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Net carbon benefit of CO₂ curing of cement from coupled machine learning and process carbon accounting

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Abstract

Carbonation curing can store CO₂ in cementitious materials, but its net carbon benefit depends on the emissions associated with CO₂ supply and curing. We manually compiled and curated a literature database, harmonised uptake to an original-material mass basis including aggregates, and coupled machine learning with process carbon accounting. Using 461 records and eight material and curing descriptors, we compared eight regressors and evaluated uptake responses alongside supply, transport and curing emissions. This framework connects experimental uptake data to the conditions under which the assessed process yields a net carbon benefit. At an illustrative predicted uptake of 0.231 kg CO₂/kg original material and an assumed material mass of 2400 kg/m³, all five supply scenarios yield net benefits of 0.189–0.219 kg CO₂/kg original material with electricity at 0.05 kg CO₂/kWh. Two scenarios become net emitters at 0.40 kg CO₂/kWh. Calculated break-even electricity intensities range from 0.314 to 2.047 kg CO₂/kWh, demonstrating how supply assumptions change the conditions for a positive balance. The curated database and coupled analysis provide a basis for comparing these conditions; limited cross-study predictive performance confines the numerical results to conditional scenarios.

20 Keywords: carbonation curing; machine learning; carbon dioxide uptake; process carbon accounting; curing energy; electricity carbon intensity

Introduction

Carbonation curing exposes cementitious materials to carbon dioxide to form carbonate products. Uptake depends on the material and on how it is conditioned and exposed to the gas. Reviews describe the range of curing variables and applications [1–3]. Experimental work has examined curing regimes and microstructure in Portland cement paste [4], moisture and initial conditioning in lightweight concrete [5,6], and pressurised curing through experiments and mathematical modelling [7]. These studies motivate considering material and operating variables together when predicting uptake.

The experimental literature also covers distinct binders and products. Studies have examined metakaolin-containing bricks and pastes [8,9], volcanic-ash and other mineral additions [10,11], and calcium sulfoaluminate cement at different water-to-cement ratios [12]. Research on subsequent curing and pre-carbonation hydration addresses how carbonation interacts with continued hydration [13–16]. This diversity broadens the available evidence, but makes material composition, conditioning history and measurement basis important when combining results across studies.

Engineering applications extend from dynamic curing and masonry units [17,18] to concrete pipes, precast production and hollow-core slabs [19–21]. Durability studies consider chloride penetration and weathering carbonation [22,23], while an industrial demonstration examines mineralisation curing at a larger scale [24]. Uptake prediction is therefore one component of evaluating a curing process; performance and operating conditions also matter.

Machine learning offers a way to combine observations obtained under different experimental conditions and represent nonlinear relationships between the reported inputs and uptake. Applications in concrete science also require careful interpretation of data coverage, model validation and physical assumptions [25]. A fitted response can help examine combinations of variables, but its value for process assessment depends on the prediction task for which it has been evaluated. Random validation assesses prediction within a pooled dataset; source-group validation additionally tests transfer to withheld studies [26].

The environmental calculation introduces another requirement. Higher uptake can require more CO₂ supply, longer gas circulation or additional conditioning energy. Earlier assessment of CO₂ use in concrete showed that supply-chain emissions and material performance can change its comparison with conventional production [27]. Life-cycle assessment of direct air capture likewise demonstrates the importance of capture-related burdens [28]. A useful coupled analysis must therefore distinguish gross uptake from the balance after supply and curing emissions are deducted.

CO₂ supply introduces further variation through capture energy and process design. Reviews of direct-air-capture deployment and assessment [29,30], process-level analysis [31] and the wider negative-emissions literature [32] motivate testing alternative supply inventories. Here, we examine five numerical scenarios whose coefficients and allocation assumptions are specified in Methods and the Supplementary Information.

We compiled and curated experimental records from the literature to bring dispersed evidence on carbonation curing into a common dataset. This database links reported material and curing descriptors to uptake on a common original-material mass basis, enabling model comparison and coupling to a transparent process carbon balance. We compare eight regression models on a 461-record working dataset, use an ensemble as a predictive benchmark, and retain a monotonicity-constrained model to generate directional response scenarios. The analysis follows the chain from individual curing variables, through joint uptake responses, to the resulting net carbon balance. The constraints define the directions permitted by the model; they are not treated as independent experimental evidence of those directions.

We examine water-to-cement ratio and CO₂ pressure at exposure times of 2, 24 and 48 h, then compare five upstream supply scenarios and variations in electricity intensity and pre-curing energy. Analytical expressions

identify the break-even electricity intensity and the marginal contribution of additional uptake. The scope is supply-and-curing carbon accounting rather than a complete product life-cycle comparison. Additional source-group validation and data-provenance checks are reported in the Supplementary Information to define the limits of applying these scenarios to new materials and installations.

5 Results

Dataset structure

The working dataset contains 465 records with numeric entries for eight predictors and the uptake target. Restricting temperature to at most 150 °C excludes four records and leaves 461 observations across 33 source identifiers. Group sizes range from 1 to 56 records, and uptake ranges from 0.01% to 51.11%, with a mean of 13.68% and a standard deviation of 8.03 percentage points. Figure 1 shows uptake against the individual descriptors; the marginal distributions are examined below. Source-group counts and uptake summaries are reported in Supplementary Table S1.

The material labels cover pastes, mortars, blocks and other specimens. The largest categories are cement paste (176 records), cement mortar (76), concrete block (57) and cement binder (55). These labels are retained as dataset metadata but are not included among the eight numeric predictors. Source identity is used only to define validation groups. Uptake values were converted during data compilation to a common original-material mass basis, including sand and aggregates where present. This mass normalisation does not remove differences in composition or measurement procedures.

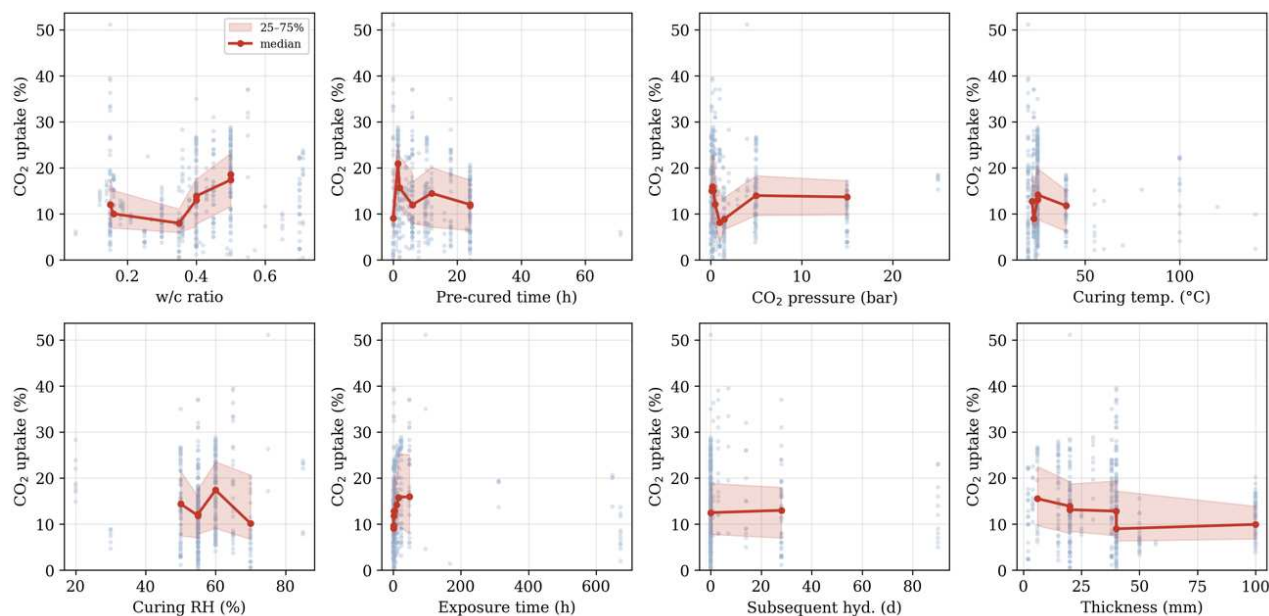


Figure 1. Recorded CO₂ uptake plotted against the eight material and curing descriptors. Points show the pooled observations and are coloured by exposure time. The red line shows the binned median and the shaded band the 25th–75th percentiles. The plotted associations combine observations from different studies.

Predictive performance of the regression models

The eight fixed model configurations are compared under random five-fold validation (Supplementary Table S3), using the same 461 observations with preprocessing fitted within each training fold. The ensemble gives pooled out-of-fold $R^2 = 0.737$ and RMSE = 4.114 percentage points. The constrained model gives $R^2 = 0.632$

and RMSE = 4.862 percentage points. Figure 2 plots the out-of-fold predictions underlying these scores, which assess prediction within the pooled literature dataset.

The random forest and gradient-boosting models give R^2 values of 0.747 and 0.744, respectively, close to the ensemble. Ridge regression gives $R^2 = 0.107$, indicating that this specified linear model captures substantially less of the recorded variation. No statistical significance test is used to rank the stronger models. The ensemble is retained as a benchmark, while the constrained model supplies all response surfaces and coupled carbon calculations. Its lower score is reported alongside its directional constraints; differing hyperparameters prevent attributing the entire score difference to the constraints alone.

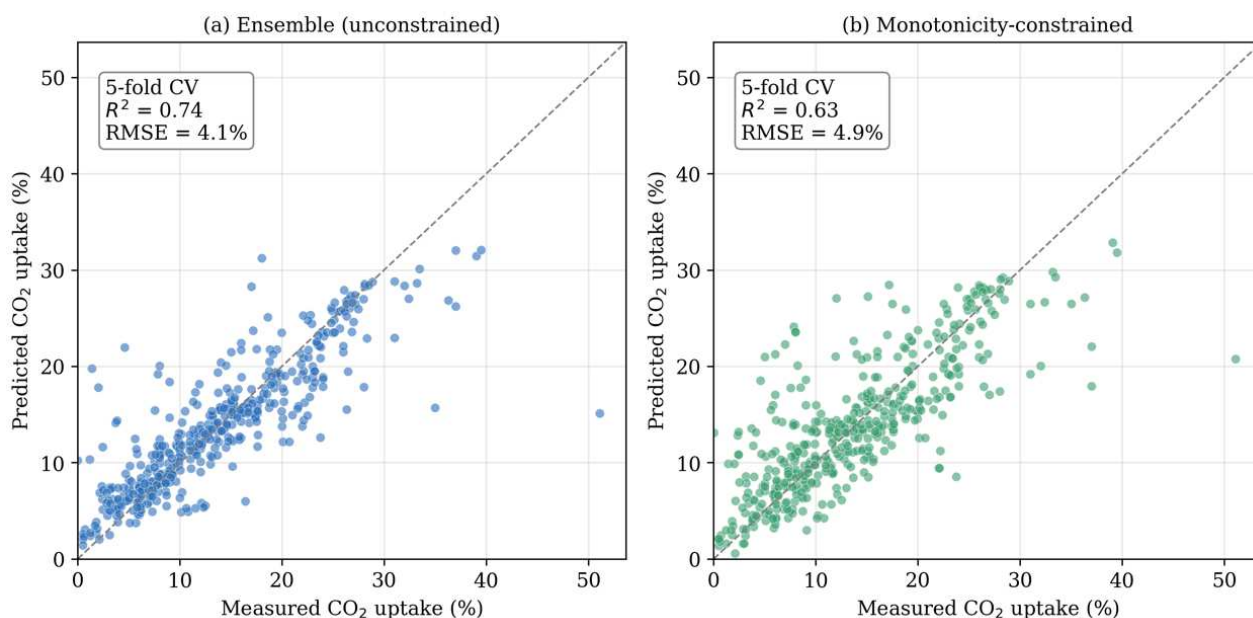


Figure 2. Random five-fold cross-validated parity plots. (a) Ensemble model. (b) Monotonicity-constrained model used for the response surfaces. Dashed lines indicate equality. The rounded annotations ($R^2 = 0.74$ and 0.63 ; RMSE = 4.1% and 4.9%) correspond to the reported pooled out-of-fold values of 0.737 and 0.632 and errors of 4.114 and 4.862 percentage points. Performance of all eight models is listed in Supplementary Table S3; source-group validation is reported in Supplementary Fig. S1.

Coverage of the material and curing descriptors

Figure 3 shows uneven coverage of the eight predictors and uptake. Most temperatures are near ambient, whereas exposure and pre-curing times have extended upper tails. Pressure observations are also concentrated within part of the available range. Predictions across these ranges therefore draw on different amounts of experimental evidence.

Some combinations used in the response surfaces have few or no close counterparts in the dataset, even when each individual input falls within its observed range. Concentrations at particular values also reflect data curation, including blank-to-zero subsequent-curing entries and blank-to-55% humidity entries (Supplementary Note “Retrospective comparison of the working tables”). Both joint coverage and these processing patterns matter when interpreting the fitted responses.

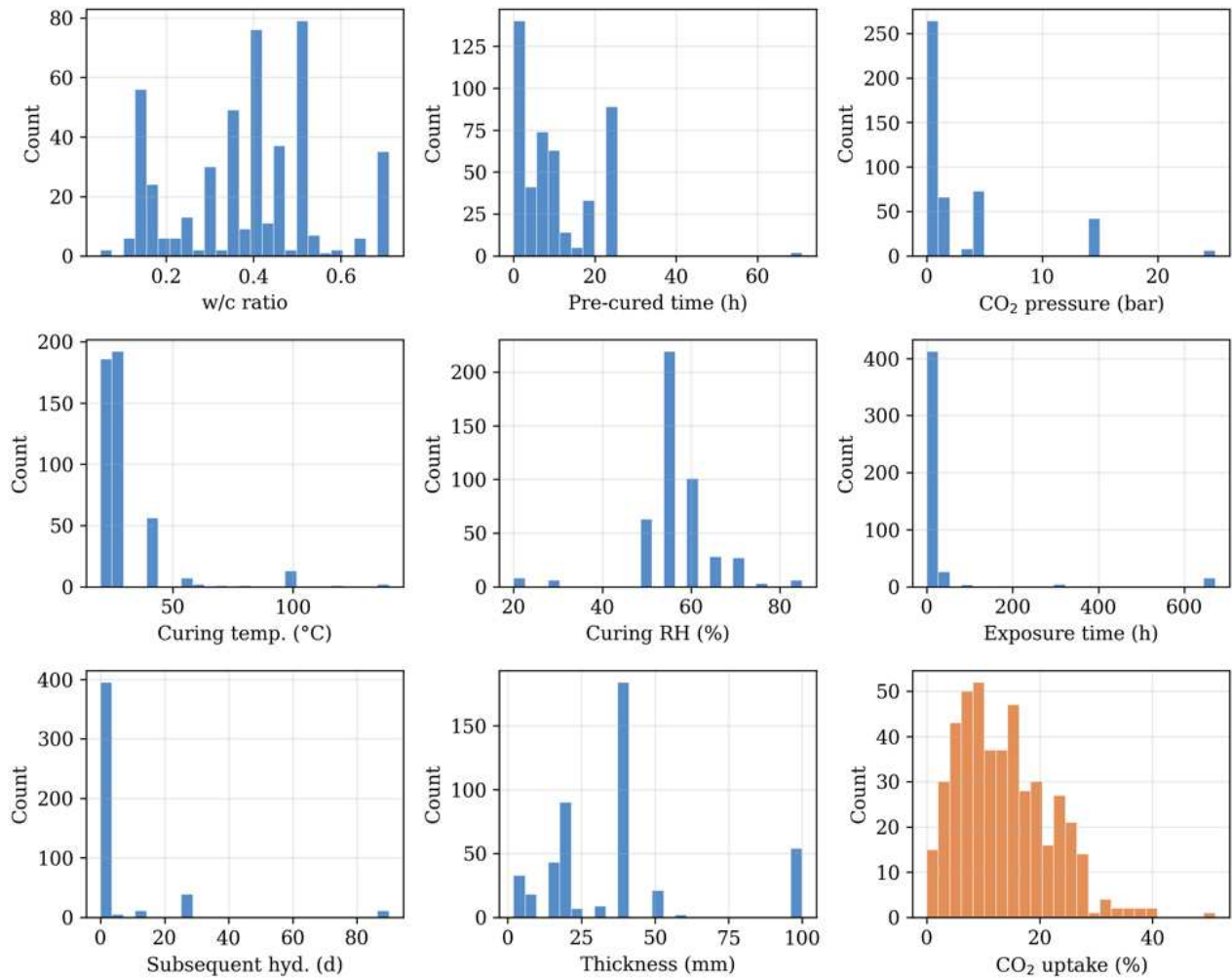


Figure 3. Marginal distributions of the eight input descriptors and the recorded CO₂ uptake target. Time, pressure and geometry use the working-table units. These marginal distributions describe uneven data coverage and do not demonstrate joint coverage of all response-surface combinations. Retrospective working-table comparisons are reported in Supplementary Note

5 “Retrospective comparison of the working tables”.

Conditional responses to individual curing factors

Figure 4 shows the constrained model’s response to each input while holding the other seven at their median settings. Predicted uptake decreases with water-to-cement ratio and thickness, and increases with pre-curing duration, CO₂ pressure and exposure time. The constraints impose these directions; the data determine the fitted magnitudes and locations of changes.

- 10 The pressure and exposure responses flatten towards the upper ends of the displayed ranges. Temperature, relative humidity and subsequent curing are unconstrained and produce different response shapes. Because the inputs span different ranges and interact with one another, these slices describe behaviour at the reference settings rather than a ranking of variable importance.

- The tree-based estimator produces stepwise curves, so plateaus and abrupt changes should not be assigned a kinetic interpretation. Positive predictions at zero exposure also reveal that the model does not enforce a zero-exposure mass-balance boundary. These features, together with the uneven joint coverage, identify where independent measurements are needed to test the fitted responses.
- 15

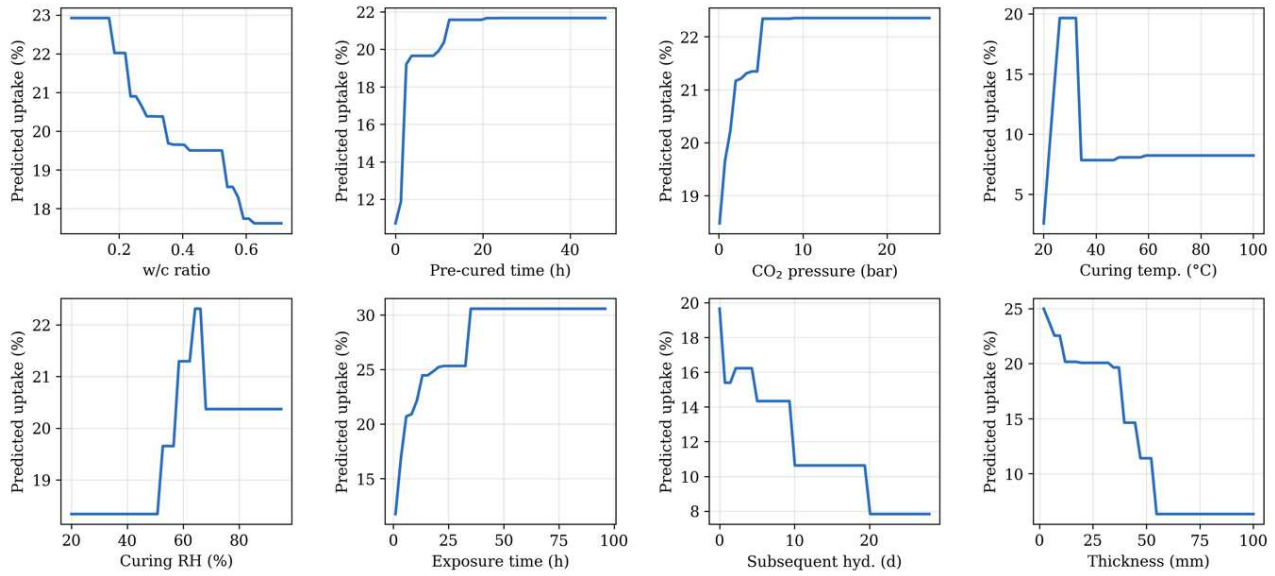


Figure 4. Single-factor responses of the deployed constrained model. Panels vary one input while the other inputs are held at the saved median settings: water-to-cement ratio 0.4, pre-curing 6 h, CO₂ partial pressure 0.6 bar, temperature 25 °C, relative humidity 55%, exposure 4 h, subsequent curing 0 d and thickness 38 mm. Axes use panel-specific ranges. Lines are conditional model predictions, not measured single-factor experiments or partial-dependence averages.

Joint responses to water-to-cement ratio, pressure and exposure

Figure 5 evaluates a two-dimensional grid of water-to-cement ratio and CO₂ pressure at exposure times of 2, 24 and 48 h. Pre-curing is fixed at 2 h and subsequent curing at 2 d, with the remaining settings specified in the caption. These scenario settings differ from the median reference used in Fig. 4. Across the grid, fitted uptake spans 9.55–23.13% at 2 h, 18.68–30.72% at 24 h and 22.66–35.25% at 48 h. The common vertical and colour scales allow the upward shift with exposure time to be compared directly.

Within each panel, uptake increases towards lower water-to-cement ratio and higher pressure, following the imposed constraints. The views from above show the plateaus and transitions more clearly. The highest predicted uptake identifies a maximum on the chosen grid; establishing a process optimum would additionally require experimental support for those input combinations and reliable prediction beyond the training studies.

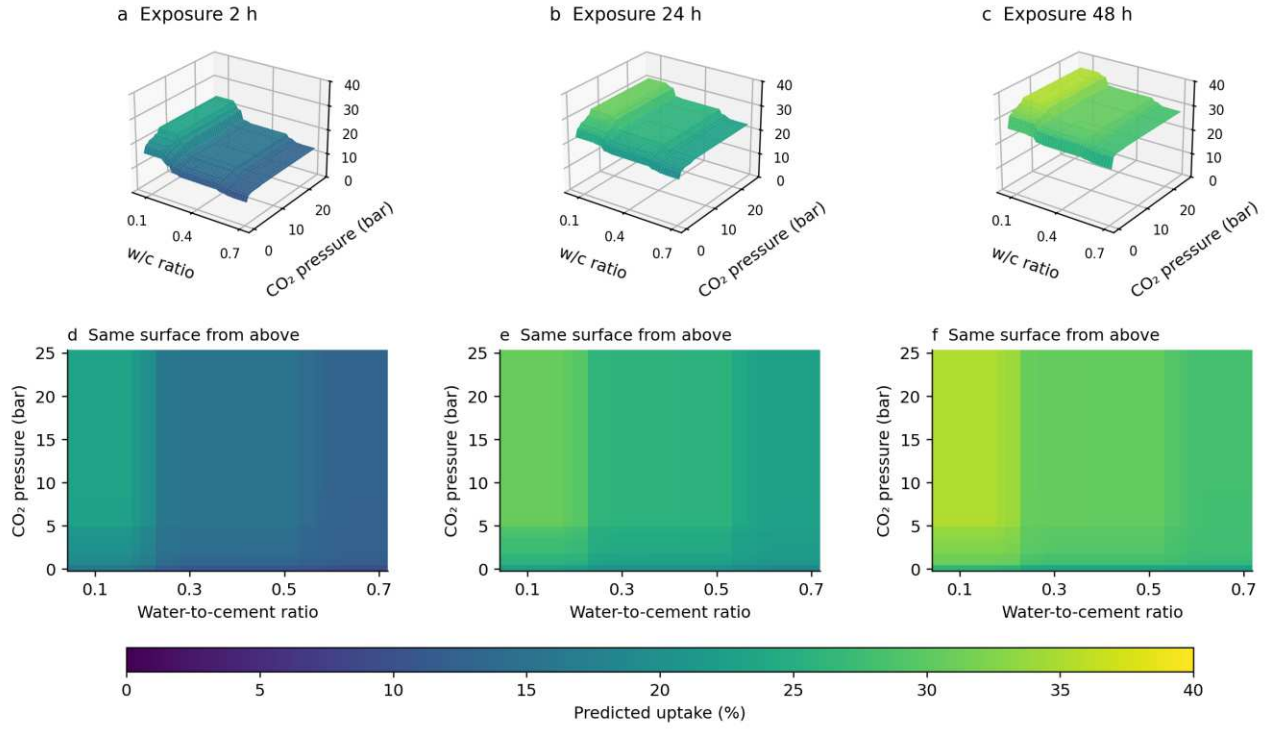


Figure 5. Conditional uptake surfaces at exposure times of 2, 24 and 48 h. Panels a–c show the fitted surfaces and d–f the same values from above. Water-to-cement ratio varies from 0.05 to 0.71 and CO₂ partial pressure from 0.1 to 25 bar on a 40 × 40 grid; the upper pressure endpoint slightly exceeds the observed maximum of 24.975 bar. Other settings are pre-curing 2 h, temperature 25 °C, relative humidity 55%, subsequent curing 2 d and thickness 38 mm. All panels share the same uptake scale. Surfaces use the full-data constrained model and are conditional predictions, not independent validation results.

Carbon balances and break-even conditions

Let U denote uptake in kg CO₂ per kg original material, η the fraction of supplied CO₂ retained, I the electricity carbon intensity, a the upstream electricity per kg CO₂ supplied, b the upstream non-electric emissions per kg CO₂ supplied, and E the curing electricity per kg original material. The process balance is

$$N = U - \frac{U}{\eta}(aI + b) - EI \quad (1)$$

Positive N denotes storage exceeding the assessed supply and curing emissions. With U , η , a , b and E held fixed, the electricity intensity at which the balance is zero is

$$I_{crit} = \frac{U(1 - b/\eta)}{aU/\eta + E} \quad (2)$$

This threshold is positive only if the numerator is positive and the denominator is non-zero. If $b \geq \eta$, the assumed non-electric burden alone prevents a positive balance for positive uptake and non-negative electricity intensity. The marginal effect of uptake, holding the inventory parameters fixed, is

$$\frac{\partial N}{\partial U} = 1 - \frac{aI + b}{\eta} \quad (3)$$

Accordingly, when $aI + b \geq \eta$, additional uptake cannot improve the balance under the assumed supply scaling. It also explains why a maximum-uptake condition need not maximise net storage. For nonzero compression that scales with supplied mass, the corresponding coefficient is given in Methods.

Net carbon response surfaces

Applying Eq. (1) to the uptake grid gives Fig. 6 for upstream scenario A at $I = 0.40 \text{ kg CO}_2/\text{kWh}$ and $\eta = 0.75$. At the assumed material mass $M = 2400 \text{ kg/m}^3$, the calculated net balance ranges from 0.0670 to 0.1765 $\text{kg CO}_2/\text{kg}$ original material at 2 h, 0.1436 to 0.2387 at 24 h, and 0.1769 to 0.2757 at 48 h. All grid points are positive under this particular inventory. This sign pattern is conditional on the supply, energy and mass-per-volume assumptions, and does not establish a positive balance for every material represented in the dataset.

For this scenario, the balance can be written $N = 0.84059U - 0.40E$. The first coefficient means that each additional unit of uptake leaves approximately 0.841 units after the assumed supply burden, before allowing for changes in curing electricity. Across the exposure panels, fan electricity rises as exposure is extended; across pressure, the mass-consistent compression term also increases above 1 bar. The net surface combines the predicted uptake with the energy required for each operating condition.

The compression calculation scales the compressed gas mass with supplied CO_2 , MU/η , where M is the mass of original material per cubic metre, and assumes pure CO_2 so that partial and total absolute pressure coincide. Relative to a fixed compressed mass of 30 kg/m^3 at the same $M = 2400 \text{ kg/m}^3$, this reduces the net balance by up to 0.0085, 0.0114 and 0.0132 $\text{kg CO}_2/\text{kg}$ original material on the respective 2, 24 and 48 h grids. No additional compression is required at the 1 bar inlet condition. Below 1 bar, vacuum demand is omitted; that part of the surface is an incomplete-energy scenario.

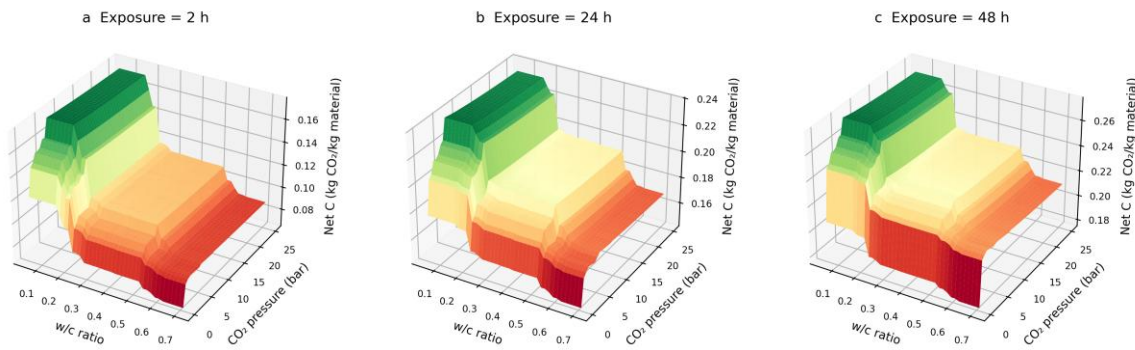


Figure 6. Conditional process carbon-balance surfaces at exposure times of 2, 24 and 48 h. Fixed settings are pre-curing 2 h, temperature 25°C , relative humidity 55%, subsequent curing 2 d and thickness 38 mm. Scenario A uses $a = 0.2473 \text{ kWh}$ per kg supplied CO_2 , $b = 0.02063488 \text{ kg CO}_2$ per kg supplied CO_2 , electricity intensity $0.40 \text{ kg CO}_2/\text{kWh}$ and utilisation 0.75. Balances use original-material mass, including aggregates, with assumed $M = 2400 \text{ kg/m}^3$. Compression uses the supplied mass and a pure-gas absolute-pressure scenario with a 1 bar inlet; vacuum demand below 1 bar is excluded. Panels have separate vertical and colour scales. All displayed balances are positive under these assumptions.

Electricity and curing inventory sensitivity

At the illustrative point $w/c = 0.4$, CO_2 partial pressure = 1 bar and exposure = 24 h, the full-data constrained model predicts $U = 0.230990$. Other inputs are pre-curing 2 h, temperature 25°C , relative humidity 55%, subsequent hydration 2 d and thickness 38 mm. The inventory assumes $\eta = 0.75$ and $E = 80.6/2400 = 0.033583 \text{ kWh}$ per kg original material. Five upstream scenarios give the balances in Table 1 and Fig. 7a. The mass conversion uses an illustrative $M = 2400 \text{ kg original material/m}^3$, not a measured density for every source study.

At $I = 0.05 \text{ kg CO}_2/\text{kWh}$ all five balances are positive, ranging from 0.189 to 0.219 $\text{kg CO}_2/\text{kg}$ original material. At $I = 0.40$, scenarios A–C remain positive and D–E are negative; at $I = 0.90$, A–B remain positive and C–E are negative. Their conditional break-even electricity intensities are 2.047, 1.116, 0.875, 0.314 and 0.330 $\text{kg CO}_2/\text{kWh}$ for A–E, respectively. At $I = 0.40$, the marginal coefficients in Eq. (3) are negative for D

and E. Increasing uptake while holding these supply assumptions fixed would therefore worsen their calculated balances.

Table 1. Conditional process carbon balances and break-even electricity intensities. $U = 0.230990$ kg CO₂/kg original material, $\eta = 0.75$ and $E = 0.033583$ kWh/kg original material. Balance columns have units kg CO₂/kg original material; intensity has units kg CO₂/kWh. Cases A–E are numerical scenarios, not verified rankings of named technologies.

Scenario	I = 0.05	I = 0.40	I = 0.90	Break-even I
A	+0.219	+0.181	+0.126	2.047
B	+0.215	+0.144	+0.044	1.116
C	+0.212	+0.122	-0.006	0.875
D	+0.189	-0.061	-0.418	0.314
E	+0.191	-0.048	-0.388	0.330

Pre-curing accounts for 77.2 of the baseline 80.6 kWh/m³ curing demand, or 95.8%, using the laboratory-conditioning coefficient described in Methods. Figure 7b varies this contribution from 0 to 120 kWh/m³ while retaining the other 3.4 kWh/m³ and the same uptake. This is an inventory sensitivity, not a prediction that uptake remains unchanged when pre-curing is altered. For scenario A at I = 0.40, omitting pre-curing electricity increases N by 0.0129 kg CO₂/kg original material. Evaluating the alternative fan and subsequent-curing coefficients in the supplied documentation gives N = 0.1771–0.1809 and break-even electricity intensity 1.892–2.053 for A (Supplementary Table S7). A–C remain positive and D–E negative at I = 0.40 across these four combinations. Varying M from 1000 to 2400 kg/m³ at fixed uptake and volumetric energy gives N = 0.1619–0.1807 for A; A–C remain positive and D–E negative at I = 0.40 (Supplementary Information).

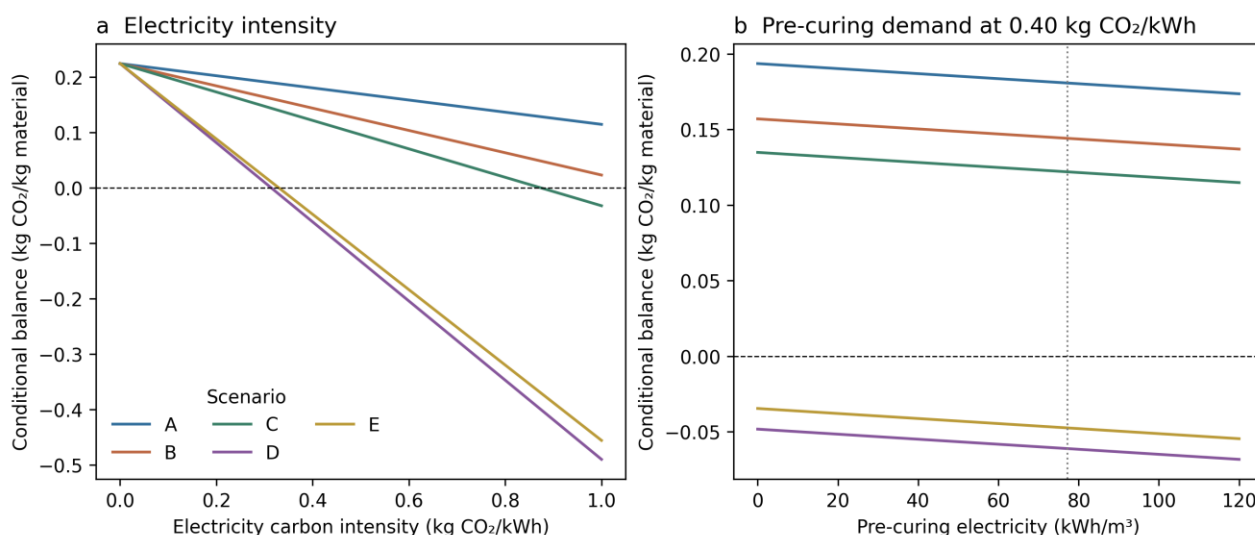


Figure 7. Conditional carbon-accounting sensitivity at $U = 0.230990$ kg CO₂/kg original material and $\eta = 0.75$. (a) Electricity intensity varies with curing electricity fixed at 80.6/2400 kWh/kg original material. (b) Pre-curing demand varies at electricity intensity 0.40 kg CO₂/kWh, retaining the other 3.4 kWh/m³ curing demand; the dotted line marks 77.2 kWh/m³. Upstream scenarios A–E are defined in Supplementary Table S4. Dashed horizontal lines mark zero balance. The calculations vary inventory assumptions at fixed uptake and do not represent confidence intervals or validated operating envelopes.

Discussion

The carbon balance explains why uptake alone is insufficient to assess the benefit of carbonation curing.

Greater uptake increases storage, but also increases CO₂ supply requirements through U/η . Curing emissions add a further dependence on operating conditions. Equation (3) separates the benefit of additional uptake from its supply burden, while Eq. (2) identifies the electricity intensity at which the remaining benefit is exhausted.

Longer exposure raises the fitted uptake under the imposed non-decreasing constraint, but also increases gas-circulation electricity. In scenario A, the uptake gain from 2 to 24 or 48 h outweighs this additional demand at the specified electricity intensity. In scenarios D and E, however, the supply burden makes the marginal uptake contribution negative at $I = 0.40$ kg CO₂/kWh. The value of increasing uptake therefore depends on how the CO₂ is supplied as well as on the material response.

The sensitivity calculations show how electricity supply and pre-curing affect the balance. All five supply scenarios are positive at the low electricity intensity; A–C remain positive at $I = 0.40$ and only A–B at $I = 0.90$ kg CO₂/kWh. Pre-curing accounts for 95.8% of baseline curing electricity, making the laboratory-derived coefficient a major component of the assumed energy demand. Varying this coefficient at fixed uptake isolates its accounting effect. Changing the physical pre-curing regime could also change uptake, which would require paired measurements of both quantities.

The difference between random and study-grouped validation is substantial. Random five-fold R^2 is 0.737 for the ensemble and 0.632 for the constrained model, but falls to -0.086 and -1.540 when source studies are kept intact. Leave-one-group-out evaluation confirms poor transfer (Supplementary Note “Cross study validation and interpretation of prediction errors” and Figs. S1–S2). The models can therefore describe patterns within the pooled data but are not validated for prediction in a new study. Monotonicity constraints control response direction; they cannot compensate for omitted composition variables, measurement differences or gaps in joint coverage. The surfaces should be interpreted as model-based scenarios rather than experimentally established optima.

The database brings dispersed experimental observations into a reusable set of modelling inputs. Harmonising uptake to original-material mass enables comparison while retaining differences among pastes, mortars and other material classes. Material composition, including binder mass fraction, and detailed measurement protocols are not among the eight predictors. The carbon inventory adds a separate set of assumptions: M represents a scenario mass per volume, the pre-curing coefficient is transferred from a laboratory experiment, and upstream allocation, circulation, subsequent curing and pressure handling follow the specified scenarios. Applying the calculation to an installation would require measurements appropriate to its materials, loading and equipment.

The accounting boundary covers CO₂ supply and selected curing operations. It excludes binder production, infrastructure, service life and end-of-life behaviour, and includes neither a strength-equivalent comparator nor an assessment of leakage and long-term storage permanence. A positive process balance therefore does not establish a carbon-negative product or avoided emissions relative to conventional concrete. Model RMSE also measures aggregate prediction error, so it is not used as a calibrated confidence interval for an individual carbon-balance estimate.

The next step is to pair the compiled uptake data with composition and detailed conditioning and measurement information, then test the coupling against independent uptake and energy measurements. This would establish whether conditions that increase uptake also improve net benefit in a specific process. The present database, equations and sensitivity calculations provide a basis for designing that evaluation.

Conclusions

We compiled a literature database and linked uptake prediction to CO₂-supply and curing emissions. The ensemble and constrained models achieve random five-fold R² values of 0.737 and 0.632, respectively. The coupled analysis shows how supply emissions, electricity intensity, utilisation and conditioning energy determine whether predicted uptake yields a positive net balance. At the example process point, the five supply scenarios give break-even electricity intensities of 0.314–2.047 kg CO₂/kWh. The database supports further analysis of carbonation curing, while the calculated thresholds make the dependence on the supply inventory explicit. Poor cross-study prediction limits the current numerical results to scenario comparison; operating recommendations require independent validation and material-specific inventories.

10 Methods

Data and preprocessing

We manually extracted reported material characteristics, curing conditions and CO₂ uptake from the source publications and curated the records into data_0519.xlsx. Uptake was converted during compilation to kilograms of CO₂ per kilogram of original material, including sand and aggregates where present, and is stored as a percentage. Supplementary Data 1 preserves the 465 curated records, eight predictors, target, material labels and source identifiers, together with workbook row numbers and inclusion flags. The broader compilation contains 548 records from 35 source identifiers. The Ref column retains the compilation's source identifiers for study-group validation; these identifiers are distinct from the numbered citations in this article.

The 35 source publications underlying the broader compilation are cited in the reference list [4–13, 15–23, 33–48], with DOI or publication details where available. They include cement and concrete, air-lime and slag-based materials. The curated workbook and broader compilation snapshot accompany the submission. The source bibliography documents the compilation as a whole; not every source contributes to the final 461-record modelling dataset.

All eight predictors and the uptake target in the curated workbook are numeric and non-missing. No further imputation is applied; earlier compilation changes are documented below. Four records above 150 °C (Number 135, 136, 144 and 145) are excluded to retain the original modelling domain. Three records repeat an earlier predictor–target vector and are retained because the table does not distinguish repeated experiments from duplicate extraction.

Supplementary Table S6 and the note “Retrospective comparison of the working tables” document changes between the broader compilation and curated workbook, including blank-to-numeric entries, range-to-scalar representations and changes to populated fields. This comparison records the development of the dataset. All analyses use the curated workbook without substituting values from the earlier version.

Predictors are ordered as water-to-cement ratio, pre-curing time, CO₂ partial pressure, temperature, relative humidity, exposure time, subsequent hydration time and thickness. Pre-curing time, pressure, exposure and subsequent hydration are transformed by $\log(1 + x)$; numerical values use the units in Supplementary Data 1. A StandardScaler is then fitted on the training data of each validation fold. The target is the recorded uptake percentage, without rescaling during regression. Division by 100 gives kg CO₂/kg original material for the carbon calculation. No further target conversion is made during this reanalysis.

Models and validation

Models are implemented with scikit-learn 1.7.2 [49]. They comprise ridge regression, a radial-basis support-vector regressor, random forest, gradient boosting, histogram-based gradient boosting, a multilayer perceptron, a weighted voting ensemble and a constrained histogram-based regressor. Supplementary Table S2 specifies

the configurations. The ensemble weights are 0.5 for histogram boosting, 0.3 for random forest and 0.2 for support-vector regression. The constrained model has 600 iterations, maximum depth 6, learning rate 0.1 and L2 regularisation 2. In predictor order, its monotonicity vector is $(-1, +1, +1, 0, 0, +1, 0, -1)$. These settings are held fixed; there is no hyperparameter search on the reported validation outcomes.

- 5 Random five-fold validation uses KFold with shuffling and `random_state = 1`. Study-grouped five-fold validation uses GroupKFold with five splits and no shuffling, keeping each Ref value intact. A pipeline containing the transformation, scaler and estimator is fitted separately in each training fold. R^2 is calculated as one minus the ratio of the pooled squared prediction errors to the sum of squared deviations from the pooled observed mean. RMSE is the square root of the mean squared prediction error; MAE is the mean absolute error. All error values are in uptake percentage points. Fold assignments and observation-level predictions accompany the code.

Additional source-group and leave-one-group-out evaluations, including a training-mean baseline and study-balanced MAE, are reported in Supplementary Note “Cross study validation and interpretation of prediction errors”. No tuning or model selection uses those outcomes. The original random 80:20 analysis is reported separately in the supplement and is not interpreted as study-level transfer.

For conditional scenario prediction, the constrained model and scaler are fitted to all 461 included observations. This full-data fit is separate from the validation fits. The full-data fit reproduces the saved model’s predictions in the specified software environment. The model is used for its imposed response directions; its study-grouped performance is reported separately.

20 **Conditional response calculations**

Figure 4 evaluates one input at a time with the other inputs fixed at their median values. Its panel-specific ranges are narrower than the full data range for some variables and extend beyond it for others. The accompanying code also provides 240-point full-range slices for numerical inspection. Both use the same fitted model.

- The two-dimensional surfaces use 40 equally spaced water-to-cement values between 0.05 and 0.71 and 40 pressure values between 0.1 and 25 bar at each of three exposure times (2, 24 and 48 h). Fixed values are pre-curing 2 h, temperature 25 °C, relative humidity 55%, subsequent curing 2 d and thickness 38 mm. The same uptake arrays feed the carbon surfaces, using scenario A and the mass-consistent compression calculation below. This is a conditional grid, not a search for experimentally admissible or optimal combinations. Figure 5 uses common plotting scales; Figure 6 uses separate panel scales. Each grid point and its comparison with the fixed-mass inventory is provided in `updated_surface_grid.csv`.

Process inventory and sensitivity calculations

- The accounting reference is 1 kg original material. Upstream terms cover assumed capture electricity, any electrified heat, liquefaction, vaporisation and a 100 km one-way diesel transport scenario. The coefficients a and b for each numerical scenario are specified in Supplementary Table S4. Thermal inputs assigned no additional burden remain allocation assumptions; numerical cases are labelled A–E rather than validated inventories for particular commercial plants. No new experiment or measured plant inventory is introduced.

- The wider inventory literature addresses concrete-construction environmental inventories [50], humidification energy [51], embodied energy of blocks [52] and freight range and congestion [53]. These references frame the processes and boundary choices that require assessment, rather than establishing the exact constants used in this scenario model. Electricity-intensity data are also available through the source cited in the original manuscript [54]; the present calculations use explicit illustrative intensities rather than updated country-specific observations.

Curing electricity is normalised by $M = 2400 \text{ kg original material/m}^3$, including sand and aggregates. This illustrative mass-per-volume value is retained from the original inventory configuration and is not a measured dry-material density for the pooled dataset. $M = 1000$ and 1800 kg/m^3 are additional sensitivity values, not inferred specimen properties. El-Hassan and Shao [55] report laboratory chamber demand of 154.58 and 695.61 kWh/m³ for 4 and 18 h conditioning, respectively (Table V, p. 291). Both imply approximately 38.6 kWh/(m³·h), retained here as a rounded coefficient. Its use at the modelled material loading and conditions is a scenario transfer, not an industrial measurement. At 25 °C, 55% relative humidity and 1 bar, heating, humidification and additional compression are zero. Pre-curing contributes 77.2 kWh/m³, fan circulation 1.0 kWh/m³, and subsequent curing 2.4 kWh/m³. Fan flow is assumed to be 0.05 m³/s per m³ processed material, at 500 Pa and efficiency 0.6; subsequent curing uses 0.05 kW/m³ for 48 h. The alternative documented flow of 0.01 and subsequent-curing power of 0.5 are evaluated separately and jointly in Supplementary Table S7.

For pressure-dependent calculations, all delivered gas $m = MU/\eta$ is compressed once after vaporisation at $P_0 = 1 \text{ bar}$. Specific compression electricity is $c(P) = RT \max[\ln(P/P_0), 0]/(3.6 \times 10^6 \eta c) \text{ kWh/kg gas}$, with $R = 188.9 \text{ J/(kg} \cdot \text{K)}$, $T = 298 \text{ K}$ and $\eta c = 0.7$. Pure CO₂ is assumed, equating the predictor to absolute total pressure; $E_{\text{comp}} = U_c(P)/\eta \text{ kWh/kg original material}$. No vacuum work, expansion credit, pressure recovery or detailed recirculation is modelled. With the other curing terms fixed, the marginal coefficient becomes $\partial N/\partial U = 1 - [aI + b + I_c(P)]/\eta$; Eq. (3) is recovered at 1 bar. Figure 7 varies electricity intensity and pre-curing demand at that point. These calculations assess the stated supply-and-curing boundary only.

Data availability

Supplementary Data 1 contains the curated modelling dataset, row-level inclusion flags and source-group identifiers. Supplementary Code and Data includes the broader compilation snapshot, fold assignments and observation-level validation predictions. The curated dataset contains the eight predictors required to reproduce the models.

Code availability

The model definitions, validation pipelines, saved model, scenario calculations and plotting scripts are supplied in Supplementary Code and Data, together with execution instructions and the software version requirements.

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Author contributions

L.C. contributed to conceptualisation, methodology, software, data curation, investigation, validation and writing the original draft. J.P. contributed to validation.

Competing interests

- 15 The authors declare no competing interests.

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