

Supplementary information for:

Ex ante life cycle assessment of bauxite residue vitrification technology

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S1 Chemical composition of Bauxite residue (BR)

Table S1 presents the normalised chemical composition of the BR considered in this study, as reported by Hertel et al. (2016). This BR is from Aluminium of Greece (AoG), Greece, and is used as the raw material in the vitrification process.

Table S1: Normalised chemical composition of bauxite residue (according to Hertel et al. (2016))

Component	Fe ₂ O ₃	Al ₂ O ₃	CaO	SiO ₂	TiO ₂	Na ₂ O	Others
Wt%	48	19	11	10	7	4	<1

Table S2 provides the typical variation in bauxite residue chemical composition, based on data from the International Aluminium Institute (2020).

Table S2: Typical chemical composition found in bauxite residue (International Aluminium Institute, 2020)

Component	Fe ₂ O ₃	Al ₂ O ₃	CaO	SiO ₂	TiO ₂	Na ₂ O
Wt%	5-60	5-30	2-14	3-50	0.3-15	1-10

S2 Life cycle inventory

The life cycle inventory (LCI) for the unit process datasets, used for the different scales (i.e., laboratory, pilot, and industrial) and industrial upscaling approaches (i.e., process modelling, regression analysis, and proxy technology) are presented in the tables S3, S4, S6-S9.

S2.1 Laboratory scale

Table S3: LCA data for the BR vitrification at the laboratory scale

Lab Scale						
Vitrification						
Material input	Quantity	Unit	Material output	Quantity	Unit	Source
Bauxite residue	1.75	kg	VBR	1.79	kg	
Limestone	0.18	kg	CO ₂	0.18	kg	
Coke	0.04	kg	Vapour	0.13	kg	
Silica sand	0.13	kg				

Energy input	Quantity	Unit				
Mixer	1.90	kWh				(HOBART, 2024)
Dryer 1	3.40	kWh				(BINDER, 2024)
Vitrification	29	kWh				(INDUTHERM, 2024)
Dryer 2	3.40	kWh				(BINDER, 2024)
Mill	8.80	kWh				(UNION PROCESS, 2024)

S2.2 Pilot scale

Table S4: LCA data for the BR vitrification at the pilot scale

Pilot Scale						
Vitrification						
Material input	Quantity	Unit	Material output	Quantity	Unit	Source
Bauxite residue	100	kg	VBR	102.06	kg	
Limestone	10.43	kg	CO ₂	10.36	kg	
Coke	2.04	kg	Vapour	7.45	kg	
Silica sand	7.40	kg				
Energy input	Quantity	Unit				
Dryer	38.40	kWh				(DESPATCH, 2024)
Mixer	2.50	kWh				(MEKA, 2024)
Vitrification	300	kWh				(OTTOJUNKER, 2024)
Mill	65.90	kWh				(UNION PROCESS, 2024)

S2.3 Industrial scale

S2.3.1 Process modelling

Process modelling was conducted using the "Solids" thermodynamic package in Aspen Plus v.11 software to simulate BR vitrification and estimate energy data across various unit operations i.e., mixer, pelletiser, preheater, furnace, cooler, and mill. Input material flows, such as bauxite residue, limestone, pet coke, and silica sand, were modelled based on their chemical composition.

The energy demand of the pelletiser was calculated based on a normal distribution of particle size distribution, with an average particle size of 1.5 cm. For the preheating step, a counter-current heat exchanger was modelled. The furnace was represented by a stoichiometric reactor to simulate the chemical reactions, such as limestone decomposition, decarbonation (at 600 - 800 °C), and the formation of sodium aluminosilicates, melilite, and spinel (at 600 - 1050 °C). This resulted in a phase composition consisting of 65% amorphous phase, 21% hercynite-magnetite, and 9% magnetite as primary phases. Phase change due to partial melting was empirically calculated and added separately. The hot melt exiting at ~1200 °C, was cooled through a series of coolers to reduce the temperature to 50 °C, with the recovered heat integrated into the preheater. The mill was modelled based on an average particle size distribution (D50) of 10µm. The final chemical composition of VBR is presented in Table S5.

Table S5: Chemical composition of VBR

Chemical composition	Percentage (%)
FeO	34.7

Al ₂ O ₃	18.7
SiO ₂	18
CaO	17.5
Na ₂ O	7
TiO ₂	2.8
Others	1.3

Table S6: LCA data for the BR vitrification at the industrial scale presents the data inventory for the upscaling of BR vitrification to industrial scale with process modelling.

Table S6: LCA data for the BR vitrification at the industrial scale

Process modelling					
Vitrification					
Material input	Quantity	Unit	Material output	Quantity	Unit
Bauxite residue	100	tonne	VBR	125.80	tonne
Limestone	22	tonne	CO ₂	25.88	tonne
Coke	2.04	tonne	Vapour	9.18	tonne
Silica sand	15	tonne			
Bentonite (binder)	1.50	tonne			
Energy input	Quantity	Unit			
Mixer	-	kWh			
Pelletiser	587	kwh			
Preheater	1700	kWh			
Vitrification	59000	kWh			
Mill	48	kWh			

S2.3.2 Regression analysis

Existing literature and industrial data sheets for unit operations (i.e., dryer, mixer, pelletiser, furnace, cooler, and mill) were used to establish correlations between material input and energy consumption. These correlations were graphically represented, and regression analysis was applied to estimate missing energy consumption data based on material inputs. Both linear and power relationships were tested to investigate the sensitivity of how difference upscaling relationships affect energy estimates, and consequently the environmental performance. Interpolation was applied within the range of available data; extrapolation was used when estimating electricity demand for capacities beyond the reported range. Data for the furnace were primarily based on industrial induction furnaces used in ceramic vitrification, selected as a relevant proxy for the BR vitrification process.

Table S7 presents the data inventory for upscaling BR vitrification to an industrial scale with power and linear regression analysis.

Table S7: LCA data for the BR vitrification at the industrial scale

Power/Linear						
Vitrification						
Material input		Quantity	Unit	Material output	Quantity	Unit
Bauxite residue		100	tonne	VBR	125.80	tonne
Limestone		22	tonne	CO ₂	25.88	tonne
Coke		2.04	tonne	Vapour	9.18	tonne
Silica sand		15	tonne			
Bentonite (binder)		1.5	tonne			
Energy input		Quantity	Unit			
Dryer 1		186/210	kWh			
Mixer		130/132	kWh			
Pelletisation		355/363	kwh			
Vitrification		68445/71347	kWh			
Cooler		25/27	kWh			

Mill		75/82	kWh			
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S2.3.3 Proxy

Table S8 presents the data inventory for upscaling BR vitrification to an industrial scale using clinker production as a proxy technology. Two scenarios are considered: scenario 1, clinker production modelled according to Centre et al., 2013 and scenario 2, modelled based on ecoinvent v3.9.1 “clinker production - Europe without Switzerland (Ecoinvent v.3.9.1, 2007a).

Table S8: LCA data for the BR vitrification at the industrial scale

Clinker production Scenario 1/ Scenario 2					
Vitrification					
Material input	Quantity	Unit	Material output	Quantity	Unit
Bauxite residue	100	tonne	VBR	125.80	tonne
Limestone	22	tonne	CO ₂	25.88	tonne
Coke	2.04	tonne	Vapour	9.18	tonne
Silica sand	15	tonne			
Bentonite (binder)	1.5	tonne			
Energy input	Quantity	Unit			
Grinder	16688/16688	kWh			
Furnace	74215/ 115304	kWh			

Table S9 presents the data inventory for upscaling BR vitrification to an industrial scale using clinker production as a proxy technology. Two scenarios are considered: scenario 3, ceramic tile production modelled according to the European Commission. (2007) and scenario 4, modelled based on ecoinvent v.3.9.1 “ceramic tile production - RoW - ceramic tile” (Ecoinvent v.3.9.1, 2007b).

Table S9: LCA data for the BR vitrification at the industrial scale

Ceramic production Scenario 3/ Scenario 4					
Vitrification					
Material input	Quantity	Unit	Material output	Quantity	Unit
Bauxite residue	100	tonne	VBR	125.80	tonne
Limestone	22	tonne	CO ₂	25.88	tonne
Coke	2.04	tonne	Vapour	9.18	tonne
Silica sand	15	tonne			
Bentonite (binder)	1.50	tonne			
Energy input	Quantity	Unit			
Grinder	17055/16688	kWh			
Pelletiser	3904/0	kWh			
Preheater	22448/0	kWh			
Furnace	120022/ 234219	kWh			

S2.3.3.1 Proxy Selection

A thorough evaluation of technologies with similar operating conditions, such as technology type (vitrification), material properties, and firing temperature, was conducted to select appropriate proxies. The selected proxies were used as reference technologies to estimate the energy demand and associated emissions from energy production. Clinker production and ceramic vitrification were identified as suitable proxies. Relevant processing stages were identified, and energy consumption data were collected on a product basis (per kilogram of vitrified clay or clinker). This addressed the variability in energy demands across different furnaces and equipment types, each with distinct residence times.

Modelling considerations for proxy technologies i.e., clinker production and ceramic tile production are presented in Table S10-S11.

Table S10. Modelling assumptions and data sources for proxy scenarios

Scenario no	Proxy material	Data source	Assumptions or specific conditions
Scenario 1	Clinker	Best Available Techniques (BAT) reference document for the production of cement, lime and magnesium oxide	- Dry process: five-stage preheater, precalciner, grate cooler, vertical raw mill - Fuel: 100 % petroleum coke - Heat consumption: 3 300 kJ/kg clinker - Pet coke (net) calorific value (NCV): 33 500 kJ/kg fuel - Furnace operating temperature: 1450 °C
Scenario 2	Clinker	ecoinvent 3.9.1 – ‘clinker production - Europe without Switzerland’	- The dataset describes the production of Portland cement clinker in the EU without Switzerland - Furnace operating temperature: 1450 °C
Scenario 3	Ceramic tile production	Best Available Techniques (BAT) Reference document for the ceramic manufacturing industry	- Fuel composition: 98.1% natural gas, 1.1% fuel oil, 0.8% heavy fuel oil - Furnace operating temperature: 1150 °C
Scenario 4		ecoinvent 3.9.1 – ‘ceramic tile production - RoW - ceramic tile’	- Technology: The infrastructure data corresponds to large-scale production in Europe, using gas-fired kiln technology - Ceramic tiles are produced by slurry processing. - Furnace operating temperature: 1150 °C

Table S11: Unit processes and data inventory for proxy scenarios

		Thermal energy		Electricity		Reference
Scenario 1	Total energy consumption	3.3	MJ/kg clinker	96	kWh/t	Centre et al., 2013
Scenario 2	Total electricity consumption			0.058	kWh/kg clinker	Ecoinvent v.3.9.1, 2007a
	Hard coal consumption	0.0354	kg/kg clinker			
	Heavy fuel oil consumption	0.0255	kg/kg clinker			
	Light fuel oil consumption	0.000374	kg/kg clinker			
	natural gas consumption	0.000175	m ³ /kg clinker			

	Petroleum coke consumption	0.00391	kg/kg clinker			
	Diesel consumption	0.0134	MJ/kg clinker			
Scenario 3	Feed preparation, dry grinding			15.28	kWh/t	European Commission, 2007
	Shaping, pressing			27.78	kWh/t	
	Drying	0.55	GJ/t	6.94	kWh/t	
	Firing	3.35	GJ/t	23.61	kWh/t	
Scenario 4	Total energy consumption	5.5765	MJ/kg	0.313	kWh/kg	Ecoinvent v.3.9.1, 2007b

S2.4 Raw materials

Life cycle inventory (LCI) data for the raw materials are shown here. The LCI data for limestone, coke, and silica sand were sourced from the ecoinvent v3.9.1 database, using the following datasets: 'limestone, crushed, for mill – RoW,' 'petroleum coke production, petroleum refinery operation – Europe without Switzerland,' and 'silica sand production – RoW.'

S2.4.1 Limestone

Table S12: LCI data for the transport of limestone

Limestone		
Name	Value	Unit
Economic inflow		
Limestone, crushed, for mill	1	kg
Transport, freight, lorry 16 -32 metric t, EURO6	0.05	t km
Economic outflow		
Limestone, crushed, for mill	1	kg
Environmental resources		
Environmental emissions		

Included activities start: This activity starts with the reception of raw materials (i.e., crushed limestone).

Included activities end: This activity ends with the crushed limestone transported in the cement facility. Packaging is not included, and no production waste is assumed.

S2.4.2 Petroleum coke

Table S13: LCI data for the transport of petroleum coke

Petroleum coke		
Name	Value	Unit
Economic inflow		
Petroleum coke	1	kg
Transport, freight, lorry 16 -32 metric t, EURO6	0.05	t km
Economic outflow		
Petroleum coke	1	kg
Environmental resources		
Environmental emissions		

Included activities start: This activity starts with the reception of raw materials (i.e., petroleum coke).

Included activities end: This activity ends with the petroleum coke transported in the cement facility. Packaging is not included, and no production waste is assumed.

S2.4.3 Silica sand

Table S14: LCI data for the transport of silica sand

Silica sand		
Name	Value	Unit
Economic inflow		
Silica sand	1	kg
Transport, freight, lorry 16 -32 metric t, EURO6	0.05	t km
Economic outflow		
Silica sand	1	kg
Environmental resources		
Environmental emissions		

Included activities start: This activity starts with the reception of raw materials (i.e., silica sand).

Included activities end: This activity ends with the silica sand transported in the cement facility. Packaging is not included, and no production waste is assumed.

While the raw materials used in this study (e.g., limestone, petroleum coke, and silica sand) were selected to yield a VBR with a desired chemical composition, quality, and reactivity, this work remains a case study of a potential processing pathway rather than a definitive route. The primary focus of this work is on technological upscaling and its influence on environmental performance, rather than on the optimisation of raw material selection or process conditions for technical performance of the specific processing route used here (vitrification using an induction furnace).

The selected raw mix formulation used in this case study demonstrated the feasibility of producing a glassy SCM with high Fe content, thereby demonstrating that viable SCMs can be produced beyond the typical Ca-, Al-, and Si-rich chemical systems. However, future implementations may involve different raw materials. For example, basic oxygen furnace (BOF) slags could serve as alternative Ca, Fe, and Si sources. The use of such materials introduces additional considerations, including their potential to reduce CO₂ emissions associated with limestone calcination and coke combustion, used as raw materials here, as well as potential variations in the overall heat balance of the process. Depending on the composition of the metallurgical slag and the presence of metallic Fe or Fe(II) contained within the material, both the thermal profile and the final properties of the vitrified product can vary. Ongoing research is therefore exploring these alternative feedstocks with the aim of further reducing environmental burdens while maintaining the performance of the SCM.

S2.4.4 Ground granulated blast-furnace slag (GGBFS)

Table S15: LCI data for ground granulated blast furnace slag production and preparation.

Ground Granulated Blast-furnace Slag		
Name	Value	Unit
Economic inflow		
Ground Granulated Blast-furnace Slag	1	kg
Electricity, medium voltage	0.095	kWh
Transport, freight, lorry 16 -32 metric t, EURO6	0.05	t km
Economic outflow		
Ground Granulated Blast-furnace Slag (treated)	1	kg
Environmental resources		
Environmental emissions		
(Petek Gursel et al., 2014)		

Included activities start: This activity starts with the reception of raw materials (i.e., by-product of iron and steelmaking in a blast-furnace).

Included activities end: This activity ends with the ground granulated blast-furnace slag treated in the cement facility. Packaging is not included, and no production waste is assumed.

S2.4.4.1 Allocation of GGBFS

Ground granulated blast furnace slag (GGBFS) was modelled using the cut-off approach. Although GGBFS meets all the conditions set by the European Union Directive (European Union, 2008) to be classified as an industrial by-product rather than a waste the cut-off allocation approach was used to assure a fair comparison between GGBFS and BR (which is currently classified as waste). The inventory for GGBFS production includes the (i) quenching/granulation, (ii) dewatering/ drying, (iii) crushing, and (iv) grinding of molten blast furnace slag. Treating GGBFS as a by-product by applying economic allocation to it while treating BR as a waste would create inconsistencies in the comparison. We recommend that if/once vitrified bauxite residue achieves industrial scale production, economic allocation of GGBFS and BR should be applied to a more appropriately evaluate the environmental performance of these SCMs.

In this study, we modelled the vitrification process to yield VBR with similar quality and reactivity to GGBFS, and this assumption is consistently applied across all scales (laboratory, pilot, and industrial).

S3 Background electricity scenarios (according to SSPs)

The electricity mix used as the primary energy source for the vitrification technology was modelled using base-load electricity supplied from the European grid (modelled as containing electricity from Denmark (14.7%), France (14.7%), Great Britain (9.0%), and Italy (8.7%) in 2020. Table S16 provides the country-specific electricity mixes.

The electricity mix in 2020 (Table S16) and its corresponding carbon intensity evolution under different SSPs scenarios from 2020 to 2050 are detailed in Table S17.

Table S16: Electricity mix of main location-specific electricity sources in 2020

	Country			
Electricity flow	Denmark (14.7%)	France (14.7%)	Great Britain (9.0%)	Italy (8.7%)
Electricity production, lignite	19.5%	-	-	-
Electricity production, wind	21.6%	5.9%	18.0%	4.6%
Electricity production, nuclear	10.8%	71.3%	19.5%	-
Electricity production, hard coal	8.2%	-	2.4%	6.4%
Electricity production, hydro	6.9%	10.6%	-	16.3%
Electricity production, natural gas	6.0%	3.5%	39.5	42.6%

Table S17: Carbon intensity of background electricity generation scenarios (SSP2 baseline, SSP2 RCP 2.6, and SSP2 RCP 1.9) from 2020 to 2050

	2020	2050		
		SSP2 Baseline	SSP2 RCP 2.6	SSP2 RCP 1.9
Carbon intensity of electricity production kg CO ₂ /kWh	0.41	0.6	0.26	0.22

S4 Limitations in upscaling methodology

Limitations in upscaling emerging technologies depend on the upscaling approach (process modelling, regression analysis, and proxy technology).

Using Aspen Plus presents challenges due to the lack of components (waste flows, emerging materials) such as bauxite residue in its database, leading to missing thermodynamic properties (e.g., heat capacities). Hence, average data from existing literature must be used. In process simulation, bauxite residue was modelled based on its oxide composition, according to Hertel et al. (2016). This shows the need for further development of representative datasets to enhance the accuracy and comprehensiveness of emerging technology simulations. Similar constraints have been reported in prior ex-ante studies, such as Cuéllar-Franca et al. (2016). Another limitation of Aspen Plus is the inability to capture phase transitions and the enthalpy changes during the conversion of a solid to a partially melted slag (as in VBR). Hence, thermodynamic calculations were used to estimate the heat transfer required during phase changes and phase formation (Giels, 2023).

Limitations in proxy technologies involve adapting established processes to novel applications, assuming analogous performance based on existing data (e.g., efficiencies, yields, and material flows) (Buyle et al., 2019). Proxy technologies may not capture process synergies, such as heat integration and recovery or carbon capture and storage techniques, designed to minimise energy demands and associated process emissions.

Regression analysis has limitations in capturing non-linear relationships between uncertain process parameters such as efficiencies and yields (Buyle et al., 2019). These parameters are linked not only to scale but also to technical performance. Additional limitations include the inability to consider process dynamics, thermodynamic changes, and process synergies.

S5 Furnace technology

S5.1 Semi-quantitative discussion on furnace technology selection

Selecting suitable industrial equipment is crucial for process system productivity, efficiency, and safety (Paramasivam et al., 2011). The equipment selection process aims to achieve desired quality levels, cost-effectiveness, and reliability ensuring sustainable industrial operations. In furnace selection, close collaboration with industrial experts and technology developers is essential. In the present study, we employed a generic electric-powered furnace model for BR vitrification. Possible electric-powered furnace examples include induction furnaces, electric arc furnaces, microwaving and submerged arc furnaces.

Despite being electric-powered, electric arc and submerged arc furnaces, both alter the chemistry and mineralogy of the final VBR. These furnaces increase the reduction of Fe^{3+} , resulting in the co-production of metallic iron and an Fe-depleted VBR. While the reactivity of the Fe-depleted VBR is acceptable, its composition differs from the VBR studied here, hence these furnace types are not considered further in this study. Induction furnaces, however, produce a single product; a VBR with the desired FeO content, consistent with the composition used in this work. This composition has been validated through lab and pilot-scale testing using an induction furnace within the scope of the project (ReActiv). Therefore, selecting the appropriate furnace requires a thorough assessment of factors such as product (VBR) quality, properties (i.e., reactivity) and processing parameters (cost, and efficiency) for each furnace type.

A rotary kiln furnace is another viable option that can ensure the desired Fe content. However, as a fuel-powered technology, its environmental performance particularly the climate change impact, depends on the fuel mix composition. While we did not directly model a rotary kiln scenario in the industrial-scale case for VBR, the influence of furnace type and energy source is implicitly captured through the modelling of the proxy scenarios. In particular, the clinker proxy technology was modelled using a rotary kiln system, with the energy consumption being 3.3 and 2.33 MJ/kg of clinker, in Table S10, where both scenarios 1 and 2 correspond to clinker production. As discussed in Section 3.2, the decarbonisation of the electricity grid plays a critical role in the environmental performance of the vitrification process.

In this study, the future decarbonisation scenarios were applied only to the electricity-based industrial model developed through process modelling. This focus was selected because electrified systems are directly impacted by projected changes in the electricity grid, which is expected to decarbonise significantly under SSP2-based pathways. In contrast, fuel-based systems such as rotary kilns, would require a different decarbonisation strategy involving changes in the fuel mix such as increased use of alternative fuels like biomass, waste-derived fuels, or hydrogen. In the cement industry, the use of alternative materials varies regionally, with a global average

replacement of ~6%. Common waste-derived fuels include tyres, oils, plastics, and textiles, while increasing demand for biomass, such as waste wood and sawdust, plays a significant role in reducing CO₂ emissions. While such transitions are possible and already employed in the cement industry, modelling future fuel mix shifts was outside the scope of this study. We acknowledge that a full comparison between electricity- and fuel-based kiln technologies, under different decarbonisation pathways, is an important area for future research.

Plasma technology is a promising alternative, generating a hot beam of ionised plasma that reaches temperatures from 1500°C to over 7000°C. However, plasma technology has not yet been implemented in industrial-scale cement manufacturing, with only a few conceptual applications and methods explored, including ongoing projects on plasma-heated cement kilns (Schneider et al., 2023; ELECTRA, 2025)

Selecting an appropriate furnace technology also involves evaluating scalability and practicality. The rotary kiln furnace is well-established in various industries, particularly in cement production and may appear more suitable compared to the induction furnace in certain applications.

The thermal efficiency and scalability of industrial, electric-powered furnaces vary by type, leading to differences in energy demands. Microwaving shows an efficiency range of 55% to 70% with some cases reaching up to 82% (Priecel and Lopez-Sanchez, 2019). Electric arc furnaces achieve efficiency rates between 36% and 93% (Pfeifer et al., 2005; Kirschen et al., 2009). Induction furnaces typically operate at 20% to 50% efficiency but can attain 75% with best operating practices (IPPC Bureau et al., 2022). Shaft furnaces, used in glass, ceramic, automotive and aviation industries, exhibit efficiency rates of 40% to 50% for non-ferrous applications, while reverberatory furnaces range from 15% to 40% (Cusano et al., 2017). These wide efficiency ranges highlight the critical importance of considering energy efficiency factors when selecting kiln types.

S6 Results

S6.1 Effect of technology scale

Table S18 presents the effects of upscaling from the laboratory to pilot and industrial scale. The industrial scale results represent the average values based on the seven upscaling scenarios explored.

Table S18: ReCiPe 2016 midpoint impact results of laboratory, pilot and industrial (mean) scale vitrification technology

Impact categories	Units	Laboratory	Pilot	Industrial (mean)
Terrestrial acidification potential (TAP)	kg SO ₂ -eq.	0.035	0.005	0.001
Global warming potential (GWP100) ^a	kg CO ₂ -eq.	10.092	1.688	0.559
Freshwater ecotoxicity potential (FETP)	kg 1,4-D, C, B-eq.	1.095	0.060	0.007
Marine ecotoxicity potential (METP)	kg 1,4-D, C, B-eq.	1.389	0.079	0.010
Terrestrial ecotoxicity potential (TETP)	kg 1,4-D, C, B-eq.	52.696	2.361	0.414
Fossil fuel potential (FFP)	kg oil-eq.	2.436	0.418	0.103
Freshwater eutrophication potential (FEP)	kg P-eq.	8.22×10^{-3}	1.29×10^{-3}	1.59×10^{-4}
Marine eutrophication potential (MEP)	kg N-eq.	6.08×10^{-4}	9.96×10^{-5}	1.24×10^{-5}
Human toxicity potential (HTPc)	kg 1,4-D, C, B-eq.	0.632	0.101	0.014
Human toxicity potential (HTPnc)	kg 1,4-D, C, B-eq.	16.722	1.747	0.236
Ionising radiation potential (IRP)	kg Co-60-eq.	5.096	0.843	0.071

Agricultural land occupation (LOP)	m ² a crop-eq.	0.285	0.043	0.005
Material resources: metals/minerals surplus ore potential (SOP)	kg Cu-eq.	0.079	0.010	0.002
Ozone depletion potential (ODPinfinite) ^b	kg CFC-11-eq.	4.08×10^{-6}	6.60×10^{-7}	8.00×10^{-8}
Particulate matter formation potential (PMFP) ^c	kg PM2.5-eq.	0.014	0.002	4.13×10^{-4}
Photochemical oxidant formation potential: humans (HOFp)	kg NO _x -eq.	0.016	0.003	5.94×10^{-4}
Photochemical oxidant formation potential: ecosystems (EOFp)	kg NO _x -eq.	0.017	0.003	6.31×10^{-4}
Water consumption potential (WCP)	m ³	0.153	0.018	0.002

^a Reported using global warming potential over a 100-year horizon (GWP100).

^b Measured in kg CFC-11-eq.; Chlorofluorocarbons (CFCs)

^c Measured in kg PM2.5-eq.; Particulate matter (PM).

S6.1.1 Contribution analysis

At the laboratory and pilot scales, milling and drying contribute significantly to the total climate change impact due to more process inefficiency at smaller scale (Figure S1). For example, at the laboratory scale, milling and drying processes together accounted for 34% of the climate change impact (19.5% and 14.5%, respectively). In contrast, at the industrial scale, process optimisations result in these contributions falling to less than 4% of the total impact, with the primary contribution arising from preheating (12%) and vitrification (84%).

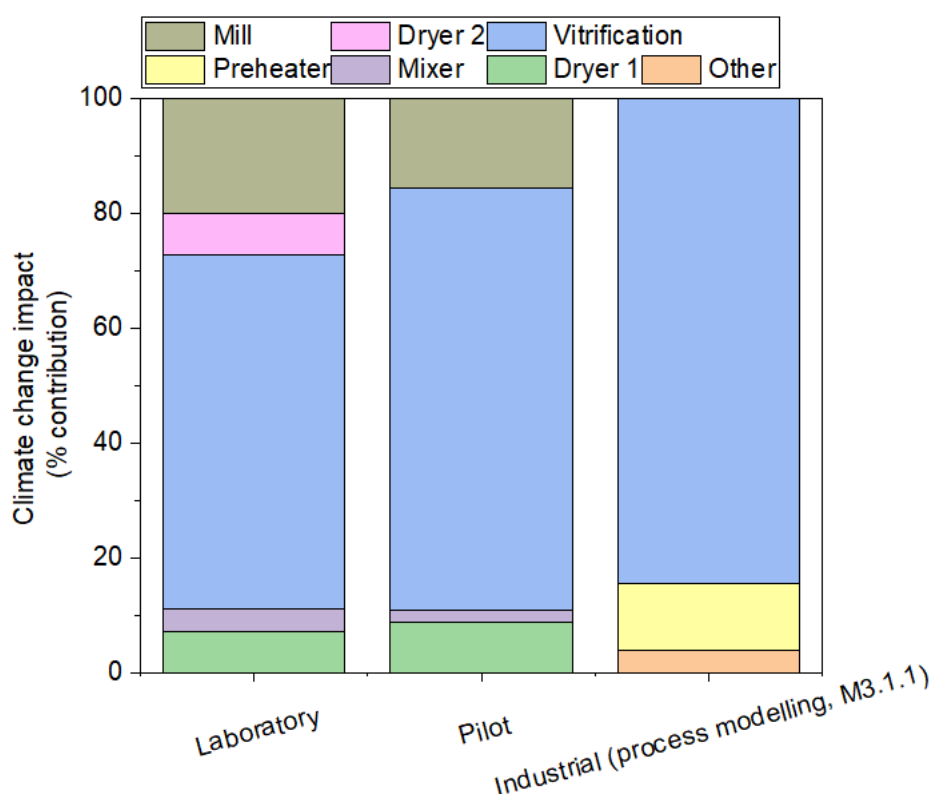


Figure S1: Contribution analysis of climate change impacts (% contribution) for laboratory, pilot, and industrial (obtained via process modelling) scale production of vitrified bauxite residue

S6.2 Effect of upscaling approach

Table S19 presents the impacts of industrial upscaling scenarios, which include; process simulation (M3.1.1), linear regression (M3.2.1), power regression (M3.2.2), clinker production modelled based on Centre et al. (2013), (M3.3.1), clinker production modelled based on Ecoinvent v.3.9.1. (2007a), (M3.3.2), ceramic vitrification modelled based on European Commission. 2007 M3.3.1), ceramic vitrification modelled based on Ecoinvent v.3.9.1. (2007b), (M3.3.2).

Table S19: ReCiPe 2016 midpoint impact results of individual upscaling scenarios for industrial scale vitrification technology

Impact categories	Units	M3.1.1	M3.2.1	M3.2.2	M3.3.1	M3.3.2	M3.3.3	M3.3.4
Terrestrial acidification potential (TAP)	kg SO ₂ -eq.	8.20 × 10 ⁻⁴	7.50 × 10 ⁻⁴	7.80 × 10 ⁻⁴	1.38 × 10 ⁻³	2.79 × 10 ⁻³	3.30 × 10 ⁻³	6.60 × 10 ⁻⁴
Global warming potential (GWP100) ^a	kg CO ₂ -eq.	0.472	0.448	0.458	0.480	0.709	0.563	0.785
Freshwater ecotoxicity potential (FETP)	kg 1,4-D, C, B-eq.	0.009	0.008	0.009	0.005	0.010	0.003	0.007
Marine ecotoxicity potential (METP)	kg 1,4-D, C, B-eq.	0.012	0.011	0.012	0.006	0.014	0.004	0.010
Terrestrial ecotoxicity potential (TETP)	kg 1,4-D, C, B-eq.	0.403	0.370	0.383	0.620	0.442	0.286	0.393
Fossil fuel potential (FFP)	kg oil-eq.	0.076	0.070	0.073	0.073	0.110	0.125	0.192
Freshwater eutrophication potential (FEP)	kg P-eq.	2.00 × 10 ⁻⁴	1.80 × 10 ⁻⁴	1.90 × 10 ⁻⁴	1.00 × 10 ⁻³	2.70 × 10 ⁻³	5.00 × 10 ⁻⁴	1.30 × 10 ⁻⁴
Marine eutrophication potential (MEP)	kg N-eq.	1.61 × 10 ⁻⁵	1.46 × 10 ⁻⁵	1.52 × 10 ⁻⁵	8.97 × 10 ⁻⁶	1.76 × 10 ⁻⁵	3.97 × 10 ⁻⁶	1.01 × 10 ⁻⁵
Human toxicity potential (HTPc)	kg 1,4-D, C, B-eq.	0.015	0.014	0.014	0.009	0.021	0.008	0.015
Human toxicity potential (HTPnc)	kg 1,4-D, C, B-eq.	0.273	0.247	0.258	0.172	0.427	0.084	0.195
Ionising radiation potential (IRP)	kg Co-60-eq.	0.129	0.117	0.122	0.015	0.027	0.016	0.069
Agricultural land occupation (LOP)	m ² a crop-eq.	0.007	0.007	0.007	0.003	0.005	0.002	0.005
Material resources: metals/minerals surplus ore potential (SOP)	kg Cu-eq.	0.002	0.002	0.002	0.001	0.001	0.002	0.004
Ozone depletion potential (ODPinfinite) ^b	kg CFC-11-eq.	1.06 × 10 ⁻⁷	9.61 × 10 ⁻⁸	1.00 × 10 ⁻⁷	5.00 × 10 ⁻⁸	9.14 × 10 ⁻⁸	4.44 × 10 ⁻⁸	9.53 × 10 ⁻⁸
Particulate matter formation potential (PMFP) ^c	kg PM2.5-eq.	3.30 × 10 ⁻⁴	3.00 × 10 ⁻⁴	3.10 × 10 ⁻⁴	5.10 × 10 ⁻⁴	9.80 × 10 ⁻⁴	1.70 × 10 ⁻⁴	3.00 × 10 ⁻⁴
Photochemical oxidant formation potential: humans (HOFp)	kg NO _x -eq.	4.60 × 10 ⁻⁴	4.20 × 10 ⁻⁴	4.40 × 10 ⁻⁴	6.00 × 10 ⁻⁴	1.00 × 10 ⁻³	3.90 × 10 ⁻⁴	6.40 × 10 ⁻⁴
Photochemical oxidant formation	kg NO _x -eq.	4.80 × 10 ⁻⁴	4.40 × 10 ⁻⁴	4.60 × 10 ⁻⁴	6.40 × 10 ⁻⁴	1.00 × 10 ⁻³	4.40 × 10 ⁻⁴	7.10 × 10 ⁻⁴

potential: ecosystems (EOFP)								
Water consumption potential (WCP)	m ³	0.003	0.002	0.003	0.001	8.60 × 10 ⁻⁴	6.60 × 10 ⁻⁴	0.002

^a Reported using global warming potential over a 100-year horizon (GWP100).

^b Measured in kg CFC-11-eq.; Chlorofluorocarbons (CFCs)

^c Measured in kg PM2.5-eq.; Particulate matter (PM).

Table S20 provides the mean, standard deviation, and coefficient of variation (CV %) for each environmental impact category across the seven upscaling approaches. CV is used in Section 3.2 to identify impact categories more sensitive to the choice of upscaling approach.

Table S20: Mean, standard deviation, and coefficient of variation (CV %) for each environmental impact category across the seven upscaling approaches.

Impact categories	Mean	Standard deviation	Coefficient of variance (CV, %)
Terrestrial acidification potential (TAP)	1.07×10^{-3}	8.16×10^{-4}	76
Global warming potential (GWP100) ^a	0.559	0.135	24
Freshwater ecotoxicity potential (FETP)	7.36×10^{-3}	2.56×10^{-3}	35
Marine ecotoxicity potential (METP)	9.93×10^{-3}	3.37×10^{-3}	34
Terrestrial ecotoxicity potential (TETP)	0.414	0.102	25
Fossil fuel potential (FFP)	0.103	0.045	44
Freshwater eutrophication potential (FEP)	1.59×10^{-4}	7.26×10^{-5}	46
Marine eutrophication potential (MEP)	1.24×10^{-5}	4.85×10^{-6}	39
Human toxicity potential (HTPc)	0.014	4.38×10^{-3}	32
Human toxicity potential (HTPnc)	0.236	0.106	45
Ionising radiation potential (IRP)	0.071	0.052	74
Agricultural land occupation (LOP)	4.97×10^{-3}	2.17×10^{-3}	44
Material resources: metals/minerals: surplus ore potential (SOP)	1.92×10^{-3}	8.61×10^{-4}	45
Ozone depletion potential (ODPinfinite) ^b	8.33×10^{-8}	2.51×10^{-8}	30
Particulate matter formation potential (PMFP) ^c	4.13×10^{-4}	2.69×10^{-4}	65
Photochemical oxidant formation potential: humans (HOFP)	5.94×10^{-4}	2.92×10^{-4}	49
Photochemical oxidant formation potential: ecosystems (EOFP)	6.31×10^{-4}	2.93×10^{-4}	47
Water consumption potential (WCP)	1.67×10^{-3}	9.56×10^{-4}	57

Table S21 reports the process contributions in each upscaling scenario, including process simulation, regression analysis, and proxy technology.

Table S21: Process contributions in terms of kg CO₂-eq. emissions of VBR processed at industrial scale according to upscaling scenarios; process simulation, regression analysis, and proxy technology. “Other” represents the impact of upstream background activities such as hard coal preparation, and petroleum/natural gas production.

Climate change (kg CO ₂ -eq. emissions)	M3.1.1	M3.2.1	M3.2.2	M3.3.1	M3.3.2	M3.3.3	M3.3.4
Other	0.05	0.05	0.05	0.07	0.07	0.10	0.13
Furnace (electricity consumption)	0.21	0.19	0.20	0.03	0.05	0.03	0.12
Furnace (heat consumption, natural gas)						0.23	0.33
Furnace (heat consumption, other than natural gas)				0.18	0.38		
Furnace (direct process emissions)	0.21	0.21	0.21	0.21	0.21	0.21	0.21

S6.3 Prospective evaluation of future decarbonisation potential in the entire value chain of VBR for cementitious applications

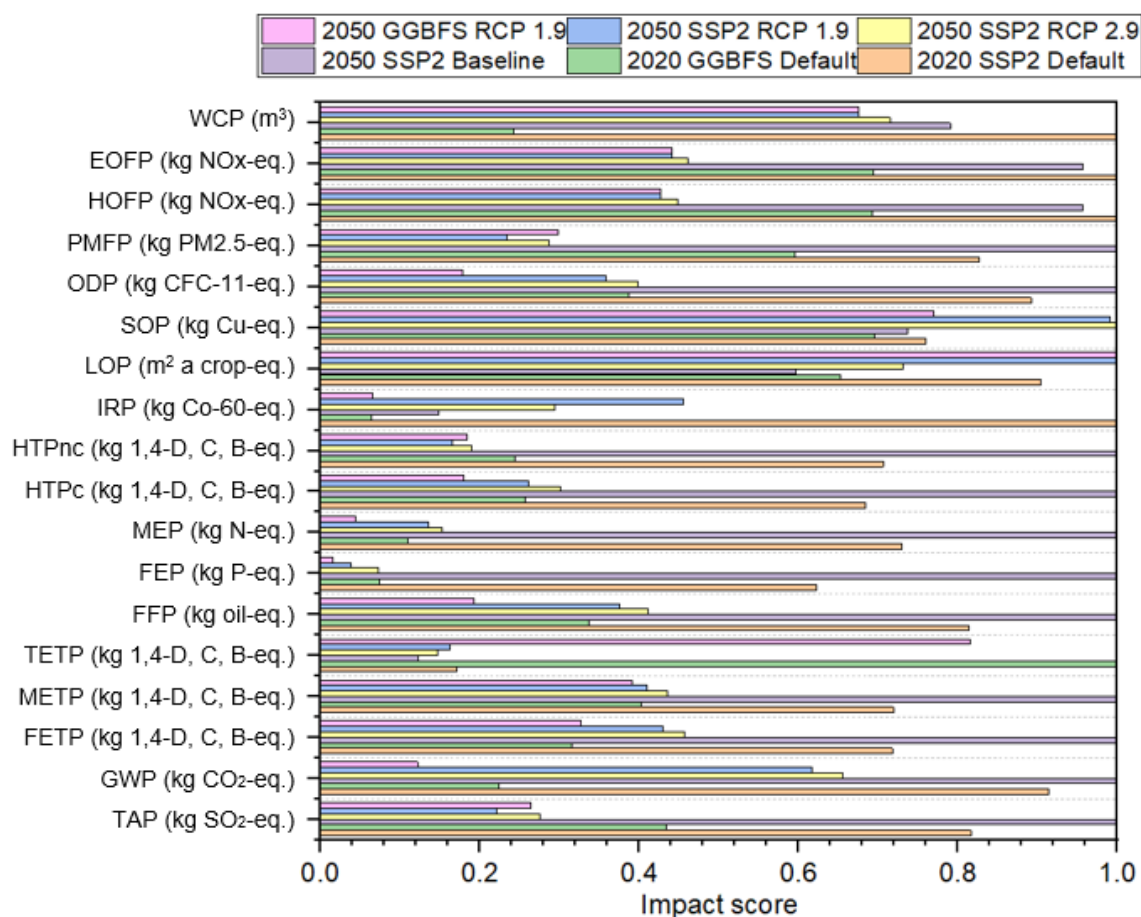
Table S22 and Figure 2 present the normalised environmental impact values for VBR production across different upscaling scenarios, adapted from Table 3 in the main manuscript. The comparison includes different timeframes (2020 vs. 2050) and background electricity scenarios based on Shared Socioeconomic Pathways (SSP2). The scenarios include SSP2 Default (2020), SSP2 Baseline (2050), and future projections under different climate policies: SSP2 RCP 2.9 and SSP2 RCP 1.9 (2050).

Table S22: Normalised environmental impact comparison across scenarios for VBR production and GGBFS. The impact scores are normalised to the highest value within each category to facilitate comparison. The scenarios represent different timeframes (2020 vs. 2050) and background electricity assumptions (SSP2 Default, SSP2 Baseline, SSP2 RCP 2.9, SSP2 RCP 1.9) for both VBR and GGBFS.

		2020		2050			2050 GGBFS
Impact categories	Units	SSP2 default	GGBFS default	SSP2 baseline	SSP2 RCP 2.9	SSP2 RCP 1.9	SSP2 RCP 1.9
Terrestrial acidification potential (TAP)	kg SO ₂ -eq.	0.82	0.43	1.00	0.28	0.22	0.26
Global warming potential (GWP100) ^d	kg CO ₂ -eq.	0.91	0.22	1.00	0.66	0.62	0.12
Freshwater ecotoxicity potential (FETP)	kg 1,4-D, C, B-eq.	0.72	0.32	1.00	0.46	0.43	0.33
Marine ecotoxicity potential (METP)	kg 1,4-D, C, B-eq.	0.72	0.40	1.00	0.43	0.41	0.39
Terrestrial ecotoxicity potential (TETP)	kg 1,4-D, C, B-eq.	0.17	1.00	0.12	0.15	0.16	0.82
Fossil fuel potential (FFP)	kg oil-eq.	0.81	0.34	1.00	0.41	0.38	0.19
Freshwater eutrophication potential (FEP)	kg P-eq.	0.62	0.07	1.00	0.07	0.04	0.02
Marine eutrophication potential (MEP)	kg N-eq.	0.73	0.11	1.00	0.15	0.14	0.04
Human toxicity potential (HTPc)	kg 1,4-D, C, B-eq.	0.68	0.26	1.00	0.30	0.26	0.18
Human toxicity potential (HTPnc)	kg 1,4-D, C, B-eq.	0.71	0.24	1.00	0.19	0.17	0.18
Ionising radiation potential (IRP)	kg Co-60-eq.	1.00	0.06	0.15	0.29	0.46	0.07
Agricultural land occupation (LOP)	m ² a crop-eq.	0.90	0.65	0.60	0.73	1.00	1.00
Material resources: metals/minerals surplus ore potential (SOP)	kg Cu-eq.	0.76	0.70	0.74	1.00	0.99	0.77

Ozone depletion potential (ODP _{infinite}) ^e	kg CFC-11-eq.	0.89	0.39	1.00	0.40	0.36	0.18
Particulate matter formation potential (PMFP) ^f	kg PM2.5-eq.	0.83	0.59	1.00	0.29	0.23	0.30
Photochemical oxidant formation potential: humans (HOFP)	kg NO _x -eq.	1.00	0.69	0.96	0.45	0.43	0.43
Photochemical oxidant formation potential: ecosystems (EOFP)	kg NO _x -eq.	1.00	0.69	0.96	0.46	0.44	0.44
Water consumption potential (WCP)	m ³	1.00	0.24	0.79	0.71	0.68	0.68

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Figure 2: Normalised environmental impact comparison across scenarios for VBR production and GGBFS. The impact scores are normalised to the highest value within each category to facilitate comparison. The scenarios represent different timeframes (2020 vs. 2050) and background electricity assumptions (SSP2 Default, SSP2 Baseline, SSP2 RCP 2.9, SSP2 RCP 1.9) for both VBR and GGBFS.

Table S23 provides the mean, standard deviation, and coefficient of variation (CV %) for each environmental impact category across the three future electricity scenarios in 2050 (i.e., SSP2 RCP1.9, SSP2 RCP2.6, and SSP2 Baseline).

Table S23: Mean, standard deviation, and coefficient of variation (CV %) for each environmental impact category across the three future electricity scenarios in 2050 (i.e., SSP2 RCP1.9, SSP2 RCP2.6, and SSP2 Baseline).

Impact categories	Mean	Standard deviation	Coefficient of variance (CV, %)
Terrestrial acidification potential (TAP)	5.91×10^{-4}	6.80×10^{-4}	87
Global warming potential (GWP100) ^a	0.122	0.44	28
Freshwater ecotoxicity potential (FETP)	5.02×10^{-3}	9.81×10^{-3}	51
Marine ecotoxicity potential (METP)	7.01×10^{-3}	0.013	54
Terrestrial ecotoxicity potential (TETP)	0.079	0.57	14
Fossil fuel potential (FFP)	0.038	0.065	59
Freshwater eutrophication potential (FEP)	2.42×10^{-4}	1.64×10^{-4}	147
Marine eutrophication potential (MEP)	1.43×10^{-5}	1.24×10^{-5}	115
Human toxicity potential (HTPc)	0.012	0.015	80
Human toxicity potential (HTPnc)	0.248	0.235	105
Ionising radiation potential (IRP)	0.018	0.035	51
Agricultural land occupation (LOP)	1.07×10^{-3}	4.03×10^{-3}	27
Material resources: metals/minerals: surplus ore potential (SOP)	3.24×10^{-4}	1.97×10^{-3}	16
Ozone depletion potential (ODPinfinite) ^b	3.26×10^{-8}	5.32×10^{-8}	61
Particulate matter formation potential (PMFP) ^c	1.85×10^{-4}	2.19×10^{-4}	84
Photochemical oxidant formation potential: humans (HOFP)	1.55×10^{-4}	3.15×10^{-4}	49
Photochemical oxidant formation potential: ecosystems (EOFP)	1.56×10^{-4}	3.32×10^{-4}	47
Water consumption potential (WCP)	1.63×10^{-4}	2.01×10^{-3}	8

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