

Thermodynamic modelling of cements clinkering process as a tool for optimising the proportioning of raw meals containing alternative materials

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Supplementary information

Example of determining the equations for modelling

Table S1 shows a simplified example of the oxide composition of the raw materials to illustrate the calculation of the input equations for the dosing method by thermodynamic modelling. The example considers co-processing 10 wt.% SFCC and the alumina modulus set to 1.6.

Oxides (%)	SFCC	CaCO ₃ AP	SiO ₂ AP	Fe ₂ O ₃ AP
SiO ₂	55.00	1.00	100.00	0.00
Al ₂ O ₃	44.00	1.00	0.00	1.00
Fe ₂ O ₃	1.00	0.00	0.00	98.00
CaO	0.00	56.00	0.00	1.00
CO ₂	0.00	42.00	0.00	0.00

Table S1. Oxide composition of the raw materials for the simplified example.

The determination of the fixed Fe₂O₃ AP content is shown in equation S1.

$$F_{\text{fixed}} = \frac{10 \cdot 44.00}{1.6 \cdot 98.00} = 2.81\% \quad (\text{S1})$$

The angular coefficients for the input equations are calculated as in equation S2.

$$\begin{bmatrix} A_{\text{SiO}_2} \\ A_{\text{Al}_2\text{O}_3} \\ A_{\text{Fe}_2\text{O}_3} \\ A_{\text{CaO}} \\ A_{\text{CO}_2} \end{bmatrix} = \begin{bmatrix} 0.55 & 0.01 & 1.00 & 0.00 \\ 0.44 & 0.01 & 0.00 & 0.01 \\ 0.01 & 0.00 & 0.00 & 0.98 \\ 0.00 & 0.56 & 0.00 & 0.01 \\ -0.00 & 0.42 & 0.00 & 0.00 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.99 \\ -0.01 \\ 0.00 \\ -0.56 \\ -0.42 \end{bmatrix} \quad (\text{S2})$$

The linear coefficient for each oxide is calculated from Equation S3. Where S_{fixed} was the fixed SFCC content for the system (10 wt.%), C_{max} was the maximum CaCO₃ AP content in the raw meal (100 - S_{fixed} - F_{fixed} = 87.19), S_{min} was the minimum content of SiO₂ AP (0 wt.%), and F_{fixed} was the content of Fe₂O₃ AP fixed in the system (2.81 wt.%).

$$\begin{bmatrix} B_{\text{SiO}_2} \\ B_{\text{Al}_2\text{O}_3} \\ B_{\text{Fe}_2\text{O}_3} \\ B_{\text{CaO}} \\ B_{\text{CO}_2} \end{bmatrix} = \begin{bmatrix} 0.55 & 0.01 & 1.00 & 0.00 \\ 0.44 & 0.01 & 0.00 & 0.01 \\ 0.01 & 0.00 & 0.00 & 0.98 \\ 0.00 & 0.56 & 0.00 & 0.01 \\ -0.00 & 0.42 & 0.00 & 0.00 \end{bmatrix} \cdot \begin{bmatrix} 10.00 \\ 87.19 \\ 0.00 \\ 2.81 \end{bmatrix} = \begin{bmatrix} 6.37 \\ 5.30 \\ 2.85 \\ 48.85 \\ 36.62 \end{bmatrix} \quad (\text{S3})$$

In this context, the linear equations applied as inputs in FactSage would be indicated below (S4 to S8). The variable *x* (SiO₂ AP content) would be configured in the software to go through values from 0 to 22.5% with a step of 0.5, covering 46 scenarios (raw meal compositions).

$$Y_{\text{SiO}_2} = 6.37 + 0.99x \quad (\text{S4})$$

$$Y_{\text{Al}_2\text{O}_3} = 5.30 - 0.01x \quad (\text{S5})$$

$$Y_{\text{Fe}_2\text{O}_3} = 2.85 \quad (\text{S6})$$

$$Y_{\text{CaO}} = 48.85 - 0.56x \quad (\text{S7})$$

$$Y_{\text{CO}_2} = 36.62 - 0.42x \quad (\text{S8})$$

Oxide composition of modelled systems

Table S2 details the oxide composition of the clinker raw meals dosed in this study.

Sample	CaO	SiO ₂	Fe ₂ O ₃	Al ₂ O ₃	MgO	SO ₃	P ₂ O ₅	Na ₂ O	ZnO	K ₂ O	NiO	TiO ₂	MnO	CO ₂
S5	46.02	15.99	0.09	2.33	0.25	0.06	0.08	0.13	0.00	0.01	0.05	0.03	0.00	34.96
S7.5	45.74	15.30	0.11	3.44	0.25	0.06	0.09	0.13	0.00	0.02	0.07	0.05	0.00	34.74
S10	45.46	14.60	0.14	4.55	0.25	0.06	0.10	0.13	0.00	0.02	0.10	0.06	0.01	34.53
S15	44.61	13.71	0.20	6.77	0.24	0.05	0.12	0.14	0.00	0.03	0.14	0.09	0.01	33.89
S20	44.05	12.32	0.26	8.99	0.24	0.05	0.14	0.14	0.00	0.04	0.19	0.11	0.01	33.46
R5	46.00	15.98	0.09	2.33	0.25	0.07	0.06	0.13	0.00	0.01	0.00	0.00	0.00	34.95
R7.5	45.78	15.32	0.14	3.47	0.25	0.07	0.05	0.13	0.00	0.01	0.00	0.00	0.00	34.78
R10	45.44	14.60	0.15	4.55	0.24	0.06	0.05	0.13	0.00	0.01	0.00	0.00	0.00	34.53
R15	44.60	13.71	0.20	6.77	0.24	0.06	0.05	0.13	0.00	0.01	0.00	0.00	0.00	33.88
R20	44.04	12.32	0.26	8.99	0.24	0.06	0.05	0.13	0.00	0.01	0.00	0.00	0.00	33.46
S5F	45.73	15.12	1.45	2.33	0.25	0.07	0.08	0.12	0.00	0.01	0.05	0.03	0.01	34.74
S7.5F	45.17	14.23	2.17	3.44	0.24	0.07	0.09	0.13	0.00	0.02	0.07	0.04	0.01	34.32
S10F	44.61	13.35	2.88	4.55	0.24	0.07	0.10	0.13	0.00	0.02	0.10	0.06	0.01	33.89
S15F	43.49	11.60	4.30	6.76	0.24	0.07	0.12	0.13	0.00	0.03	0.14	0.09	0.01	33.03
S20F	42.06	10.36	5.73	8.98	0.23	0.07	0.14	0.13	0.01	0.04	0.19	0.11	0.02	31.94
R5F	45.76	15.14	1.47	2.35	0.25	0.07	0.06	0.12	0.00	0.01	0.00	0.00	0.01	34.77
R7.5F	45.22	14.26	2.19	3.46	0.24	0.07	0.05	0.12	0.00	0.01	0.00	0.00	0.01	34.35
R10F	44.67	13.39	2.91	4.58	0.24	0.07	0.05	0.12	0.00	0.01	0.00	0.00	0.01	33.94
R15F	43.57	11.65	4.35	6.81	0.23	0.08	0.05	0.12	0.00	0.01	0.00	0.00	0.01	33.10
R20F	42.18	10.42	5.80	9.05	0.23	0.08	0.05	0.12	0.00	0.01	0.00	0.00	0.01	32.04

Table S2. Oxide composition of the clinker raw meals optimised by the proposed dosing method.

Table S3 presents the oxide composition of clinker raw meals from previous studies simulated for method validation.

ID	CaO	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	K ₂ O	Na ₂ O	MgO	TiO ₂	SrO	SO ₃	P ₂ O ₅	V ₂ O ₅	Cr ₂ O ₃	MnO	ZnO	Cl	F	T (°C)	Ref
01	58.16	16.17	5.05	5.39	1.04	0.65	8.08	0.25	0.00	0.85	3.25	0.04	0.08	0.42	0.04	0.03	0.51	1380	31
02	64.75	21.37	4.31	5.42	0.64	0.32	2.87	0.00	0.00	0.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1450	73
03	68.91	24.48	3.22	0.82	0.39	0.67	1.51	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1500	72
04	65.29	24.28	4.90	4.38	0.32	0.01	0.73	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1470	70
05	65.50	23.75	4.80	4.32	0.31	0.14	0.87	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1470	70
06	65.68	20.82	4.44	2.79	1.29	0.21	2.77	0.23	0.00	1.64	0.03	0.00	0.00	0.00	0.02	0.09	0.00	1500	23
07	66.56	21.25	6.34	5.23	0.27	0.13	0.07	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1450	74
08	61.74	24.56	6.23	5.13	2.01	0.12	0.06	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1360	74
09	62.59	24.90	6.31	5.21	0.27	0.50	0.07	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1360	74
10	62.81	25.00	6.34	5.23	0.27	0.13	0.07	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1360	75
11	62.35	24.81	6.29	5.19	1.01	0.13	0.07	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1360	75
12	61.97	24.65	6.25	5.15	0.26	1.50	0.07	0.01	0.09	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	1360	75
13	53.90	36.10	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
14	47.90	32.10	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
15	56.40	33.60	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
16	50.10	29.90	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
17	58.60	31.40	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
18	62.20	27.80	10.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
19	56.70	23.30	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
20	57.90	22.10	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71
21	58.90	21.10	20.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1400	71

Table S3. Oxide composition of clinker raw meals simulated for method validation.