

SUPPLEMENTARY MATERIAL

Title: Life cycle assessment of ternary cement production based on calcined clay and marble residue

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11 Pages, 5 Tables, 2 Equations and 1 Figure

S1 INVENTORY OF THE PROCESSES

Table S.1 Inventory of the processes used in the evaluated scenarios and additional information.

Main Process	Flow type	Flow	Quant.	Unit	Source
OPC, LC ³ and LC ³ -R	Inputs	Clinker	Variable	t	[35]; [10]
		Gypsum	5.00E-02	t	
		Materials	Calcined clay	3.00E-01	Except for OPC
			Limestone filler	1.50E-01	Only for LC ³ [10]
			Marble residue	1.50E-01	Only for LC ³ -R
	Electricity	Cement grinding (electricity, medium voltage)	4.97E+01	kWh	[31] [Total 113 kWh/t]
		Packing and loading (electricity, medium voltage)	3.39E+00	kWh	
	Processing	Packing, cement	1.00E+00	t	Ecoinvent 3.6 [43]
	Outputs	Transport to the landfill	7.50E+01	t*km	Except for LC ³ -R
		Waste management	Marble residue in an inert landfill	1.50E-01	Except for LC ³ -R
Clinker	Inputs	Emissions	Particulates, <10,0 um	9.00E-05	[33]
			Limestone, crushed, for mill	1.42E+00	Ecoinvet v3.6 [40]
			Clay	1.20E-01	
		Electricity	Iron ore, crude ore, 46% Fe	6.07E-03	
			Sand	8.34E-03	
			Water, unspecified natural origin	2.43E-01	
			Water, harvested from rainwater	5.38E-03	
			Petroleum coke	6.90E-02	
			Charcoal	4.00E-03	
			Hard coal	4.40E-03	
		Thermal energy	Bundle, energy wood	5.00E-03	Estimate based on [32] [3,605 GJ/t-clinker]
			Heavy fuel oil	3.00E-04	
			Natural gas, low pressure	9.00E-05	
			Diesel	8.70E-04	
			Raw material grinding (electricity, medium voltage)	2.71E+01	
		Electricity	Fuel grinding (electricity, medium voltage)	4.52E+00	[31] [Total 113 kWh/t]

Clinker	Outputs	Emissions	Kiln operation (electricity, medium voltage)	2.94E+01	kWh	Ecoinvet v3.6 [40]
			Carbon dioxide	8.63E-01	t	
			Carbon monoxide, fossil	7.66E-04	t	
			Nitrogen oxides	2.27E-03	t	
			Sulfur oxides	9.16E-04	t	
			Particulate Matter, < 2.5 um	8.22E-05	t	
			Particulate Matter, > 2.5 um and < 10um	2.70E-05	t	
			Particulate Matter, > 10 um	1.93E-05	t	
			Water, Emission to air	2.49E-01	t	
			Wastewater, average	1.92E-03	m ³	
			Water, Emission to air	2.49E-04	t	
			Antimony ion	8.48E-09	t	
			Arsenic ion	8.93E-09	t	
			Beryllium II	8.27E-09	t	
			Cadmium II	5.74E-09	t	
			Chromium	3.91E-07	t	
			Cobalt II	1.23E-08	t	
			Copper ion	9.07E-08	t	
			Dioxins, measured as 2,3,7,8- tetrachlorodibenzo- p-dioxin	7.18E-14	t	
			Hydrocarbons, unspecified	1.85E-05	t	
			Hydrogen chloride	5.48E-06	t	
			Hydrogen fluoride	7.97E-07	t	
			Lead II	8.71E-08	t	
			Manganese II	8.19E-07	t	
			Mercury II	4.62E-09	t	
			Nickel II	2.88E-07	t	
			Selenium IV	1.20E-08	t	
			Thallium I	8.64E-09	t	
			Tin ion	2.34E-07	t	
			Zinc II	2.18E-06	t	
Gypsum	Inputs	Materials	Gypsum	1.00E+00	t	Ecoinvent v.3.6 [43]
Calcined clay	Inputs	Materials	Clay	1.30E+00	t	Ecoinvent v.3.6
		Thermal energy	Petroleum coke	6.31E+01	t	
		Electricity	Electricity, medium voltage	2.50E+01	kWh	

Limestone, unprocess ed	Outputs	Emissions	Carbon dioxide	2.00E+02	t	
			Methane, fossil	6.15E-03	t	
			Dinitrogen monoxide	1.23E-03	t	
			Water, Emission to air	3.00E-01	t	
	Inputs	Materials	Calcite	1.00E+00	t	Ecoinvent 3.6 [44]
			Water, unspecified natural origin	2.14E-02	m ³	Ecoinvent 3.6 [43]
		Soil	Occupation, mineral extraction site	1.34E+00	m ² a	Ecoinvent 3.3 [44]
		Excavation	Blasting	1.82E-02	t	
		Electricity	Electricity, medium voltage	2.73E-02	kWh	
		Thermal energy	Diesel, burned in building machine	3.33E+01	MJ	
			Occupation, mineral extraction site	9.56E-03	m ²	
		Transformati on	Transformation, from forest, unspecified	9.56E-03	m ²	
		Infrastructure	Recultivation, limestone mine	9.56E-03	m ²	
			Limestone quarry infrastructure	8.20E-09	item(s)	
			Water, unspecified natural origin	2.14E-02	m ³	Ecoinvent 3.6 [43]
			Particulate Matter, < 2.5 um	6.08E-03	t	Ecoinvent 3.3 [44]
Crushed limestone	Outputs	Emissions	Particulate Matter, >2.5 um and < 10um	5.89E-02	t	
			Particulate Matter, > 10 um	1.59E-01	t	
	Inputs	Materials	Limestone, unprocessed	1.00E+00	t	No losses assumed
		Electricity	Electricity, medium voltage	2.55E-01	kWh	Ecoinvent 3.6 [45]
		Thermal energy	Diesel, burned in building machine	3.40E+00	MJ	
	Outputs	Emissions	Particulate Matter, < 2.5 um	1.75E-02	t	
			2.5 um < Particulate < 10 um	7.51E-02	t	

			Particulate Matter, > 10 um	1.48E-01	t	
Filler limestone	Inputs	Materials	Crushed limestone	1.00E+00	t	No losses assumed
		Electricity	Electricity, medium voltage	6.33E+01	kWh	[33]
Marble residue	Inputs	Materials	Residue	1.00E+00	t	-
		Electricity	Electricity	6.33E+01	kWh	[33]
	Outputs	Waste management	Transport to the landfill	0	t*km	-
			Marble residue in an inert landfill	0	t	-

S2 DATA QUALITY

According to ISO 14044 (ABNT, 2014b), defining the desired level of data representativeness is essential for guiding the inventory data collection.

Table S.2 Representativeness of foreground inventory data in this study

Aspect	Description
Reliability (R)	Priority order: 1) Average data from national reports; 2) Literature data; 3) Database
Completeness (C)	Data that consider variations in the Brazilian market
Time coverage (T)	Less than 6 years – Base year: 2023
Geographical coverage (G)	Brazil
Technological coverage (F)	Technology available in the Brazilian market

According to Rosenbaum et al. [70], the basic uncertainty and the pedigree uncertainty of each inventory flow are combined using Equation S.1, resulting in the combined uncertainty of the data (ranging from 1 to 2)

Equation S.1

$$GSD_X^2 = e^{\sqrt{\sum_{i=1}^n [\ln(GSD_{X_i}^2)]^2}}$$

Where:

- GSD_X^2 : uncertainty associated with the individual flow within the set of inventory flows;
- n : total number of inventory flows.

This uncertainty is then converted into a 68% confidence interval using Equation S.2, which adjusts the confidence values:

Equation S.2

$$GSD_X = \sqrt{GSD_X^2}$$

These formulas are applied in OpenLCA® to incorporate uncertainties into the input data, using a lognormal distribution for each flow, as described in Table S.3. The Monte Carlo simulation is then performed with 501 and 1001 iterations to generate a distribution of results [70, 71].

Table S.3 Basic and pedigree uncertainty of inventory flows for the proposed scenario.

Material	Flow (Name in OpenLCA® v.2.3)	Basic uncertainty in GSD²	Pedigree score R C T G F	Pedigree uncertainty in GSD²
OPC; LC³; LC³-R	Clinker	1.15	4 1 3 2 3	1.20 1.00 1.10 1.01 1.20
	Gypsum	1.15	4 1 3 2 3	1.20 1.00 1.10 1.01 1.20
	Calcined clay	1.15	4 1 3 2 3	1.20 1.00 1.10 1.01 1.20
	Limestone filler	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Marble residue	1.12	3 4 2 2 3	1.10 1.10 1.03 1.01 1.20
	Electricity, medium voltage	1.43	4 1 2 2 5	1.20 1.00 1.03 1.01 2.00
	Packing, cement	1.38	5 5 5 5 3	1.50 1.20 1.50 1.10 1.20
	Particulates, <10 um	1.51	4 1 2 2 5	1.20 1.00 1.03 1.01 2.00
Clinker	Petroleum coke	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Charcoal	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Hard coal	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Bundle, energy wood	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Heavy fuel oil	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Natural gas, low pressure	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Diesel	1.14	4 1 2 2 3	1.20 1.00 1.03 1.01 1.20
	Electricity, medium voltage	1.43	4 1 2 2 5	1.20 1.00 1.03 1.01 2.00
Crushed limestone	Limestone, unprocessed	1.26	5 4 1 1 3	1.50 1.10 1.00 1.00 1.20
	Electricity, medium voltage	1.15	2 5 2 5 3	1.05 1.20 1.03 1.10 1.20
	Diesel, burned in building machine	1.15	2 5 2 5 3	1.05 1.20 1.03 1.10 1.20
	Particulate Matter, < 2.5 um	1.76	2 5 2 5 3	1.05 1.20 1.03 1.10 1.20
	2.5 um < Particulate < 10 um	1.45	2 5 2 5 3	1.05 1.20 1.03 1.10 1.20
	Particulate Matter, > 10 um	1.28	2 5 2 5 3	1.05 1.20 1.03 1.10 1.20
Limestone filler	Crushed limestone		5 4 1 1 3	
	Electricity, medium voltage	1.04	2 1 1 1 1	1.05 1.00 1.00 1.00 1.00

Marble Residue	Residue	1.02	1 1 1 1 1	1.00 1.00 1.00 1.00 1.00
	Electricity, medium voltage	1.26	4 2 3 2 4	1.20 1.02 1.10 1.01 1.50
	Transport to landfill	1.6	5 5 4 2 4	1.50 1.20 1.20 1.01 1.50
	Waste in inert landfill	1.34	5 4 1 1 1	1.50 1.10 1.00 1.00 1.00
	Inert waste, for final disposal	1.37	5 5 4 2 4	1.50 1.20 1.20 1.01 1.50

The results presented in Table S.4 allow for the comparison of environmental impacts among OPC, LC³, and LC³-R cements, considering different numbers of interactions (0; 501; 1001). When analyzing the results of the Monte Carlo Simulation interactions for the evaluated scenarios, it is observed that the averages generated in simulations 501 and 1001 present variations that should be considered when interpreting the data. In particular, the HTP category shows a significant change in the average, which may be attributed to the high uncertainty of the flows contributing to this category, directly affecting the values obtained.

Moreover, it is important to examine the overlap of value ranges (5% to 95%) between scenarios for each evaluated category. When there is overlap, the results do not show statistically significant differences, indicating that despite the variations, one scenario cannot be considered superior to the other with full certainty.

Table S.4 Results of Monte Carlo Simulation interactions for the scenarios under study in the evaluated categories.

Categories	Interactions								
	0		501			1001			
	-	5%	95%	Mean	Median	5%	95%	Mean	Median
CPC									
ADP	4,76E-04	4.16E-04	1.16E-03	7.21E-04	6.79E-04	4.38E-04	1.11E-03	7.11E-04	6.50E-04
ADP-ff	3.30E+03	3.32E+03	5.86E+03	4.45E+03	4.38E+03	3.26E+03	5.82E+03	4.43E+03	4.34E+03
GWP 100a	8.83E+02	6.98E+02	1.15E+03	9.13E+02	9.05E+02	6.95E+02	1.17E+03	9.14E+02	8.96E+02
ODP	3.93E-05	3.32E-05	1.39E-04	7.18E-05	6.29E-05	3.19E-05	1.30E-04	6.76E-05	6.00E-05
HTP	6.26E+01	-4.39E+01	5.94E+01	1.56E+01	1.95E+01	-3.14E+01	6.08E+01	1.59E+01	1.97E+01
AP	1.69E+00	7.99E-01	3.79E+00	1.85E+00	1.58E+00	7.54E-01	3.64E+00	1.83E+00	1.60E+00
LC ³									
ADP	3.48E-04	3.18E-04	7.25E-04	4.90E-04	4.63E-04	3.24E-04	6.89E-04	4.83E-04	4.60E-04
ADP-ff	2.65E+03	2.58E+03	4.17E+03	3.27E+03	3.20E+03	2.60E+04	4.06E+04	3.26E+03	3.19E+03
GWP 100a	5.52E+02	4.51E+02	7.01E+02	5.59E+02	5.50E+02	4.40E+02	7.08E+02	5.60E+02	5.51E+02
ODP	3.18E-05	2.45E-05	1.05E-04	5.29E-05	4.53E-05	2.41E-05	9.11E-05	4.95E-05	4.54E-05
HTP	4.19E+01	-2.56E+01	2.97E+01	-2.10E+00	8.73E+00	-2.41E+01	3.22E+01	2.53E+00	8.79E+00
AP	1.06E+00	5.39E-01	2.21E+00	1.09E+00	9.26E-01	4.98E-01	2.07E+00	1.06E+00	9.05E-01
LC ³ -R									
ADP	2.93E-04	2.62E-04	6.00E-04	4.04E-04	3.83E-04	2.72E-04	6.15E-04	4.11E-04	3.84E-04
ADP-ff	2.51E+03	2.48E+03	3.94E+03	3.09E+03	3.04E+03	2.45E+03	3.81E+03	3.08E+03	3.03E+03
GWP 100a	5.43E+02	4.25E+02	6.64E+02	5.45E+02	5.43E+02	4.32E+02	6.87E+02	5.43E+02	5.38E+02
ODP	2.99E-05	2.36E-05	9.11E-05	4.80E-05	4.24E-05	2.30E-05	8.87E-05	4.70E-05	4.20E-05
HTP	4.02E+01	-2.73E+01	2.82E+01	3.90E+01	7.60E+00	-2.67E+01	2.82E+01	-5.57E+00	7.64E+00
AP	1.02E+00	4.56E-01	2.10E+00	1.04E+00	9.37E-01	4.93E-01	2.10E+00	1.05E+00	9.00E-01

S3 COMPARISON OF THE ENVIRONMENTAL IMPACTS

Table S.5 Comparison of the environmental impacts of the analyzed cements using clinker from the database (Ecoinvent v.2.3) and clinker adapted for this study.

Categories	OPC	OPC - BD	LC ³	LC ³ -BD	LC ³ -R	LC ³ -R - BD
ADP	4.75E-04	5.15E-04	3.48E-04	3.66E-04	2.93E-04	3.12E-04
ADP-ff	3.30E+03	3.86E+03	2.65E+03	2.94E+03	2.51E+03	2.80E+03
GWP 100a	8.83E+02	8.96E+02	5.52E+02	5.59E+02	5.43E+02	5.50E+02
ODP	3.93E-05	4.75E-05	3.18E-05	3.61E-05	3.00E-05	3.42E-05
HTP	6.26E+01	6.47E+01	4.19E+01	4.30E+01	4.02E+01	4.13E+01
AP	1.69E+00	1.76E+00	1.06E+00	1.10E+00	1.02E+00	1.06E+00

Note: ADP – Abiotic depletion; ADP-ff – Abiotic depletion (fossil fuels); GWP 100a – Global warming potential; ODP – Ozone layer depletion; HTP – Human toxicity potential; AP – Acidification potential. OPC-BD: ordinary Portland cement (database); OPC: ordinary Portland cement; LC³-BD: limestone calcined clay cement (database); LC³: limestone calcined clay cement; LC³-R-BD: calcined clay and marble residue cement (database); LC³-R: calcined clay and marble residue cement.

Figure S.1 Graphical representation of Table S.1. OPC-BD: ordinary Portland cement (database); OPC: ordinary Portland cement; LC³-BD: limestone calcined clay cement (database); LC³: limestone calcined clay cement; LC³-R-BD: calcined clay and Beige Bahia marble waste cement (database); LC³-R: calcined clay and marble residue cement.

