

Table 1. Training data. Values given are averages

Mix	Cement type	Cement [CEM -]	Cement [%]	Cement crushed gravel [%]	Sharp sand [%]	Water [%]	Estimated mass/m ³ [kg/m ³]	Pre-conditioning time [days]	Carbonation coefficient, $K_{4\%}$ [mm/day ^{1/2}]	Environmental impact [kgCO ₂ e/kg]	Compressive strength, f_{cube} [MPa]	Water sat. density [kg/m ³]	Cost [£/kg]
C25 I	IIA 32.5 R	11.1	52.8	28.1	7.8	2414	141	1.742	0.095	27.46	2337	0.025	
C25 II	IIA 32.5 R	11.1	52.8	28.1	7.8	2414	138	2.301	0.095	21.30	2317	0.025	
C25 III	IIA 32.5 R	11.1	52.8	28.1	7.8	2414	16	1.648	0.095	28.35	2300	0.025	
C25 IV	IIA 32.5 R	11.1	52.8	28.1	7.8	2414	16	2.081	0.095	29.87	2297	0.025	
C20 I	IIA 32.5 R	10.0	56.0	27.4	6.5	2448	141	3.493	0.087	22.49	2263	0.024	
C18 I	IIA 32.5 R	12.0	52.9	27.3	7.8	2409	138	2.414	0.102	20.31	2260	0.026	
C30 I	IIA 32.5 R	14.2	52.5	25.5	7.8	2409	16	1.045	0.119	35.14	2247	0.027	
C40 I	IIA 32.5 R	17.4	51.4	23.4	7.8	2411	16	0.558	0.145	42.85	2220	0.029	
C45 I	I 52.5 N	14.6	48.5	28.2	8.7	2344	-	-	0.139	49.90	2287	0.027	
C55 I	I 52.5 N	13.7	51.5	27.2	7.6	2374	-	-	0.131	61.62	2333	0.027	
C50 I	I 52.5 N	16.6	44.6	28.9	9.9	2312	-	-	0.157	53.48	2300	0.029	
C20 II	I 52.5 N	10.3	47.7	33.2	8.7	2343	-	-	0.100	25.30	2237	0.024	
C35 I	I 52.5 N	8.9	50.4	33.1	7.6	2374	-	-	0.088	38.76	2290	0.024	
C30 II	I 52.5 N	9.2	50.9	32.4	7.3	2452	8	2.341	0.090	32.12	2240	0.024	
C45 II	I 52.5 N	13.4	49.5	28.9	8.1	2421	8	1.304	0.128	48.26	2357	0.027	
C30 III	I 52.5 N	9.2	50.9	32.4	7.3	2452	14	1.349	0.090	32.21	2343	0.024	
C45 III	I 52.5 N	13.4	49.5	28.9	8.1	2421	14	0.806	0.128	48.53	2360	0.027	
C25 V	I 52.5 N	10.6	48.3	32.1	9.1	2411	17	1.732	0.103	31.93	2310	0.025	
C30 IV	I 52.5 N	12.2	48.8	29.9	9.1	2408	17	1.212	0.117	37.85	2307	0.026	
C45 IV	I 52.5 N	14.2	48.9	27.9	9.0	2409	17	0.403	0.135	51.01	2330	0.027	
C55 II	I 52.5 N	17.0	48.4	25.7	9.0	2409	17	0.062	0.161	59.83	2327	0.029	

B.

Table 2. Hyperparameters of single-layer linear model, single-layer random forest model, and two-layer random forest model. Name of each hyperparameter in Scikit-learn is in italics. For each layer of the two-layer random forest model, hyperparameters are identical.

	Single-layer linear model	Single-layer random forest model	Two-layer random forest model	Imputation model
Number of trees <i>n_estimators</i>	–	200	512	512
Maximum number of features <i>max_features</i>	8	3	6	13
Minimum number of samples required to split a node <i>min_samples_split</i>	–	2	2	2

C.

Table 3. Relative feature importances of input variables (columns) for predicting each target variable (rows). Darker shades of pink correspond to higher feature importances.

	Cement type	Cement	Crushed gravel	Sharp sand	Water	Water/ cement	Total aggr./ cement	Sharp sand/ total aggr.	Precondi- tioning time
Carbonation coefficient	0.00	0.28	0.23	0.00	0.08	0.00	0.35	0.00	0.06
Environmental impact	0.04	0.45	0.27	0.24	0.00	0.00	0.00	0.00	0.00
Compressive strength	0.06	0.22	0.19	0.00	0.00	0.22	0.22	0.00	0.09
Density	0.11	0.00	0.28	0.00	0.22	0.00	0.00	0.39	0.00
Cost	0.00	0.50	0.00	0.35	0.15	0.00	0.00	0.00	0.00

D.

Table 4. Assumed embodied emissions and prices of constituent materials. Sources: Fibo Intercon, 2019; Jones and Hammond, 2019

Material, i	kgCO ₂ e/kg, e	£/kg, c
Cement CEM IIA	0.799	0.089
Cement CEM I	0.912	0.089
Gravel/Sand	0.007	0.018
Water	0.0008	0.007