5E-03
Water use	m^3 world eq.	849	1180	912	1083	4677	2947

Calculation of critical categories for CA production with ReCiPe 2016

The critical impact categories of CA production identified using the EF 3.1 impact assessment method are compared with those obtained through ReCiPe 2016 v1.1 Midpoint (H) to validate the robustness of the results. The comparison specifically assesses whether uncertainties in human toxicity characterization models affect the prioritization of impact categories across impact assessment methods. Characterized and normalized results are reported in Table S7, using midpoint, world, non-biogenic carbon normalization factors.

Table S7 LCIA characterized and normalized results of calcined (CA) production.
ReCiPe 2016 v1.1 Midpoint (H), reference unit 1 ton.

	Characterized results		**Normalized results (persons equivalent)**
	Unit	**Value**	
Climate change, default, excl biogenic carbon	[kg CO2 eq.]	1,8E+03	2,2E-01
Fine Particulate Matter Formation	[kg PM2.5 eq.]	3,5E+00	1,4E-01
Fossil depletion	[kg oil eq.]	4,7E+02	4,7E-01
Freshwater Consumption	[m3]	7,7E+00	2,9E-02
Freshwater ecotoxicity	[kg 1,4 DB eq.]	2,6E+01	1,0E+00
Freshwater Eutrophication	[kg P eq.]	8,8E-01	1,3E+00
Human toxicity, cancer	[kg 1,4-DB eq.]	1,8E+03	1,7E+02
Human toxicity, non-cancer	[kg 1,4-DB eq.]	3,5E+03	1,1E-01
Ionizing Radiation	[kBq Co-60 eq. to air]	2,6E+01	5,4E-02
Land use	[Annual crop eq.·y]	2,6E+01	4,2E-03
Marine ecotoxicity	[kg 1,4-DB eq.]	3,9E+01	9,0E-01
Marine Eutrophication	[kg N eq.]	3,7E-02	8,1E-03
Metal depletion	[kg Cu eq.]	1,1E+02	9,4E-04
Photochemical Ozone Formation, Ecosystems	[kg NOx eq.]	4,8E+00	2,7E-01
Photochemical Ozone Formation, Human Health	[kg NOx eq.]	4,8E+00	2,3E-01
Stratospheric Ozone Depletion	[kg CFC-11 eq.]	3,8E-04	6,3E-03
Terrestrial Acidification	[kg SO2 eq.]	9,5E+00	2,3E-01
Terrestrial ecotoxicity	[kg 1,4-DB eq.]	2,5E+03	1,7E-01

The categories with the highest normalized impacts are, in order of magnitude: cancer human toxicity, freshwater eutrophication, freshwater ecotoxicity, marine ecotoxicity, and fossil depletion.