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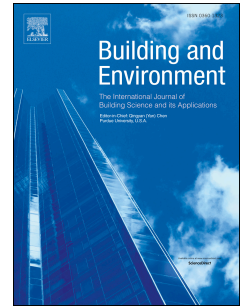
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Investigating CO₂ removal by Ca- and Mg-based sorbents with application to indoor air treatmentElliott T. Gall^{1,2,3}, Cem Sonat², William W Nazaroff^{3,4}, Cise Unluer^{2,*}¹Mechanical and Materials Engineering, Portland State University, Portland, OR 97201, USA²Civil and Environmental Engineering, Nanyang Technological University, Singapore³Berkeley Education Alliance for Research in Singapore, 1 Create Way, 138602, Singapore⁴Civil and Environmental Engineering Department, University of California, Berkeley, CA* Corresponding author. Tel.: +65 91964970, E-mail address: ucise@ntu.edu.sg**Abstract**

Indoor carbon dioxide (CO₂) levels serve as an indicator of ventilation sufficiency in relation to metabolic effluents. Recent evidence suggests that elevated CO₂ exposure (with or without other bioeffluents) may cause adverse cognitive effects. In shelter-in-place (SIP) facilities, indoor CO₂ levels may become particularly elevated. This study evaluates four low-cost alkaline earth metal oxides and hydroxides as CO₂ sorbents for potential use in indoor air cleaning applications. Sorbents studied were MgO, Mg(OH)₂, Ca(OH)₂ and commercially available soda lime. Uncarbonated sorbents characterized with nitrogen adsorption porosimetry showed BET surface areas in the 5.6-27 m²/g range. Microstructural analyses, including X-ray diffraction, thermogravimetric analysis and scanning electron microscopy confirmed the carbonation mechanisms and extent of sorption under environmental conditions typical of indoor spaces. Ca-based sorbents demonstrated higher extent of carbonation than Mg-based sorbents. Laboratory parameterizations, including rate constants (k) and carbonation yields (y), were applied in material balance models to assess the CO₂ removal potential of Ca-based sorbents in three types of indoor environments. Soda lime ($k = [2.2 - 3.6] \times 10^{-3} \text{ m}^3 \text{ mol CO}_2^{-1} \text{ h}^{-1}$, $y = 0.49-0.51$) showed potential for effective use in SIP facilities. For example, CO₂ exposure in a modeled SIP facility could be reduced by 80% for an 8-h sheltering interval and to levels below 5000 ppm for an 8-h period with a practically sized air cleaner. Predicted effectiveness was more modest for bedrooms and classrooms.

29 Keywords: Ventilation, bioeffluents, air cleaning, indoor air pollution, sorption

30

31 **1. Introduction**

32 Excluding emissions from unvented combustion, carbon dioxide (CO₂) concentrations in
33 occupied indoor spaces depend on three main factors: the CO₂ emission rate from human metaboli-
34 sm, the outdoor CO₂ concentration, and the outdoor air ventilation rate. Indoor CO₂ levels are
35 primarily managed through the replacement of indoor air with outdoor air. However, providing
36 outdoor air ventilation for buildings, while necessary to achieve indoor air quality objectives, can
37 contribute substantially to building energy use [1]. Decreasing the outdoor air exchange rate is one
38 strategy to reduce the energy demand of buildings, as mechanical ventilation requires energy input
39 to fans and may contribute to heating, cooling, and dehumidification needs, depending on site- and
40 time-specific environmental conditions. However, reducing outdoor air-exchange rates tends to
41 increase the concentrations of indoor-generated air pollutants, including CO₂. Indoor CO₂ levels may
42 also become elevated when building operation is altered temporarily (e.g. when air exchange is
43 minimized to protect occupants from hazardous outdoor conditions) including events that
44 precipitate the need for a shelter-in-place (SIP) response [2].

45 Carbon dioxide, a primary product of human metabolism, is often used as a proxy for indoor-
46 emitted air pollutants [3,4]. It is generally not considered harmful at levels routinely encountered in
47 buildings. Rather, high levels of indoor CO₂ imply that ventilation is insufficient to adequately dilute
48 air pollutants emitted by occupants or other indoor sources. However, some emerging evidence
49 suggests that exposure to elevated CO₂ at levels commonly encountered indoors may adversely
50 affect human cognition [5–7]. The matter is not yet resolved; other recent studies imply that other
51 bioeffluents or possibly some combination of CO₂ and other bioeffluents may be the causative
52 agents [8–12].

53 The US Occupational Safety and Health Administration (OSHA) has set an 8 hour (h)
54 permissible exposure limit (PEL) of 5,000 ppm for CO₂. Levels in SIP facilities might rise above this

55 threshold. One specific motivation for this study is that a household SIP facility is mandatory in
56 Singapore in all government constructed housing built after 1998 [13]. This requirement is
57 noteworthy as government housing in Singapore provides accommodation for approximately 85% of
58 the country's population [14]. A prior investigation of SIP habitability in the US context showed that
59 CO₂ levels could reach 16,000 ppm after 3 h of occupancy by five persons [15]. Exposure to such
60 levels could result in acute health consequences, as evidenced by studies investigating exposures in
61 spacecraft that show adverse effects including lethargy, malaise, and headache at CO₂
62 concentrations between 4,000 and 10,000 ppm [16]. Studies supporting the OSHA PEL showed
63 electrolyte imbalances, metabolic changes, and non-narcotic central nervous system effects for
64 short-term exposures to CO₂ in the range 10,000-30,000 ppm [16,17].

65 Given the common occurrence of elevated CO₂ concentrations in certain indoor spaces
66 combined with the possibility of acute health effects in SIP facilities and cognitive decrements in
67 other settings, this study investigates the possibility of controlling indoor CO₂ via active removal by
68 means of low-cost solid sorbents that could be integrated into a recirculating indoor air cleaner.
69 Capture of CO₂ with solid sorbents is an emerging area of research with promising potential for
70 future lower cost approaches for CO₂ control [18], including the application of sorbents that are
71 derived from waste materials [19]. Solid sorbents such as metal oxides and hydroxides are
72 considered promising candidates for removing CO₂ from flue gases through carbonation during
73 which oxides or hydroxides are converted into stable carbonates [20,21]. Sorbents under
74 development for use in carbon capture from fossil fuel combustion typically target operation at
75 higher temperatures (on the order of 400 °C or greater) and at elevated CO₂ levels (up to the order
76 of 10%), although approaches for room temperature operation at outdoor ambient CO₂ levels have
77 also been reported [22,23].

78 During the carbonation process, gaseous CO₂ dissolves in water, becoming carbonic acid,
79 which neutralizes the hydroxides (e.g. portlandite (Ca(OH)₂) or brucite (Mg(OH)₂)). Two main factors
80 control the rate and degree of carbonation of CaO and/or MgO and their derivatives: (i) sorbent

81 composition (chemical and physical properties of the solid components, water content and presence
82 of additives) and (ii) environmental conditions (CO_2 concentration and pressure, relative humidity
83 (RH), temperature and duration) [24–28]. The main factors influencing the carbonation of Ca- or Mg-
84 based sorbents can be summarized as the transport of CO_2 to the sorbent surface and its reactivity
85 with the sorbent. Transport is affected by environmental conditions (i.e. air pressure, CO_2
86 concentration, and abundance of water, etc.) and the pore structure of the sorbent, whereas the
87 sorbent composition and material properties influence its reactivity. In the case of Mg-based
88 sorbents, the hydration of MgO leads to the formation of magnesium hydroxide (brucite, $\text{Mg}(\text{OH})_2$).
89 In the presence of sufficient water, brucite reacts with CO_2 , leading to the formation of hydrated
90 magnesium carbonates such as nesquehonite ($\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$), hydromagnesite
91 ($4\text{MgCO}_3 \cdot \text{Mg}(\text{OH})_2 \cdot 4\text{H}_2\text{O}$), dypingite ($4\text{MgCO}_3 \cdot \text{Mg}(\text{OH})_2 \cdot 5\text{H}_2\text{O}$) and artinite ($\text{Mg}_2\text{CO}_3 \cdot \text{Mg}(\text{OH})_2 \cdot 3\text{H}_2\text{O}$)
92 [29–33]. Higher CO_2 concentrations increase the rate and degree of carbonation at initial stages [24].
93 The presence of water within the sorbent plays an important role in the degree of hydration and
94 carbonation as the initial water content both facilitates the hydration and carbonation reactions and
95 influences the rate of CO_2 diffusion through the sorbent system. In dry CO_2 scrubbing, low water
96 content present in sorbent media and low RH in air surrounding the sorbent delay the carbonation
97 reaction, whereas an increase in the water content of the media speeds the carbonation reaction
98 but results in a decrease of CO_2 diffusion since the diffusivity of CO_2 is much slower in water than it is
99 in air (i.e. the diffusion coefficient of CO_2 is $16 \text{ mm}^2/\text{s}$ in air vs. $0.0016 \text{ mm}^2/\text{s}$ in water [34]).
100 Therefore, rapid sorption kinetics require sufficient water for hydration and subsequent carbonation
101 but not so much water as to interfere with rapid diffusion of CO_2 through the sorbent system.
102 Previous studies have shown that RH values in the approximate range 40-80% are preferable for
103 increased carbonation of the Mg and Ca oxides [35–37]. The rates of diffusion of CO_2 into the
104 sorbent matrix and its subsequent interaction with Ca and Mg are of interest in this study.

105 If solid sorbents can be integrated into stand-alone indoor air cleaners, they can be deployed
106 to control CO_2 concentrations in locations such as SIP facilities and other indoor locations where CO_2

107 levels may be temporarily elevated. Apart from SIP environments, other potentially attractive
108 locations are those where specific populations spend substantial proportions of their day in
109 conditions that may not always be sufficiently ventilated, such as bedrooms overnight and
110 classrooms during the day [38]. Several recent efforts further describe the potential and
111 opportunity of CO₂ capture techniques specifically suited for built environments [39–41]. This study
112 employs a range of experimental methods to characterize the physico-chemical properties and
113 carbonation products, kinetics and yields of four alkaline earth metal oxides and their hydroxides.
114 Also provided is an estimate of the efficacy of potentially promising sorbents when integrated into a
115 standalone air cleaner under three hypothetical scenarios. Cases considered are those in which
116 active CO₂ removal may be beneficial owing to one or more of these factors: high occupant density,
117 small room volume, low air-exchange rate, and a susceptible population. Three specific cases are
118 explored: (i) SIP facilities in residential environments, (ii) sleeping microenvironments, and (iii)
119 school classrooms.

120 **2. Materials and Methods**

121 **2.1 Sorbents**

122 A commercial CO₂ solid sorbent, SodaSorb (Grace Chemical), consisting of a mixture of
123 Ca(OH)₂, H₂O, NaOH and KOH, was purchased from Advanced Marine Pte Ltd, Singapore. The
124 performance of this sorbent was compared to three other products: MgO (commercial name
125 “calcined magnesite 92/200”) obtained from Richard Baker Harrison Ltd (UK) and high purity (>95%)
126 Ca(OH)₂ and Mg(OH)₂ purchased from Aik Moh Paints & Chemicals, Singapore.

127 Particle size distributions of three sorbents (MgO, Ca(OH)₂ and Mg(OH)₂), in the form
128 received from the manufacturer, were measured with a particle size analyzer (Mastersizer 2000,
129 Malvern). Particle size of the sorbents is reported as the d₅₀, or mass median particle size. The
130 internal physical properties of the four sorbents were measured via nitrogen adsorption porosimetry
131 conducted at 77 K (Quantachrome Quadrasorb). All four samples were ground to a fine powder in a
132 mortar and pestle prior to analysis to facilitate outgassing of samples and equilibration with N₂

133 partial pressure during adsorption or desorption cycles. Note that this results in the reporting of a
134 specific surface area, or the interior surface area normalized by mass. It is possible that transport
135 limitations will reduce the 'effective' surface area below the specific surface areas reported if
136 sorbents are implemented with larger grain size than the fine powders used in N₂ adsorption
137 porosimetry. Samples of all four sorbents were outgassed at < 0.1 Torr and 125 °C for 8 hours
138 before measuring nitrogen adsorption isotherms. Surface areas of the sorbents were determined by
139 applying Quantachrome's BET theory; their cumulative pore volumes and average pore sizes were
140 determined with Quantachrome's density functional theory.

141 **2.2 Characterizing CO₂ uptake on sorbents**

142 **2.2.1 Carbonation of sorbents**

143 The four sorbents were subjected to carbonation in a controlled laboratory apparatus as
144 shown in Figure 1. Compressed laboratory air was first passed through a membrane dryer that
145 included a 0.01 micron pre-filter (Laman MD-15LS and Laman SAM350-E, Air Parts Center Pte Ltd) to
146 remove water vapor and particulate matter present in laboratory air. Dry air was then passed
147 through an activated carbon packed bed (BPL 6 × 16, Calgon Carbon). The outlet flow was split to
148 control the humidity level, with one stream passing through a washing column filled with deionized
149 water. The flow rates through the dry and humidified air streams were regulated using mass flow
150 controllers (Omega FMA5500, Omega Singapore). In parallel, a small flow supplied from a
151 compressed gas cylinder of food-grade CO₂ (> 99% purity) was injected into the main flow to achieve
152 the desired CO₂ concentration set-point. The two flow streams were combined and directed to a
153 temperature controlled enclosure (KBE3.1, Binder GmbH). Inlet and outlet CO₂, temperature and RH
154 (Teleaire 7001, Onset Computer Corporation) were measured upstream and downstream of a
155 reaction chamber that was either a washing column loaded with a specific sorbent/water ratio or a
156 packed bed reactor loaded with dry sorbent.

157 A calibration curve was developed between the two CO₂ monitors by collocating the
158 monitors and recording responses at five CO₂ levels ranging between 0 and 2500 ppm. The resulting
159 linear equation was applied to adjust the readings of the downstream CO₂ monitor.

160 Sorbents were tested in two sets of experiments. Longer term tests were conducted with
161 sorbents in slurries with deionized water, at a loading rate of 0.1 g sorbent per gram of deionized
162 water in a total volume of 100 cm³ and maintained at a constant temperature of 25 °C. The RH in the
163 inlet air stream was elevated to > 75% to limit the evaporation of water from the slurry. Tests were
164 conducted for 7 days at a flow rate of 2.7 L/min with a constant CO₂ concentration of 2200 ppm to
165 observe carbonation while minimizing limitations to CO₂ uptake that may result from the availability
166 of H₂O. These experiments are subsequently referred to according to experimental conditions. For
167 example, experiment 'MgO-0.1-2.7-2200' refers to the carbonation of the sorbent MgO at a loading
168 rate of 0.1 g (sorbent)/g (H₂O), flow rate of 2.7 L/min, and inlet CO₂ concentration of 2200 ppm.
169 Carbonated sorbent products were extracted from the column, centrifuged to separate the sorbent
170 from residual water and dried for 48 hours under low RH in a temperature/RH controlled chamber (T
171 = 20 °C, RH < 10%).

172 Sorbents that exhibited effective carbonation during the 7-day tests were selected for
173 further analysis to characterize uptake kinetics and reaction yields. Sorbents were tested under dry
174 and slurry conditions. Dry experiments were conducted with a loading of 5 g of media placed on a
175 wire mesh under a constant inlet RH of 75%. Slurry experiments were conducted at a loading ratio of
176 0.03 g sorbent/g water in a total volume of 100 cm³. Both dry and slurry experiments were
177 conducted at two flow rates: 1.8 and 2.7 L/min. These flow rates correspond to contact times of 0.28
178 and 0.18 seconds, respectively, in dry experiments and 0.45 and 0.3 seconds, respectively, in slurry
179 experiments. All experiments were conducted at 25 °C. Inlet and outlet temperature, RH and CO₂
180 levels were measured at five-minute intervals. Each experiment was conducted until the sample
181 appeared to be fully carbonated under the set conditions, defined as when the 1-h running average
182 inlet and outlet CO₂ concentrations were equal to within ±25 ppm.

183 Carbonation yields were determined from the time-integrated difference between inlet and
184 outlet CO₂ monitors across the duration of an experiment to determine the total mass of CO₂
185 removed. This mass of CO₂ uptake was divided by the initial mass of sorbent and converted to moles
186 to determine the molar yield, y (mol sorbed CO₂/mol sorbent initially present). For soda lime, the
187 estimate of moles of sorbent was made from the mass of only Ca(OH)₂, as the KOH and NaOH served
188 as catalysts and were not consumed in the carbonation reaction [42,43]. Measured masses of soda
189 lime were multiplied by 0.85 to obtain the mass of Ca(OH)₂ used in subsequent interpretation of
190 experimental results and modeling, according to the 85% Ca(OH)₂ content within soda lime as
191 specified by the manufacturer. Reaction rate constants, k (m³ (mol CO₂)⁻¹ h⁻¹), were determined using
192 coupled equations describing the time-varying quantities of CO₂ and unreacted sorbent in the
193 reactor. The model equations and procedures employed to estimate k and y are provided in the
194 Supporting Information; Figure S1 illustrates results for a sample experimental run.

195 **2.2.2 Microstructural analysis**

196 Selected samples from the 7-day CO₂ uptake experiments were stored in acetone for at least
197 7 days to stop hydration, followed by vacuum drying for another 7 days in preparation for X-ray
198 diffraction (XRD), thermogravimetric analysis (TGA) and scanning electron microscopy (SEM)
199 analyses. The vacuum-dried samples were ground to a powder fine enough to pass through a 75 μm
200 sieve before they were analyzed under XRD and TGA. The XRD measurements, aimed to determine
201 the crystallinity of compounds and identify and distinguish between different phases within the
202 samples, were made on a Philips PW 1800 spectrometer using Cu K_α radiation (40 kV, 30 mA) with a
203 scanning rate of 0.04° 2θ/step from 5 to 55° 2θ. TGA was conducted on a Perkin Elmer TGA 4000
204 instrument using a temperature range from 50 to 900 °C with a heating rate of 10 °C/min under
205 nitrogen flow. The vacuum-dried samples were mounted onto aluminum stubs using double-sided
206 adhesive carbon disks and coated with gold before SEM analysis. The SEM analysis was carried out
207 with a Zeiss Evo 50 microscope to investigate the morphologies of the hydration and carbonation
208 products within the prepared samples.

209 2.3 Modeling CO₂ removal in three indoor environments

210 Laboratory sorbent characterization results were used as inputs into material-balance
211 models to conduct a scaling analysis of the efficacy of hypothetical deployments of stand-alone CO₂
212 scrubbers in three types of indoor environments where CO₂ concentrations are routinely elevated:
213 shelter-in-place (SIP) facilities [15,44], bedrooms [14,45] and classrooms [46]. Model inputs
214 describing indoor spaces and occupancy were selected to be generally representative of such
215 environments in the Singapore context, as summarized in Table 1. Room volume and occupancy
216 levels for the SIP facility (5 m³ for 2 persons) were calculated considering measurements made in a
217 typical Singaporean apartment and Singapore regulations that stipulate a minimum of 1.8 m³ of
218 shelter volume per occupant [47]. Note that regulations recommend greater SIP volume than the
219 stipulated minimum for increased comfort during an emergency. Room volume for the bedroom was
220 based on measurements of a recently constructed (< 5 y old) 3-bedroom apartment that is a typical
221 Singapore residence; volume and occupancy levels of classrooms were taken from a study of six
222 primary school classrooms in Singapore [46]. Emission rates of CO₂ were made following the
223 procedure described by Persily et al. [48], with assumptions as described in Table 1 annotations.

224 Ventilation flow rates in the bedroom and SIP environments were determined from the
225 average value of triplicate measurements of air exchange rates calculated from the decay of CO₂ that
226 was injected into an unoccupied bedroom and household shelter. Ventilation flow rates in the
227 classroom environment were taken as the average of CO₂ tracer decay measurement results made in
228 six unoccupied, air-conditioned classrooms in primary schools in Singapore [46]. In bedrooms and
229 classrooms, windows and doors were sealed during measurements to reflect a 'low flow' condition
230 where the exchange of indoor and outdoor air is intentionally reduced to minimize intrusion of
231 warm, humid outdoor air into the buildings. In the SIP facility, measurements were made in a typical
232 household shelter and, per peacetime requirements dictated in the Singapore building code, the
233 ventilation sleeve was opened to 25% of the total sleeve area [47]. During an emergency, the sleeve

234 would be fully closed, likely reducing the air exchange rate in the household shelter to a value lower
235 than that reported here.

236 The efficacy of an air cleaner containing a CO₂-removing sorbent was evaluated for the three
237 hypothetical indoor environments by solving coupled material balance equations written for (i) the
238 concentration of CO₂ in the room, (ii) the concentration of CO₂ through a packed bed of sorbent and
239 (iii) the quantity of the unreacted sorbent in the air cleaner. These equations are presented in the
240 Supporting Information. Modeling of indoor environments was conducted for practically sized air
241 cleaners considering the mass of media, volume of air cleaner, and resulting pressure drop across
242 the packed media bed. Rates of carbonation were assumed to remain constant as total pressure
243 varied across the modeled packed bed. Prior studies indicate that total pressure influences uptake
244 but only for orders of magnitude higher changes in total pressure than are relevant in the present
245 context [49]. Flow rates through a hypothetical air cleaner were selected to maintain air-media
246 contact times for dry sorbents that matched those used in experiments described in §2.2.1. Scrubber
247 dimensions were selected to allow the contact time to be held constant while providing a volumetric
248 flow rate similar to commercial air cleaners appropriately sized for the indicated indoor
249 microenvironment.

250 **3. Results and Discussion**

251 **3.1 Physicochemical properties of sorbents**

252 Physical and chemical properties of the four sorbents considered in this investigation are
253 shown in Table 2. The MgO, Mg(OH)₂, and Ca(OH)₂ materials represent pure or nearly pure
254 compounds that are commercially available, low-cost, and may be derived from waste streams [19].
255 A stream for reusing alkaline earth metal oxides or hydroxides that simultaneously addresses an
256 indoor air quality concern could represent a valuable opportunity. The fourth sorbent considered,
257 soda lime, is mainly Ca(OH)₂; however, it is specifically designed for CO₂ scrubbing by the addition of
258 (a) two catalysts (KOH, NaOH) and (b) approximately 10% H₂O to accelerate the uptake of CO₂ and
259 subsequent conversion of Ca(OH)₂ to CaCO₃. The physical properties summarized in Table 2 reveal

260 only modest variation in properties across the four sorbents. The measured mass median particle
261 sizes (d_{50}) of the three powder samples (MgO , $\text{Mg}(\text{OH})_2$, and $\text{Ca}(\text{OH})_2$) ranged between 5 and 19 μm ,
262 whereas the grain size for the soda lime media was reported as 1 mm (by the manufacturer). Particle
263 size distributions for the powder samples are provided in Figure S2 of the Supporting Information.
264 Note that in the subsequent modeling of indoor spaces, granular media with a d_{50} of 1 mm is
265 assumed for both soda lime and $\text{Ca}(\text{OH})_2$; the implications of this assumption for the modeling of a
266 hypothetical $\text{Ca}(\text{OH})_2$ packed bed are discussed in §3.3. The specific surface areas of these materials
267 are a few orders of magnitude lower than values for other engineered sorbents for CO_2 and gas-
268 phase pollutants, such as metal organic frameworks [50,51]. Among the four sorbents considered,
269 MgO has the highest internal surface area, 28 m^2/g , a factor of five higher than the value for pure
270 $\text{Mg}(\text{OH})_2$. Increasing specific surface area may present a useful pathway for enhancing the uptake of
271 CO_2 to low-cost sorbents, as it is probable that the availability of CO_2 sorption and/or reaction sites is
272 a factor that limits uptake of CO_2 .

273 3.2 Characterizing CO_2 uptake by sorbents

274 3.2.1 X-ray diffraction

275 XRD patterns of Ca- and Mg-based sorbents subjected to a flow rate of 2.7 L/min under a
276 constant CO_2 concentration of 2200 ppm for 7 days are shown in Figures 2 (a) and (b), respectively.
277 Sorbents containing $\text{Ca}(\text{OH})_2$ and soda lime indicate the formation of the carbonation product
278 calcite, whose main peak is observed at $29.4^\circ 2\theta$ along with several secondary peaks. The absence of
279 the major hydroxide phase portlandite ($\text{Ca}(\text{OH})_2$) in the presented patterns is a clear indication that
280 the prepared samples have fully carbonated during the 7 days of exposure. As these samples were
281 subjected to accelerated carbonation conditions under an elevated CO_2 concentration and flow rate,
282 the hydroxide phases within the soda lime and $\text{Ca}(\text{OH})_2$ based sorbents have been transformed into
283 calcite, as observed in the XRD patterns.

284 The crystalline phases forming after the carbonation of Mg-based sorbents are shown in
285 Figure 2(b). In addition to magnesium carbonate, some of the common carbonation products

286 observed were hydrated magnesium carbonates (HMCs) such as dypingite and hydromagnesite.
287 Dypingite (powder diffraction file (PDF) #029-0857) has its four highest intensity peaks at 15°, 30.4°,
288 13.7° and 21° 2 θ followed by peaks at 12°, 20°, 27.9°, 41.3°, 45.5°, and 44.8° 2 θ . Most of the strong
289 peaks and many of the weaker ones can be seen in the XRD patterns presented, confirming the
290 presence of dypingite. Hydromagnesite (PDF #025-0513) has its highest intensity peaks at 15.3°,
291 30.8° and 13.7° 2 θ , which are similar to those of dypingite and hence are expected to overlap in the
292 XRD spectra. Hydromagnesite (PDF #003-0093) also has sharp peaks in the high-angle region at 42°
293 and 45.5° 2 θ , where small peaks can be seen in the presented diffractograms. These peaks confirm
294 the presence of hydromagnesite in the samples.

295 Other than the carbonation products, the presence of brucite is observed in both samples,
296 where unhydrated MgO peaks can be seen in the MgO-based sorbent. The presence of the MgO
297 peak at 42.9° 2 θ indicates incomplete hydration, whereas the brucite peak at 38° 2 θ is an indication
298 of incomplete carbonation of both samples. These results clearly indicate that the carbonation
299 conditions utilized in this study were not sufficient for the Mg-based samples to fully carbonate
300 within the given exposure period. In principle, improved carbonation could be realized via (i) the use
301 of a higher reactivity MgO with a larger specific surface area to increase the rate and degree of
302 hydration and the subsequent carbonation process and (ii) optimization of the carbonation
303 conditions to increase the rate and amount of CO₂ diffusion within the samples.

304 3.2.2 Thermogravimetric analysis

305 The TGA results for the Ca- and Mg-based sorbents are shown in Figure 3(a) and (b),
306 respectively. As can be seen in Figure 3(a), the thermal decomposition of Ca-based sorbents
307 followed a regular pattern, indicating the decomposition of the main carbonate phase, calcite. This
308 decomposition occurred between temperatures of 650 and 830 °C as expected, resulting in a weight
309 loss of about 44% in both samples. Corroborating the XRD results, this outcome shows that both
310 samples have fully carbonated as the molar mass calculations of the carbonation reaction indicate
311 that CO₂ (44 g/mol) represents 44% of the overall mass of calcite (100 g/mol). The similar

312 decarbonation behavior and weight loss of soda lime and $\text{Ca}(\text{OH})_2$ -based samples is a clear indication
313 that they demonstrated similar carbonation capabilities notwithstanding the additives (i.e. NaOH
314 and KOH) included in the commercial soda lime sorbent.

315 The thermal decomposition behavior of Mg-based samples, shown in Figure 3(b), is slightly
316 more complex as in addition to uncarbonated brucite, these samples contain several carbonate
317 phases with different decomposition patterns. According to the weight lost shown in the TGA curves,
318 the decomposition steps of Mg-based samples can be divided into 3 main stages, whose details are
319 listed in Table 3: (i) < 300 °C: loss of unbound water and water of crystallization of HMCs associated
320 with their dehydration; (ii) 300-500 °C: dehydroxylation of HMCs and decomposition of any
321 uncarbonated brucite; and (iii) > 500 °C: decarbonation process involving the decomposition of
322 HMCs into MgO.

323 The two endothermic peaks corresponding to the loss of unbound water and dehydration of
324 water bonded to HMCs were observed at ~ 120 and 250 °C, respectively. A strong endothermic peak
325 reflecting the decomposition of uncarbonated brucite accompanied by the dehydroxylation of HMCs
326 (hydromagnesite and dypingite) was observed at ~ 450 °C. This transformation was followed by a
327 broader peak corresponding to the decarbonation of HMCs at ~ 680 °C. The similar decomposition
328 patterns and final weights demonstrated by the MgO and $\text{Mg}(\text{OH})_2$ samples clearly indicate their
329 comparable extents of carbonation. The presence of the large brucite peak within both samples is a
330 clear indication of incomplete carbonation, which was in agreement with the XRD patterns.

331 **3.2.3 Scanning electron microscopy**

332 Figure 4 shows the microstructures of the 4 samples analyzed by XRD and TGA. The SEM
333 images of the soda lime (Figure 4(a) and (b)) and $\text{Ca}(\text{OH})_2$ -based samples (Figure 4(c) and (d)) reveal
334 similar morphologies at both magnifications. The formation of tightly packed calcite crystals of
335 different sizes can be observed in both samples. Hexagonal calcite crystals are accompanied by
336 sparsely distributed crystals of acicular shape in the $\text{Ca}(\text{OH})_2$ based sample, as shown in Figure 4(c).

337 In general, both samples indicate a dense formation of calcite, in agreement with the results of the
338 TGA and XRD analyses.

339 As depicted in Figure 4(e)-(h), the microstructure of MgO and Mg(OH)₂ based samples are
340 dominated with rosette-like formations of brucite, as was indicated by the TGA and XRD analyses.
341 The main difference between the two samples is the size and density of brucite formations. The
342 direct hydration of MgO results in the dense formation of brucite particles that are fused into large
343 agglomerates. The direct inclusion of Mg(OH)₂ produces a porous distribution of brucite particles
344 with smaller sizes. However, the morphology of these brucite formations did not influence their
345 carbonation potential as both samples demonstrated similar carbonation behaviours and capacities.
346 Minor formations of hydromagnesite and dypingite are observed around the brucite crystals, which
347 is a clear indication of limited carbonation within these samples.

348 **3.2.4 Kinetics and capacity of CO₂ uptake by Ca-based sorbents**

349 This section describes the results of the uptake experiments for the Ca-containing sorbents.
350 The Mg-containing sorbents did not sufficiently carbonate under the experimental conditions to
351 justify characterizing their kinetic and yield parameters. Some combination of catalysis (as in the
352 case of soda lime) or alteration of physical parameters (e.g., increasing the specific surface area)
353 would be required to increase the kinetics and capacity such that MgO or Mg(OH)₂ based sorbents
354 may be considered effective for CO₂ removal under conditions relevant to indoor environments.

355 Experimental conditions, rate constants and carbonation yields for soda lime and pure
356 Ca(OH)₂ are reported in Table 4. Rate constants and yields are generally higher for soda lime than for
357 Ca(OH)₂, which is as expected given the presence of two catalysts plus water in soda lime to facilitate
358 the carbonation reaction. Under dry conditions (i.e., for solid sorbents with inlet airflow at 75% RH),
359 low yields were determined for Ca(OH)₂. As will be further explored in §3.3, these limitations
360 constrain the effectiveness of dry Ca(OH)₂ as a CO₂ sorbent under representative indoor conditions.
361 However, when the experimental flow rate was increased from 1.8 to 2.8 L/min, the reaction rate of
362 CO₂ with Ca(OH)₂ increased to nearly that of soda lime, albeit with substantially lower yield. This

363 increase in kinetics illustrates potential for subsequent optimization of air cleaners utilizing $\text{Ca}(\text{OH})_2$
364 media in indoor air treatment applications.

365 We explored the role of water availability by conducting experiments in both slurry and
366 packed dry-bed configurations. Under slurry conditions, the carbonation yield for $\text{Ca}(\text{OH})_2$ is
367 substantially higher than for dry-bed conditions, approaching that of soda lime. A slurry
368 configuration is likely infeasible for indoor air cleaning applications owing to high pressure drops
369 across a water column and the high-humidity effluent. However, future research could be
370 worthwhile to pursue, investigating in more detail the role of water or water vapor influencing the
371 uptake of CO_2 by Ca-containing sorbents with the goal of increasing CO_2 removal rates on low-cost
372 sorbents.

373 **3.3 Modeling indoor CO_2 removal**

374 Modeled indoor CO_2 concentrations for the three hypothetical scenarios (SIP, bedroom, and
375 classroom settings) are shown in Figure 5. In each case, a duration of 8 h is simulated, to
376 approximate a single-event occupancy in each of the three types of spaces. In this section, results for
377 CO_2 removal for 8-h model durations are described for each scenario, focusing on conditions that
378 result in greater observed removal of CO_2 from the hypothetical indoor environments. A sensitivity
379 analysis is then presented for the most efficacious scenario. Finally, implications of model results
380 regarding feasibility of $\text{Ca}(\text{OH})_2$ as a reagent for indoor CO_2 removal are discussed.

381 The application of active CO_2 control to the shelter-in-place (SIP) scenario shown in Figure 5
382 illustrates the most efficacious outcome among the scenarios considered. This favorable result is a
383 consequence of the small volume and relatively low air exchange rate of the modeled SIP facility. For
384 the SIP scenario with a soda lime containing air cleaner, the CO_2 level is maintained below 5000 ppm
385 until 7-8.5 h after initial occupancy. After 10 h of operation, the soda lime packed bed is effectively
386 spent (see Figures S4-S6 of the Supporting Information), and the SIP CO_2 concentration begins to
387 increase, exceeding 10,000 ppm shortly after 10 h of occupancy (see Figure S4). These times contrast
388 with the no air cleaning case, where the 5000 ppm CO_2 level is reached after only 1.1 h of sheltering

389 and 10,000 ppm is reached after only 1.9 h. Without air cleaning, concentrations of CO₂ in the SIP
390 environment would reach values in excess of 25,000 ppm after 8 h of occupancy. These results imply
391 that occupancy under the “no scrubber” condition shown in Figure 5 for more than a few hours may
392 result in CO₂ exposures that can produce acute adverse health effects [17].

393 Bedrooms represent an important microenvironment contributing to daily exposures of CO₂,
394 as shown in a recent study of personal exposures to CO₂ in Singapore [52]. As can be observed in
395 Figure 5, in the absence of air cleaning, levels of CO₂ in the bedroom scenario exceed 1000 ppm after
396 just 1 h of exposure. An air cleaner containing a soda lime packed bed, operating either at low or
397 high flow rate, can maintain sub-1000 ppm CO₂ concentrations in the bedroom for the duration of
398 the 8-h sleeping period. As with the SIP scenario, an air cleaner containing a pure Ca(OH)₂ dry
399 sorbent appears to have more modest impacts on indoor CO₂ concentrations. However, worth
400 noting is that the average CO₂ concentration during the 8-h sleeping period for the high flow rate
401 Ca(OH)₂ treatment is approximately 950 ppm.

402 In the case of classrooms, due to the larger room volume and higher air exchange rate than
403 the bedroom and SIP scenarios, the presence of the air-treatment unit has a relatively small impact
404 on CO₂ concentrations. Levels of CO₂ in the classroom after 8 h of operation in absence of air
405 cleaning would be approximately 1400 ppm, compared to a range 900-1050 ppm with a soda lime
406 air cleaner. Since a classroom would not typically be occupied continuously for 8-h periods, the CO₂
407 concentrations presented in Figure 5 for the classroom case may be considered as an upper limit.
408 Given the modest reductions in classroom CO₂ levels for a substantial mass of media and volume of
409 air cleaner (see Table 1), the results indicate that the classroom scenario described here does not
410 appear to present a good opportunity for active CO₂ removal given the present state of sorbent
411 development.

412 Model runs for longer durations (16 h, 40 h, and 40 h, respectively, in the SIP, bedroom, and
413 classroom) assuming continuous occupancy are shown in Figure S3 (Supporting Information) with
414 pertinent results of the sensitivity analysis summarized in Table 5. Removal of CO₂ under the

415 conditions of the SIP facility occurs over a range of achievable pressure drops (150-435 Pa) when
416 compared with commercially available air cleaners. Because of the small volume and low air
417 exchange rate, impacts of air cleaning on CO₂ concentrations are substantial: the time to reach a
418 10,000 ppm threshold is extended by 4-12 hours, and cumulative 8-h exposures are reduced by 60-
419 90%. However, the relatively small mass of media combined with the high CO₂ concentrations results
420 in substantial media usage; in all cases the scrubber media is exhausted after 13 h of continuous
421 operation.

422 In the bedroom scenario, the scrubber appears effective over the range of media masses
423 considered, with pressure drops ranging from 120-290 Pa. Reductions in cumulative exposures are
424 again substantial, in the range 50-66%, and at higher sorbent masses appear to exhibit cumulative
425 run-times that are 40 h or greater. Note that these estimates are conservative, as an air-cleaner
426 deployed to a bedroom would not operate continuously for 40 h, and would likely be utilized in
427 sequential 8-h periods that begin with CO₂ concentration nearer to ambient levels.

428 Model results for a Ca(OH)₂ containing air cleaner across all three scenarios illustrate more
429 modest removal of CO₂ from the indoor space than for soda lime. While the cost of Ca(OH)₂ itself is
430 relatively low and the efficacy of the air cleaner could be increased by recirculating air at higher flow
431 rates through the Ca(OH)₂ bed, effectively increasing the removal rate of CO₂ could become
432 prohibitive with respect to energy use owing to the nonlinear relationship between flow rate and
433 pressure drop. Also worth noting is that the estimates of k and γ for Ca(OH)₂ are likely best-case
434 values with respect to room-scale air cleaning. The Ca(OH)₂ used in laboratory parameterizations
435 was purchased from a commercial supplier and was of a finer grain than the granular media that
436 would typically be used in an air cleaner; transport limitations resulting from the geometry of a
437 larger Ca(OH)₂ granule may reduce the effective yield, rate constant or both, possibly a result of the
438 formation of a diffusion limiting carbonate shell [53]. Achieving the uptake reported from laboratory
439 tests in the applied scenarios by use of a fine grain Ca(OH)₂ may, in practice, create prohibitively
440 large pressure drops across the air cleaner. Testing granular Ca(OH)₂ with varying physical

441 properties, including size of particles as deployed in the packed bed, would more fully inform the
442 potential use of $\text{Ca}(\text{OH})_2$ as a low cost sorbent for active indoor CO_2 control.

443 **4. Conclusions**

444 This study investigated the ability of Mg- and Ca-based sorbents to take up gaseous carbon
445 dioxide through the formation of solid carbonates. The work establish links between a range of
446 controlling parameters and the progress of carbonation through a sorbent matrix. Four alkaline
447 earth metal oxides or hydroxides were characterized for their potential as CO_2 sorbents in an active
448 indoor air cleaning application. A comparison between Mg- and Ca-based sorbents was provided in
449 terms of carbonation degree, microstructure and parameterizations of carbonation kinetics and
450 yields from laboratory experiments. These results were supported by XRD, TGA and SEM analyses,
451 which provided information on the hydration and carbonation phases, the progress and degree of
452 carbonation and the morphology of the sorbents.

453 Results indicate that extensive carbonation of sorbents occurred at conditions typical of
454 indoor spaces ($25\text{ }^\circ\text{C}$ and CO_2 levels of approximately 2200 ppm), although Mg-containing sorbents
455 carbonated slowly such that parameterization of kinetics and capacity were not pursued. Modeling
456 of hypothetical scenarios in which packed beds of sorbents were part of an active indoor air cleaner
457 show potential for the substantial removal of CO_2 from SIP facilities with the use of soda lime.
458 Reductions in integrated CO_2 exposures of over 80% are predicted and indoor CO_2 levels are
459 maintained below the OSHA PEL for an assumed 8-h period of occupancy. These reductions were
460 accomplished with reasonable masses of soda lime (1.7 kg) and at a pressure drop (approximately
461 300 Pa) achievable by fans similar to those present in a typical HEPA filter-containing portable air
462 cleaner. Modeling for low-ventilation bedrooms showed that meaningful reductions are also
463 possible in this setting, with reductions in CO_2 levels after 8 hours of occupancy from 2500 ppm (with
464 no air cleaner) to 550-750 ppm for a continuously operating soda-lime containing air cleaner.
465 However, regular occupancy in bedrooms would necessitate the weekly replacement of the sorbent
466 media as the model shows nearly full exhaustion of the media after 40 hours of operation. The

467 relatively large mass of sorbent needed in bedrooms could make the use of soda lime cost-
468 prohibitive, a disadvantage that could potentially be removed by enhancing the kinetics and capacity
469 of the lower cost sorbents ($\text{Ca}(\text{OH})_2$, MgO and $\text{Mg}(\text{OH})_2$).

470 The empirical kinetic and yield findings were supported by detailed microstructural and
471 thermal analyses, which enabled a thorough comparison of the different media studied. Mg-based
472 sorbents experienced low carbonation rates in the conditions utilized in this study. The carbonation
473 of Mg-based sorbents could be further enhanced via the use of a higher reactivity MgO with a larger
474 specific surface area to induce hydration and the subsequent carbonation process and optimization
475 of the carbonation conditions to increase the rate and amount of CO_2 diffusion within the samples.
476 Efforts to develop sorbents tailored for CO_2 removal in conditions typical of indoor spaces could
477 enable practical utilization of new methods of removing CO_2 from indoor spaces, which appear
478 especially promising in special circumstances where increasing air exchange is infeasible owing to
479 adverse outdoor conditions, such as shelter-in-place facilities.

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643

Table 1. Summary of model inputs to three scenarios considered for active CO₂ removal ^a

| Building and air cleaner parameters | Shelter-in-place | Bedroom | Classroom |
|--|------------------|----------|-----------|
| Room volume, V (m ³) | 5 | 50 | 150 |
| Occupancy (# of persons) | 2 | 2 | 40 |
| CO ₂ emission rate, E (mol CO ₂ /h) ^a | 1.4 | 1.4 | 19 |
| Outdoor air ventilation, Q (m ³ /h) (Air exchange rate, (h ⁻¹)) | 1 (0.2) | 15 (0.3) | 450 (3) |
| Air cleaner flow rate, low/high Q_f (m ³ /h) | 13/21 | 40/61 | 198/306 |
| Packed bed diameter (m) | 0.15 | 0.25 | 0.45 |
| Packed bed length (m) | 0.11 | 0.12 | 0.09 |
| Media mass (kg) ^b | 1.7 | 5 | 25 |

^a Total emission rate of CO₂. For classrooms, the average age of occupant was taken to be 10 years, weight of 35 kg, height of 1.4 m, Dubois surface area of 1.1 m², activity level of 1.2 met, and respiratory quotient of 0.83. For bedroom and shelter-in-place, age was taken to be 35 years, weight of 60 kg, height of 1.65 m, Dubois surface area of 1.7, activity level of 1.2 met, and respiratory quotient of 0.83.

^b Media packing density for both sorbents in the scrubber was taken to be 900 kg/m³, as per soda lime manufacturer specifications.

Table 2. Summary of physical and chemical properties of tested sorbents

| Sorbent | Chemical composition (% by mass) | Physical characterization | | | |
|------------------------|---|---|--|-------------------------|--|
| | | Specific surface area [m ² /g] | Total pore volume [cm ³ /g] | Avg. pore diameter [nm] | Mass median particle size (d ₅₀) (μm) ^d |
| MgO | >91.5% MgO, 4% LOI ^b , 2% SiO ₂ , 1.6% CaO, 1% R ₂ O ₃ ^c | 27 | 7.2 × 10 ⁻² | 0.56 | 16 |
| Mg(OH) ₂ | >99% Mg(OH) ₂ | 5.6 | 8.7 × 10 ⁻³ | 0.24 | 5.4 |
| Ca(OH) ₂ | >99% Ca(OH) ₂ | 15 | 3.9 × 10 ⁻³ | 0.18 | 19 |
| Soda lime ^a | 85% Ca(OH) ₂ , 10% H ₂ O, 3% KOH, 2% NaOH | 7.1 | 1.6 × 10 ⁻² | 0.15 | 1000 ^e |

^a Chemical composition determined as described by Gall et al. [54]

^b LOI is loss on ignition, a determination of the amount of volatile substances within the sorbent composition.

^c R₂O₃ refers to the group of oxides generally consisting of Al₂O₃, Fe₂O₃, and B₂O₃, and are impurities in the sorbent composition.

^d Median particle size of unground media reported from particle size analyzer

^e Median size of soda lime granules as reported by manufacturer.

Table 3. Thermal decomposition of hydrate and carbonate phases within Mg-based sorbents

| Phases | Decomposition reactions | | |
|--|---|---|--|
| | 50 – 300 °C | 300 – 500 °C | 500 – 900 °C |
| Brucite Mg(OH)_2 | - | $\text{Mg(OH)}_2 \rightarrow \text{MgO} + \text{H}_2\text{O}$ | - |
| Hydromagnesite $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O}$ | $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 4\text{H}_2\text{O} \rightarrow 4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 + 4\text{H}_2\text{O}$ | $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \rightarrow 4\text{MgCO}_3 + \text{MgO} + \text{H}_2\text{O}$ | $\text{MgCO}_3 \rightarrow \text{MgO} + \text{CO}_2$ |
| Dypingite $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 5\text{H}_2\text{O}$ | $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 5\text{H}_2\text{O} \rightarrow 4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 + 5\text{H}_2\text{O}$ | $4\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \rightarrow 4\text{MgCO}_3 + \text{MgO} + \text{H}_2\text{O}$ | $\text{MgCO}_3 \rightarrow \text{MgO} + \text{CO}_2$ |

Table 4. Summary of experimental conditions, reaction rate constants, k , and yields, y , for CO₂ uptake experiments to soda lime and Ca(OH)₂.

| Sorbent | Experimental condition | Temperature | Q | Contact time | Inlet [CO ₂] | Reaction rate constant, k | Yield, y |
|---------------------|------------------------|-------------|---------|--------------|--------------------------|---|------------------------------------|
| | | [°C] | [L/min] | [s] | [ppm] | [m ³ mol CO ₂ ⁻¹ h ⁻¹] | [mol CO ₂ /mol sorbent] |
| Soda lime | Dry packed | 26.1 | 1.8 | 0.28 | 1870 | 2.2 | 0.49 |
| | bed | 25.2 | 2.8 | 0.18 | 1890 | 3.6 | 0.51 |
| | Slurry | 25.2 | 1.8 | 0.28 | 2100 | 1.9 | 0.74 |
| | | 25.2 | 2.7 | 0.18 | 2110 | 1.6 | 0.79 |
| Ca(OH) ₂ | Dry packed | 25.2 | 1.8 | 0.28 | 2200 | 1.0 | 0.05 |
| | bed | 24.8 | 2.8 | 0.18 | 2310 | 3.3 | 0.18 |
| | Slurry | 25.0 | 1.8 | 0.28 | 2200 | 1.6 | 0.65 |
| | | 25.0 | 2.7 | 0.18 | 2200 | 2.4 | 0.65 |

Table 5. Summary of sensitivity analysis of model output of indoor CO₂ concentrations in three scenarios of active CO₂ removal from indoor spaces.

| Shelter-in-place, Soda lime, Scrubber diameter = 0.12 m | | | | |
|--|-------------------------------|---------------------------------|------------------------|---------------------------|
| Mass of media (kg) | Contact time (s) [#] | Pressure drop (Pa) [§] | Time to 10,000 ppm (h) | ∫ exposure, 0-8 h (ppm-h) |
| - | - | 0 | 1.9 | 139000 |
| 0.9 | 0.09 | 157 | 6.5 | 46150 |
| 1.3 | 0.14 | 226 | 8.4 | 27080 |
| 1.7* | 0.18 | 296 | 10.1 | 26200 |
| 2.1 | 0.22 | 365 | 12.1 | 17780 |
| 2.5 | 0.26 | 435 | 13.8 | 17080 |
| Bedroom, Soda lime, Scrubber diameter = 0.25 m | | | | |
| Mass of media (kg) | Contact time (s) | Pressure drop (Pa) | Time to 1,000 ppm (h) | ∫ exposure, 0-8 h (ppm-h) |
| - | - | 0 | 0.9 | 14730 |
| 3 | 0.11 | 122 | 13 | 5370 |
| 4 | 0.14 | 163 | 18 | 5000 |
| 5 | 0.18 | 204 | 22 | 4820 |
| 6 | 0.22 | 245 | 27 | 4730 |
| 7 | 0.25 | 285 | 29 | 4730 |
| Classroom, Soda lime, Scrubber diameter = 0.45 m | | | | |
| Mass of media (kg) | Contact time (s) | Pressure drop (Pa) | Time to 1,000 ppm (h) | ∫ exposure, 0-8 h (ppm-h) |
| - | - | - | 0.4 | 11100 |
| 15 | 0.11 | 170 | 4.0 | 7950 |
| 20 | 0.14 | 337 | 6.6 | 7630 |
| 25 | 0.18 | 580 | 8.9 | 7460 |
| 30 | 0.22 | 910 | 11 | 7360 |
| 35 | 0.25 | 1340 | 12 | 7340 |

[#] Values for k and y at indicated contact time were determined by linearly interpolating/extrapolating from experimentally determined values.

[§] Pressure drop was calculated using the Ergun equation [55] with an equivalent spherical particle diameter of 1 mm and a packed bed porosity of 0.55.

* Conditions in bold are the 'base-case' conditions.

Figures

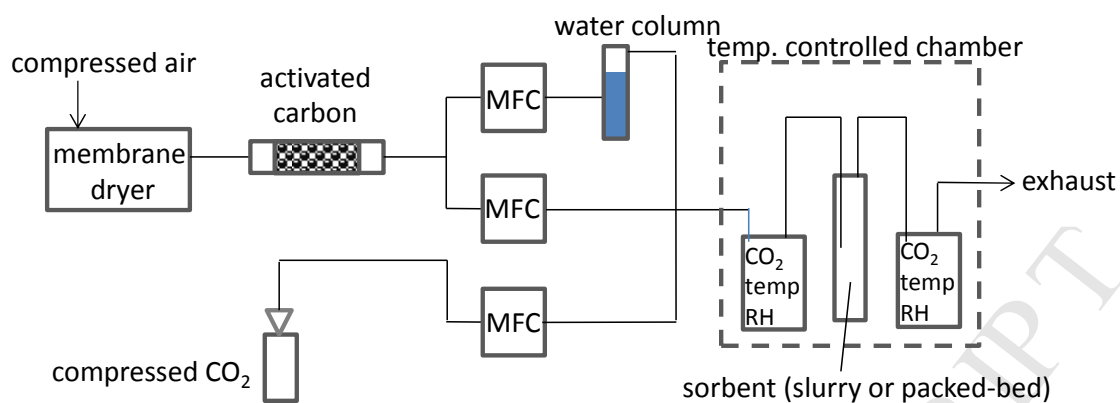
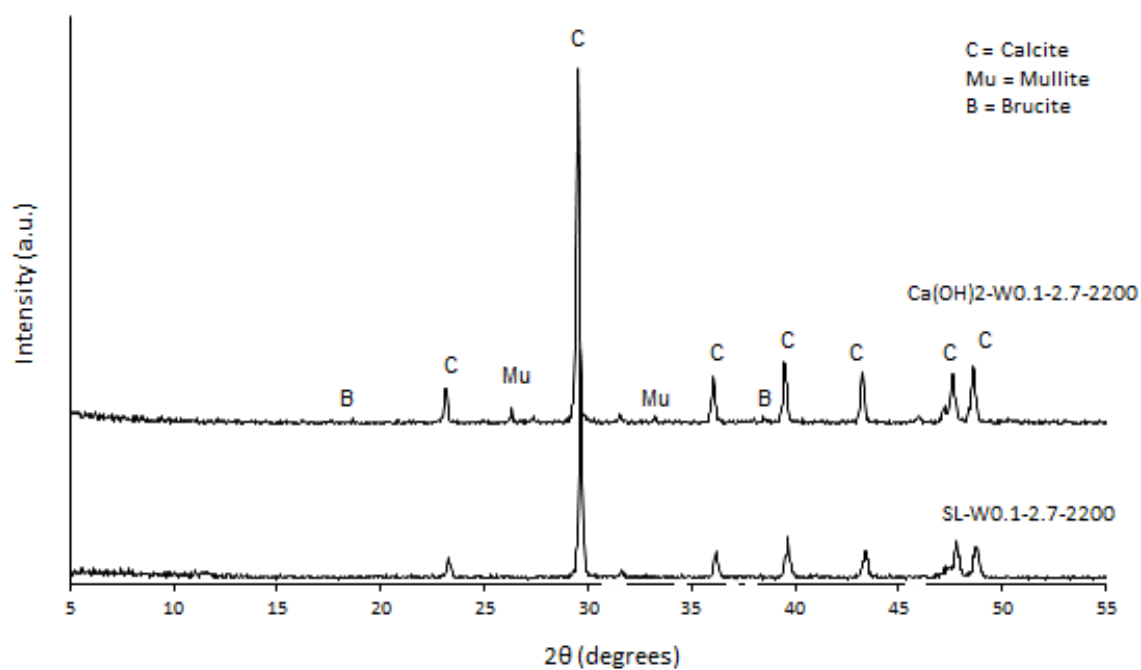
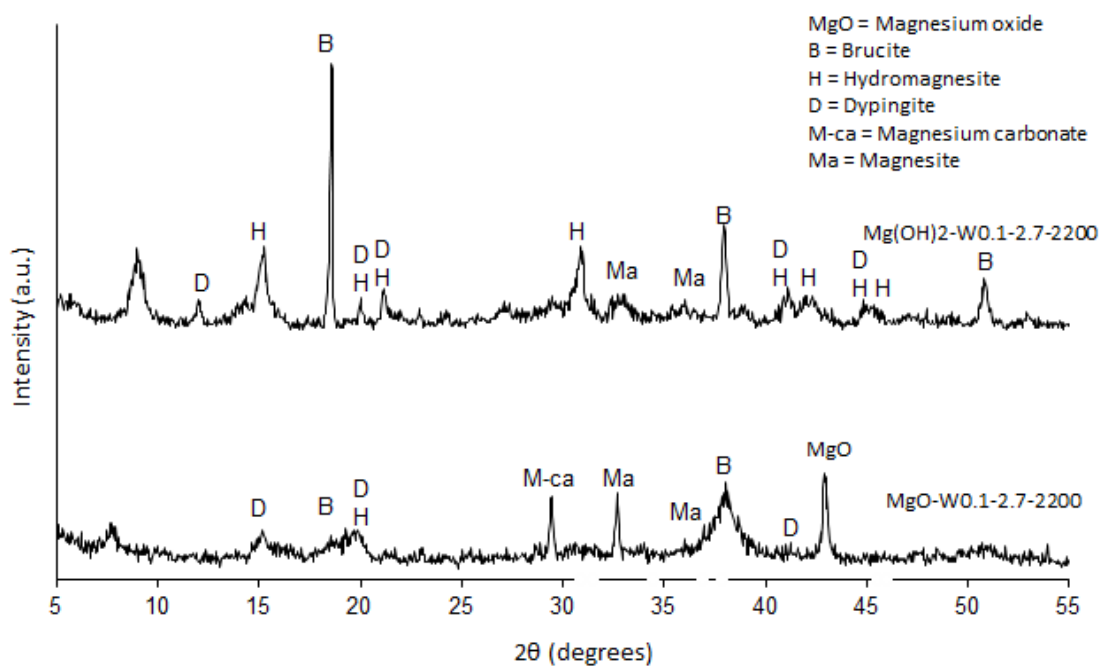


Figure 1. Schematic of laboratory apparatus used for carbonation experiments with controlled temperature, humidity and CO₂ levels. MFC = mass flow controller, temp. = temperature, RH = relative humidity.

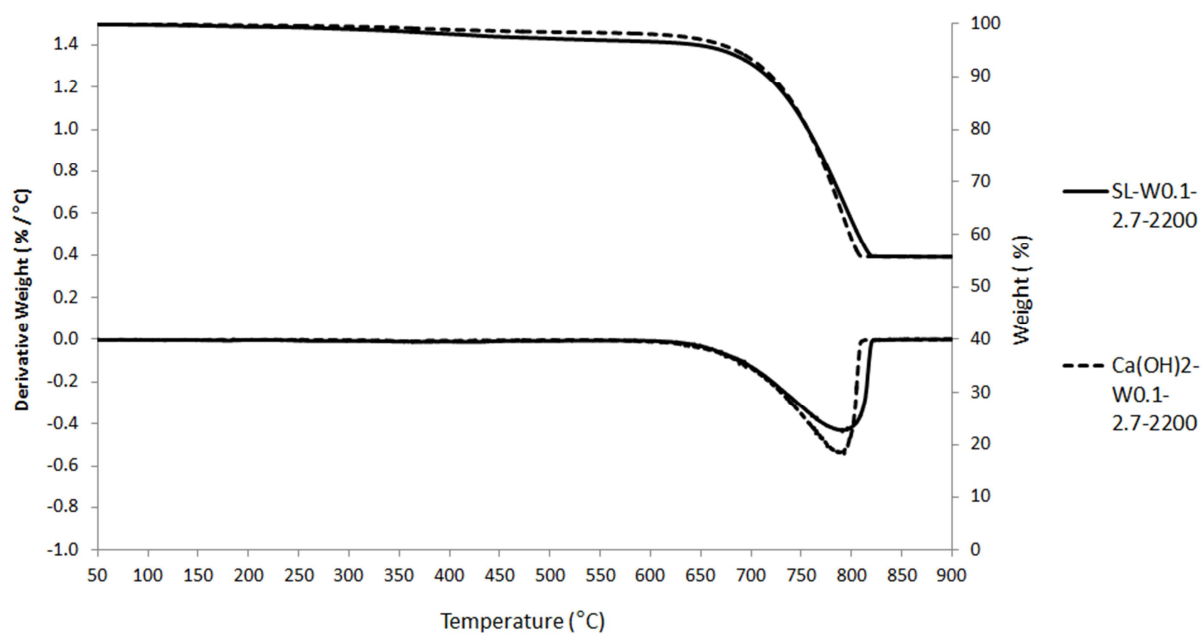


(a)

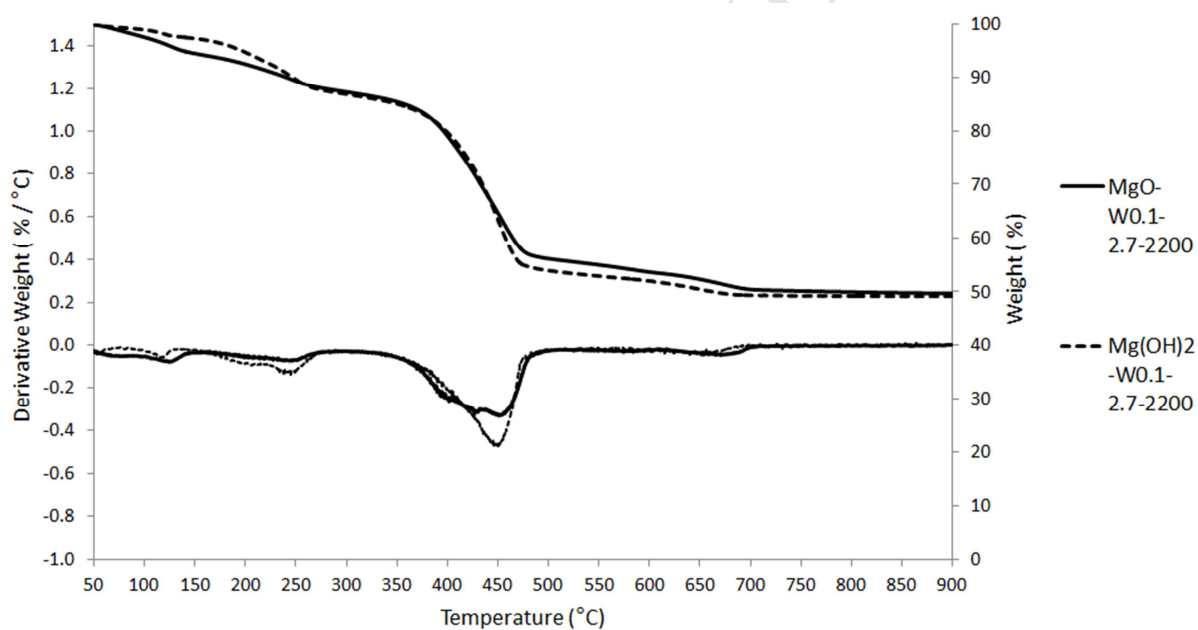


(b)

Figure 2. X-ray diffraction patterns of (a) Ca- and (b) Mg-based sorbents after exposure to CO₂.



(a)



(b)

Figure 3. Thermogravimetric analysis graphs of (a) Ca- and (b) Mg-based sorbents (the primary y-axis (on the left) refers to the lower traces of derivative weight; the secondary y-axis (on the right) refers to the upper traces of percentage weight).

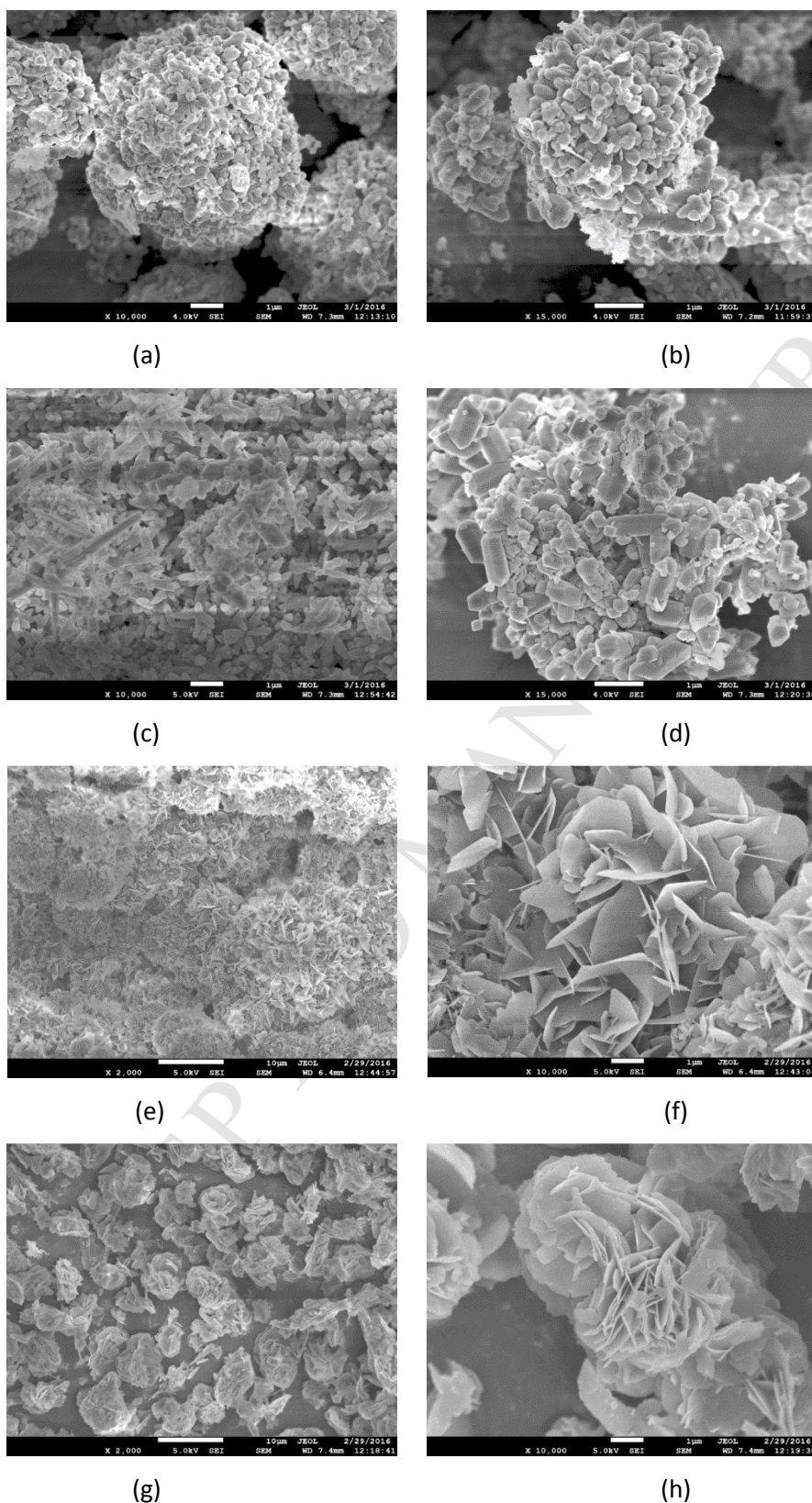


Figure 4. Scanning electron microscopy images of (a)-(b) SL-WO.1-2.7-2200, (c)-(d) Ca(OH)_2 -WO.1-2.7-2200, (e)-(f) MgO-WO.1-2.7-2200 and (g)-(h) Mg(OH)_2 -WO.1-2.7-2200. The white bar at the bottom of each photograph indicates the scale: 1 μm (a-d, f, h) or 10 μm (e, g). These images were acquired after exposure of the sorbents to CO_2 .

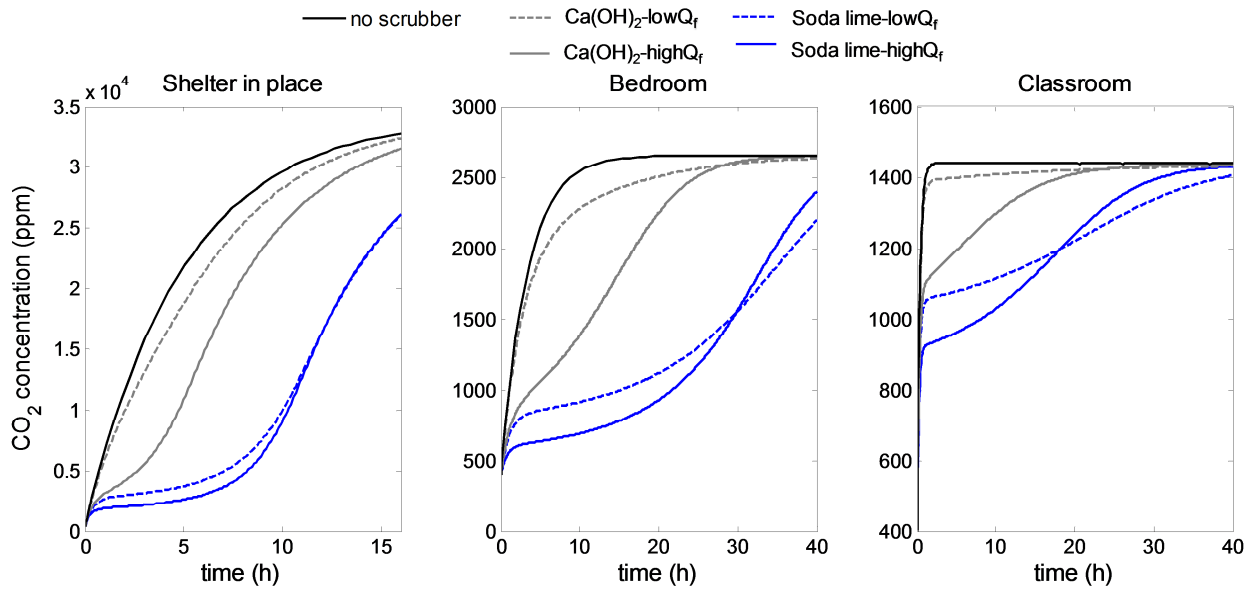


Figure 5. Modeled indoor CO₂ concentrations for three hypothetical indoor environments: a shelter-in-place facility, a bedroom and a classroom with and without the presence of an air cleaner that includes a CO₂ scrubbing bed. Relevant built environment and air cleaner parameters for each of the three indoor environments are provided in Table 1. ‘LowQ_f’ refers to the low air cleaner flow rate condition, ‘highQ_f’ refers to the high air cleaner flow rate condition.

Highlights:

- CO₂ can accumulate in indoor spaces with low air exchange, e.g. in shelter-in-place
- Various Ca- or Mg- based sorbents are investigated as potential air cleaner media
- Ca containing sorbents carbonated under conditions relevant to indoor spaces
- Active removal may substantially reduce CO₂ exposure in shelter-in-place facilities