

Environmental model and optimisation pathway for Potassium Silicate and Metakaolin based geopolymer with earth additions for 3D printing

Corentin Le Gall [1], Charlotte Roux [1], Julien Archez [1], [Adélaïde Fresnet-Férraille \[1\]](#), Jean-François Caron [1]

[1] Navier Laboratory, Gustave Eiffel University, Ecole des Ponts ParisTech, CNRS, Champ sur Marne, France

Supporting information

S1 PROCESS DETAILED MODELISATION

Parameters used in formula description

Notation	Comments
Q_MK	Metakaolin massic share in matrix (default = 0.5)
Q_LKMK	Low-kaolinite Metakaolin massic share in matrix (default = 0)
Q_GeoS	Geosil massic share in matrix (default =0.5)
D_MK	Transport distance for metakaolin
D_PSS	Transport distance for Geosil (potassium silicate)
S0/S1..Sn	UpScale scenario

Geopolymer GP-SE (m3)

Amount	Unit	Product	Activity	Location	Database	Formula
751.8	kg	GP matrix	GP matrix	FR	geopolymers	375.9*2
496.2	kg	Steamed earth	Steamed earth	GLO	geopolymers	
255.6	kg	sand	market for sand	CH	cutoff371	

GP matrix (1 kg)

Amount	Unit	Product	Activity	Location	Database	Formula
0.5	kg	Geosil 14515	Geosil 14515	FR	geopolymers	Q_GeoS
0.0	kg	LK Metakaolin	LK Metakaolin	FR	geopolymers	Q_MK*(S4 + S5)
0.5	kg	Metakaolin	Metakaolin	FR	geopolymers	Q_MK*(S0+S1+S2+S3)
0.006993	kWh	electricity, low voltage	market electricity, low voltage	FR	cutoff371	0.006993*(S0+S1+S2+S3+S4)
0.2675	t.km	transport, freight, lorry 3.5-7.5 metric ton, EURO4	market transport, freight, lorry 3.5-7.5 metric ton, EURO4	RER	cutoff371	D_MK*(Q_MK+Q_LKMK)/1000 * S0
0.252	t.km	transport, freight, lorry 3.5-7.5 metric ton, EURO4	market transport, freight, lorry 3.5-7.5 metric ton, EURO4	RER	cutoff371	D_PSS*Q_GeoS /1000 * S0

0.0	t.km	transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified	RER	cutoff371	$D_MK * (Q_MK + Q_LKMK) / 1000 * (S1)$
0.0	t.km	transport, freight, lorry, unspecified	market for transport, freight, lorry, unspecified	RER	cutoff371	$D_PSS * Q_GeoS / 1000 * (S1)$
0.0	t.km	transport, freight, lorry, unspecified	transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified	RER	cutoff371	$D_MK * (Q_MK + Q_LKMK) / 1000 * (S2 + S3 + S4 + S5)$
0.0	t.km	transport, freight, lorry, unspecified	transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified	RER	cutoff371	$D_PSS * Q_GeoS / 1000 * (S2 + S3 + S4 + S5)$
0.0	kWh	electricity, low voltage, label-certified	market for electricity, low voltage, label-certified	CH	cutoff371	$0.006993 * (S5)$

Steamed earth (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
1.3	kg	Raw earth	Raw earth	GLO	geopolymers	
0.1	kilowatt hour	electricity, low voltage	market for electricity, low voltage	FR	cutoff371	

Raw earth (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
1.0	kilogram	clay	clay pit operation	CH	cutoff371	

Geosil 14515 (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
0.45	kg	Potassium silicate, WITHOUT WATER, 48% solution	Potassium silicate, WITHOUT WATER, 48% solution	FR	geopolymers	
0.55	kilogram	tap water	market for tap water	Europe without Switzerland	cutoff371	

Potassium silicate based on ecoinvent activity Sodium Silicate. Molar equivalent for the quantity of potassium hydroxide. Contextualization: in activity "Potassium silicate, WITHOUT WATER, 48% solution" from the ecoinvent database, changing market for potassium hydroxide, GLO by RER market, removing container ship freight and production from RoW.

Raw earth (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
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0.45	kg	Potassium silicate, WITHOUT WATER, 48% solution	Potassium silicate, WITHOUT WATER, 48% solution	FR		geopolymers
0.55	kilogram	tap water	market for tap water	Europe Switzerland	without	cutoff371

Metakaolin (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
2.5	MJ	heat, district or industrial, natural gas	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	FR	cutoff371	$2.5*(S0+S1+S2)$
1.16	kg	kaolin	kaolin production	FR	geopolymers	
1.0	MJ	heat, central or small-scale, other than natural gas	heat and power co-generation, biogas, gas engine	FR	cutoff371	$2.5*(S3+S4)$
1e-10	unit	ceramic factory	ceramic factory construction	CH	cutoff371	

Kaolin production has been derived from the ecoinvent process RER contextualized to French conditions, changing the electricity mix

Low kaolinite metakaolin (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
1e-10	unit	ceramic factory	ceramic factory construction	CH	cutoff371	
1.16	kg	clay	clay pit operation	CH	cutoff371	
2.5	MJ	heat, district or industrial, natural gas	heat and power co-generation, natural gas, conventional power plant, 100MW electrical	FR	cutoff371	$2.5*(S0+S1+S2+S3+S4)$
1.0	kg	packing, clay product	packing, clay product	CH	cutoff371	
0.0	MJ	heat, central or small-scale, other than natural gas	heat and power co-generation, biogas, gas engine	FR	cutoff371	$2.5*S5$

GP-GfW (kg)

Amount	Unit	Product	Activity	Location	Database	Formula
0.45	kg	Geosil 14515	Geosil 14515	FR	geopolymers	
0.55	kg	Metakaolin	Metakaolin	FR	geopolymers	
0.006993	kWh	electricity, low voltage	market for electricity, low voltage	FR	cutoff371	
0.296	t.km	transport, freight, lorry 3.5-7.5 metric ton, EURO4	market for transport, freight, lorry 3.5-7.5 metric ton, EURO4	RER	cutoff371	

Market for wollastonite (kg)

From market for asbestos, chrysotile type in ecoinvent database. Transport distance modified: <https://www.searates.com/services/distances-time/>

Wollastonite from Mexico : 315 km by lorry to coast, 12871.5 container ship, 33.5 km lorry

Wollastonite production : Proxy based on asbestos production in ecoinvent v3.7.1, asbestos production, chrysotile type. Changes made: removing biosphere flow: Chrysotile, in ground 1.11, adding -> wollastonite, in ground not possible. Only in ReCiPe2016. adding, "clay, unspecified" 1.11

Amount	Unit	Product	Activity	Location	Database	Formula
0.45	kg	Potassium silicate, WITHOUT WATER, 48% solution	Potassium silicate, WITHOUT WATER, 48% solution	FR	geopolymers	
0.55	kilogram	tap water	market for tap water	Europe Switzerland	without cutoff371	

Market for glass fibre (kg)

Market for glass fibre, adapted from market for fibre, GLO to account for French providers. Production site : LAUDUN L'ARDOISE 30290 -> 700 km

Glass fibre production: from glass fibre production, RER, contextualized with a French electricity mix (medium voltage)

Amount	Unit	Product	Activity	Location	Database	Formula
0.7	t.km	transport, freight, lorry, unspecified	market group for transport, freight, lorry, unspecified	GLO	cutoff371	
1.0	kg	glass fibre	glass fibre production	FR	geopolymers	

S2 IMPACT CATEGORIES

ILCD indicators and used abbreviations

Impact Category	Abreviation	unit
climate change total	CC	kg CO2-Eq
freshwater and terrestrial acidification	FTA	mol H+-Eq
freshwater ecotoxicity	FEx	CTU
freshwater eutrophication	FEu	kg P-Eq
marine eutrophication	MEu	kg N-Eq
terrestrial eutrophication	TEu	mol N-Eq
carcinogenic effects	CE	CTUh
ionising radiation	IR	kg U235-Eq
non-carcinogenic effects	nCE	CTUh
ozone layer depletion	OD	kg CFC-11.
photochemical ozone creation	POCP	kg NMVOC-.
respiratory effects, inorganics	RE	disease i.
resources, dissipated water	DW	m3 water-.
resources, fossils	RF	megajoule
resources, land use	RLU	points
resources, minerals and metals	RMM	kg Sb-Eq

cumulative Energy Demand	CED	MJ-Eq
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Exhaustive results for unit element

		CC	FTA	FEx	FEu	MEu	TEu	CE	IR	nCE
process	unit	kg CO2-Eq	mol H+-Eq	CTU	kg P-Eq	kg N-Eq	mol N-Eq	CTUh	kg U235-Eq	CTUh
cement, Portland	kg	8.57E-01	1.95E-03	8.98E-02	8.67E-05	5.33E-04	6.04E-03	4.18E-09	3.34E-02	3.82E-08
tap water	kg	3.44E-04	1.87E-06	1.04E-03	2.48E-07	3.70E-07	3.47E-06	9.05E-11	1.19E-04	1.51E-10
sand	kg	4.92E-03	3.47E-05	1.16E-02	7.25E-07	1.29E-05	1.44E-04	3.56E-10	9.90E-04	6.80E-10
electricity, low voltage	kWh	1.16E-01	5.54E-04	1.12E-01	3.72E-05	1.38E-04	1.12E-03	5.32E-09	5.43E-01	1.79E-08
Metakaolin	kg	2.74E-01	1.12E-03	7.73E-02	1.04E-04	1.77E-04	1.73E-03	2.62E-09	5.20E-02	2.21E-08
Potassium silicate solution (Geosil 14515)	kg	6.18E-01	3.19E-03	6.33E-01	3.16E-04	6.68E-04	7.01E-03	2.40E-08	1.36E-01	8.57E-08
transport, freight, lorry 3.5-7.5 metric ton, EURO4	t.km	5.08E-01	2.38E-03	9.72E-01	4.94E-05	7.81E-04	8.50E-03	1.50E-08	4.31E-02	6.29E-08
glass fibre	kg	1.74E+00	1.38E-02	4.49E+00	1.98E-04	3.14E-03	3.29E-02	5.60E-08	8.87E-01	9.02E-07
wollastonite	kg	2.62E-01	4.76E-03	2.46E-01	3.19E-05	1.21E-03	1.35E-02	8.05E-09	1.87E-02	1.85E-08
Steamed earth	kg	2.07E-02	1.35E-04	5.15E-02	7.28E-06	3.87E-05	4.25E-04	3.91E-09	5.49E-02	4.18E-09
Raw earth	kg	7.03E-03	6.15E-05	3.10E-02	2.74E-06	1.92E-05	2.41E-04	2.60E-09	4.67E-04	1.84E-09
silica fume, densified	kg	3.15E-03	2.02E-05	8.04E-03	3.30E-07	7.40E-06	8.07E-05	1.00E-10	2.31E-04	4.44E-10
calcium nitrate	kg	1.62E+00	9.68E-03	1.29E+00	3.16E-04	1.17E-03	3.43E-02	6.38E-08	6.96E-02	1.76E-07
plasticiser, for concrete, based on sulfonated melamine formaldehyde	kg	1.38E+00	8.98E-03	1.18E+00	4.41E-04	1.38E-03	1.44E-02	2.96E-08	9.71E-02	2.08E-07
transport, concrete 50MPa, m3	m3	2.63E+01	1.46E-01	5.95E+01	2.74E-03	5.21E-02	5.69E-01	7.88E-07	2.34E+00	3.52E-06

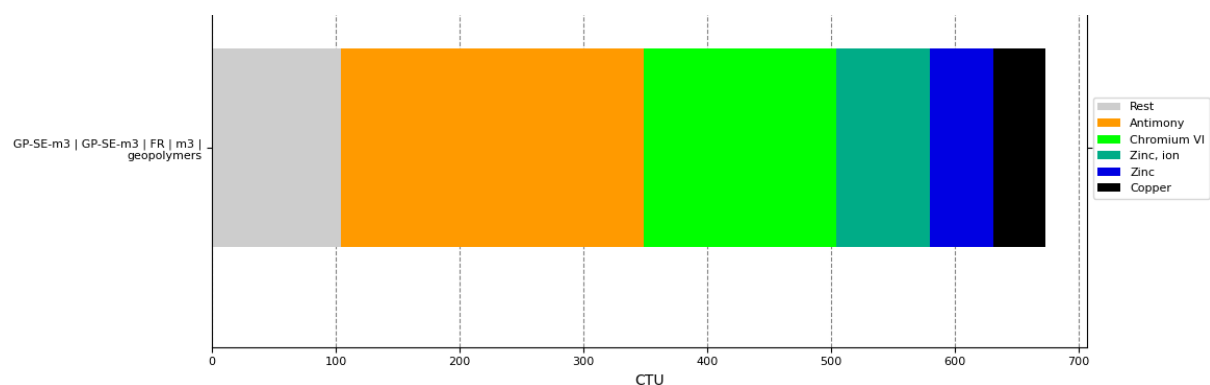
		OD	POCP	RE	DW	RF	RLU	RMM	CED
process	unit	kg CFC-11.	kg NMVOC.	disease i.	m3 water.	MJ	points	kg Sb-Eq	MJ-Eq
cement, Portland	kg	2.58E-08	1.52E-03	9.20E-09	7.33E-02	3.77E+00	1.14E+00	1.27E-06	3.7
tap water	kg	2.29E-11	1.12E-06	1.61E-11	2.51E-04	6.72E-03	2.38E-03	1.55E-09	0.0
sand	kg	9.81E-10	3.94E-05	6.99E-10	1.72E-03	8.11E-02	1.75E-01	4.13E-08	0.1
electricity, low voltage	kWh	1.21E-08	3.08E-04	4.78E-09	1.41E-01	1.24E+01	9.66E-01	3.35E-06	13.2
Metakaolin	kg	4.05E-08	5.07E-04	5.61E-09	1.70E-01	5.01E+00	1.19E+00	7.27E-07	5.9
Potassium silicate solution (Geosil 14515)	kg	6.97E-08	1.94E-03	2.56E-08	2.34E-01	1.11E+01	8.81E+00	1.53E-05	11.9
transport, freight, lorry 3.5-7.5 metric ton, EURO4	t.km	1.09E-07	2.45E-03	2.75E-08	4.50E-02	7.69E+00	5.22E+00	3.21E-06	8.2
glass fibre	kg	1.82E-07	9.17E-03	1.10E-07	6.29E-01	4.11E+01	8.10E+00	1.94E-05	43.7
wollastonite	kg	4.73E-08	3.58E-03	1.86E-08	2.08E-02	3.63E+00	1.81E+00	1.29E-06	3.8
Steamed earth	kg	2.36E-09	1.07E-04	2.02E-09	1.69E-02	1.36E+00	3.75E-01	9.00E-07	1.4
Raw earth	kg	8.89E-10	5.89E-05	1.19E-09	2.12E-03	9.12E-02	2.14E-01	4.34E-07	0.1

silica fume, densified	kg	6.50E-10	2.26E-05	3.01E-10	2.61E-04	4.74E-02	5.90E-02	1.08E-08	0.0
calcium nitrate	kg	1.43E-07	2.79E-03	5.73E-08	1.03E+00	1.84E+01	9.02E+00	5.34E-05	20.0
plasticiser, for concrete, based on sulfonated melamine formaldehyde	kg	2.23E-07	5.65E-03	7.02E-08	9.87E-01	3.38E+01	5.88E+00	1.74E-05	34.7
transport, concrete 50MPa, m3	m3	5.79E-06	1.67E-01	2.42E-06	2.30E+00	4.04E+02	4.40E+02	1.81E-04	432.7

S3 LCA RESULTS: STRESSOR CONTRIBUTION TO ECOTOXICITY

Graphs below give stressor contribution detail for freshwater ecotoxicity for both characterisation methods used: ILCD 2018 ad ImpactWorld+. It shows that contributing stressors highly differs. While copper is present and significant in both case, Antimony, Chromium VI and Zinc dominate for ILCD and Aluminium clearly drives the impact for both short and long term in ImpactWorld+.

Stressor contribution to freshwater ecotoxicity, ILCD



Stressor contribution to freshwater ecotoxicity, long term Impact World +

