Mineral carbonation as a design project for green chemical engineering education

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Abstract. Accelerated mineral carbonation is a promising CO₂ sequestration technology that is strongly linked to concepts of sustainability and Green Chemistry, and its process requirements apply principles of reaction kinetics, transport phenomena, and materials characterization. The present work aimed to develop educational tools for including accelerated mineral carbonation in chemical engineering curricula. To this end, an experimental investigation laboratory procedure and a design project outline have been conceived. As a way to further engage students in this learning experience, the process conditions for the laboratory work are varied between groups of students, and the experimental data obtained are pooled to be used by every group for the subsequent design exercise. This is meant to give students motivation to generate accurate data that they knew would be useful for the entire class and, at the same time, provide students with the opportunity to use data generated by colleagues, much in the same way the design work is done in the industry. In the design project, students use the experimental data obtained by themselves and classmates on the accelerated mineral carbonation of wollastonite, to determine if this is a feasible process for industry to sequester carbon dioxide, in view of mitigating climate change. Also, they use the experimental data, acquired using a range of process conditions, to study the effect of the process variables (CO₂ pressure and mixing rate) on the carbonation kinetics and mass transfer rate. The focus of our previously published article was on the experimental investigation, while the focus of this conference paper is on the design project.

Keywords: Chemical engineering, green design, green chemistry, carbon dioxide

1. Introduction

One of the biggest concerns with the accelerated mineral carbonation technology is that if it is implemented as an industrial process, it will not deliver net CO₂ sequestration. The reason behind this is that all process equipment in the industry requires energy to function, and, in most cases, that energy is supplied from CO₂-intensive processes. Even so-called “green energy” has a CO₂ footprint. Hydroelectric fares the best, at 4 g, CO₂-eq/kWhe, while wind and solar emit (over the life-cycle) 12 and 22 g, CO₂-eq/kWhe, respectively (CO₂-eq stands for CO₂-equivalent, and kWhe is the rate of electrical energy generation) [1]. At the other end of the spectrum, the median CO₂ intensity of coal power generation, the worst performer, is a whopping 1001 g, CO₂-eq/kWhe. Thus, if too much energy is used for accelerating mineral carbonation, the process may end up emitting more CO₂ than sequestering it.
Due to the energetic challenges posed, it is vital to conduct an energetic analysis of any proposed accelerated mineral carbonation process. For example, Santos et al. [2] found that, for an ultrasound-enhanced mineral carbonation process (at lab-scale), for every 2.3 g of CO$_2$ sequestered, 79.2 g would be emitted (based on the energy-mix of Belgium). They proposed some strategies to reduce the CO$_2$ emissions further at the industrial-scale, such as securing a less CO$_2$-intensive energy source, increasing the solids loading in the reactor (i.e., more solids per volume of liquid), and improving the design of the reactor to maximize the utilization of sonication energy. Still, a 100-factor reduction in CO$_2$-intensity would be necessary to achieve net CO$_2$ sequestration, so it is not easy and perhaps not feasible.

More recently, for a more conventional carbonation process, utilizing steelmaking slag as the carbon sink, Costa et al. [3] estimated an energy requirement of 272−1750 kWh/tonne CO$_2$ sequestered. Based on the aforementioned energy-intensity of wind power generation, this would represent 38 kg, CO$_2$ emitted per 1000 kg, CO$_2$ sequestered. Hence, this would be a feasible process for net CO$_2$ sequestration. It should be noted, however, that steelmaking slags require less intense carbonation conditions compared to wollastonite (as the material is more reactive). Unfortunately, there is far less steelmaking slag being produced than CO$_2$ being emitted by steelmaking, so this material alone cannot substantially reduce emissions from this CO$_2$-intensive industry. Thus, natural materials, such as wollastonite, more abundantly available (though more expensive due to mining and transportation costs), are required to curtail industrial emissions.

So the question is, can accelerated carbonation of wollastonite become a feasible industrial process for net CO$_2$ sequestration? This can be addressed in an educational setting through a design project, herein proposed. This project is suitable for implementation in upper-year undergraduate (Bachelor or Advanced Diploma) engineering and engineering technology programs, and also for graduate courses at the Master’s level.

2. Design project procedure

The following paragraphs highlight the main steps in the design procedure.

First, assemble a process flowsheet for sequestering CO$_2$ using wollastonite. The process starts with mined, coarse grade (80% passing 8 mm) wollastonite, and CO$_2$ that has been captured from a flue gas source. Capturing means concentrating the CO$_2$ from an industrial source (typically 10-30% CO$_2$ by volume) into a pure (>99 vol%) CO$_2$ stream). You must take the energy consumption of the capturing step into account (see table A1, in the Appendix), but you can ignore the energy consumption of wollastonite mining and transport. The process must use the following equipment (listed in arbitrary order):

- a. pressurized, jacket heated, continuously stirred tank reactor.
- b. CO$_2$ multi-stage compressor.
- c. slurry pump(s).
- d. heat exchanger(s).
- e. solid/liquid separator (unspecified type).
- f. size reduction grinder/mill (unspecified type).

Second, determine what process conditions you will use. Choose the combination of process conditions, from the experiments conducted by all students, that yielded the highest carbonation conversion, and conversely the highest CO$_2$ uptake.

The third step is to determine the scale of the process. That is, how much CO$_2$ is to be sequestered. For this, ideally, you should choose a rate of CO$_2$ sequestration that matches the rate of CO$_2$ emissions from a particular industrial facility (e.g., coal power plant, steelmaking mill, cement factory, pulp and paper plant, to name a few). Your flowsheet will have a single reactor, which should have a feasible size, so choose an emissions source that will fit the scale of the process you are able to design, or propose to capture only a fraction of the emissions with the single reactor if the scale is too large. It is your task to research emissions values and make an appropriate design choice. Assume that all CO$_2$
that is compressed will be sequestered (i.e., there are no gaseous emissions). Based on the amount of 
CO₂ to be sequestered (tonnes/day), and the maximal CO₂ uptake (tonnes, CO₂/tonne, wollastonite) 
you are able to achieve (from the previous step), you can determine the amount of wollastonite 
(tonnes/day) that you will need to process.

Fourth is step is that once you know the amount of wollastonite that you will need to process, you 
can determine slurry volume and consequently the size of the reactor. Remember that the reactor is a 
batch process, so there is only so much wollastonite slurry that can be processed per batch, and only so 
many batches that can be processed per day (based on filling, heating and emptying times). Use your 
lab experiment experience, and your batch reactor theory and design knowledge, to make a suitable 
determination of the reactor size. You will not need to size any of the other equipment for this design 
exercise; it will be assumed that each equipment’s energy consumption depends only on throughput 
and not on physical size.

In the fifth step, calculate the energy consumption of each process/equipment using the equations 
given in Table A. Table A presents the equations needed, along with definitions and units of each 
equation parameter, and suggestive values for some parameters. Other parameter values will come 
from the process conditions used in the lab experiment (that gave the best carbonation conversion), 
such as the mixing rate (G, in s⁻¹). Other parameters will have to be researched or assumed (e.g., the 
dynamic viscosity (µ) of the slurry); use justifiable assumptions. You can neglect the slurry pumping 
power. Note that the units for each energy term differ (kWh/tonne, Wh, J, etc.); these will have to be 
converted to a common energy unit (kWh/tonne CO₂ sequestered) before being summed to obtain the 
total energy consumption value.

In the sixth step, for the slurry heating power, take into account how much exothermic energy is 
produced in the reactor during the reaction, how much energy is lost to the environment by natural 
convection, and how much waste heat may be re-used to pre-heat the feed using a heat-exchanger. 
Some additional assumptions will be required (e.g., heat-exchange efficiency). Based on this analysis, 
you only need to take into account in the overall energy balance what extra heating energy is required 
that will consume external power.

For the seventh and final step, once you have the total energy consumption value, per tonne CO₂ 
sequestered, determine if the process achieves net CO₂ sequestration. That is, convert the energy 
consumption value into a carbon emission value, using an assumed CO₂-intensity value of power 
generation (find this value for Ontario), and compare the rate of emission to the rate of sequestration. 
Assume that all energy requirement for the process comes from electrical power obtained from the 
provincial grid.

2.1. Reaction rate law
In the energetic analysis, you will use experimental data to decide what the maximal CO₂ uptake of 
wollastonite is. However, during experimentation, only a limited number of experiments were 
performed. So it may be that the maximal CO₂ uptake occurs with a CO₂ pressure different than the 
values tested (maybe even higher or lower than the range covered). It is thus helpful for design 
purposes to obtain a rate law that describes how CO₂ pressure affects the carbonation rate.

In the Experimental Investigation [4], a rate law proposed by Ptáček et al. [5] was introduced, 
which accounted for the effect of temperature on the rate of carbonation. That law, which is based on 
the well-known Arrhenius equation, required experimental determination of two empirical parameters: 
the pre-exponential factor (A), and the activation energy (EA). Values for these two parameters, 
suggested by Ptáček et al., were cited: 1.8 ± 0.9·10³ s⁻¹ for A in the case of wollastonite dissolution in 
acetic acid, and 47 ± 1 kJ/mol for EA. It should be noted, however, that these values were obtained 
from experimental studies on the dissolution of wollastonite in acetic acid, rather than its dissolution 
and immediate precipitation, as it occurs when wollastonite is exposed to carbonic acid (i.e., CO₂ at 
elevated pressure in contact with an aqueous slurry of wollastonite). It should also be noted that the 
value of EA obtained experimentally is “apparent”, meaning that it is a measure value based on a 
specific set of process conditions, rather than the true activation energy based on fundamental
principles of chemistry. Thus, it is plausible that it, in addition to A, would differ for substantially different process conditions (such as the dissolution of wollastonite in carbonic acid).

To take into account the effect of CO₂ pressure, in addition to temperature, a possibly suitable rate law is an extended version of the Arrhenius equation, as follows:

$$r_{\text{min carb}} = A \cdot e^{-\frac{E_A}{RT}} \cdot (P_{CO2})^y$$

(1)

where $r_{\text{min carb}}$ is the mineral carbonation rate (mol/(m²·s)), $A$ is the pre-exponential empirical factor (mol/(m²·s⁻¹)), $E_A$ is the apparent activation energy of carbonation (kJ/mol), $R$ is the universal gas constant (kJ/(mol·K)), $T$ is the temperature (K), $P_{CO2}$ is the partial pressure of CO₂ (bar), and $y$ is the order of reaction.

Also recall that the rate of carbonation ($R_{\text{carb}}$ (mol/s)) is proportional to the available mineral surface area ($A_{\text{min init}}$ (m²)) (Eq. 2), which itself is a function of time (Eq. 3). $\xi(t)$ is the fractional extent of carbonation conversion of the mineral at the reaction time and $m_{wo,init}$ is the initial mass of wollastonite being carbonated (g), and SSA is the initial specific surface area (m²/g).

$$R_{\text{carb}} = r_{\text{min carb}} \cdot A_{\text{min init}}$$

(2)

$$A_{\text{min init}} = SSA \cdot (1 - \xi) \cdot m_{wo,init}$$

(3)

Hence, the first step in this analysis will be to convert the experimental carbonation conversions ($\xi_{\text{30min}}$) and rates of carbonation ($R_{\text{carb}}$) into reaction rates ($r_{\text{min carb}}$). The value of $R_{\text{carb}}$ will be calculated from the total CO₂ uptake value, and it will be assumed that the rate of carbonation is linear in the first 30 minutes (this is in agreement with the work of Huijgen et al. [6]).

Once values of $r_{\text{min carb}}$ are obtained for every experiment (with varying CO₂ pressures and mixing rates), the rate law will be fitted to the data to account for the effect of pressure. For this, it is best to divide the data into sets of constant mixing rate, and for each set, fit the data based on variation of pressure alone. Fitting of the data should be done by plotting experimental and calculated values of $r_{\text{min carb}}$ versus $P_{CO2}$, and adjusting parameters to minimize the difference between the lines. Having three unknowns ($A$, $E_A$, and $y$), and no data on the effect of temperature, you will need to use some discretion in adjusting these parameters to fit the available data. For example, you may wish to use the values of Ptáček et al. [5] for $A$ and $E_A$ at first, solve for $y$, and then adjust $A$ or $E_A$ to better fit the experimental data trend. Repeat this for each mixing rate set to find out if the mixing rate has a large effect on the rate law, and if so on which rate parameter.

2.2. Mass transfer analysis

Mass transfer of ions in the aqueous mineral carbonation system occurs in two mediums: the solid phase and the liquid phase. In the solid phase, ion transport is governed by the diffusivity of the ions through the mineral matrix, with porosity and ion-solid interactions playing a role in aiding or restricting ion transport compared to the simple diffusion mechanism. In the liquid phase, mixing plays an important role in inducing convection in the bulk phase, in aiding the dissolution of CO₂ from the gaseous phase (which is over the liquid surface), and in reducing the thickness of the stagnant liquid film at the surface of solid particles. This increases the driving force for the transport of ions from and to the solid surface.

In this mass transfer analysis, you will focus on the effect of mixing rate on the rate of carbonation using the experimental data set you are given. In the experimental study, the mixing rate was varied along with CO₂ partial pressure. By dividing the data set into sub-sets, you can isolate the effect of mixing rate for a given CO₂ partial pressure. One question to address is if mixing can compensate for a lower CO₂ partial pressure, as the energy consumption of mixing is expected to be lower than the energy consumption of compressing CO₂ (is this what the energetic analysis indicated?). Another question to address is what the rate limiting step of the reaction is: mineral dissolution, ion diffusion
through the solid phase, or ion diffusion in the liquid phase (either from the solid phase or from the
gaseous phase)?

To investigate the effect of the mixing rate, you will look at the Sherwood Number \((Sh)\), which
indicates if diffusion or convection dominates the mass transfer in the liquid phase. A high value of \(Sh\)
implies that there is sufficient mixing to overcome diffusion limitations. But if the carbonation rate
does not improve markedly with higher rate of mixing, it will indicate that the rate limiting step lies
elsewhere. In that case, an assessment of the rate of diffusion through the solid phase, and comparison
of that rate with the reaction rate, would further indicate if mineral dissolution or solid-phase mass
transfer is rate-limiting.

The correlation between mass transfer and agitation is made by the Sherwood Number \((Sh)\), which
is a dimensionless number that represents the ratio of the convective rate of mass transfer to the rate of
diffusive mass transport (Eq. 4) \([7]\). The value of \(Sh\) has been found to be a function of two additional
dimensionless numbers common in the field of transport phenomena (Eq. 5): the Reynolds Number
\((Re)\), defined in Eq. 6 for an impeller-stirred tank; and the Schmidt Number \((Sc)\), defined in Eq. 7.

\[
Sh = \frac{K}{L/D} \quad (4)
\]

\[
Sh = f(Re, Sc) \quad (5)
\]

\[
Re = \frac{\rho_L \cdot N \cdot D_I^2}{\mu_L} \quad (6)
\]

\[
Sc = \frac{\mu_L}{\rho_L \cdot D_L} \quad (7)
\]

where \(L\) is a characteristic length (m), which in the case of particles is the particle diameter \([7]\), \(D\)
is mass diffusivity \((\text{m}^2\text{s}^{-1})\), \(K\) is the convective mass transfer film coefficient \((\text{m} \cdot \text{s}^{-1})\), \(\rho_L\) is the density
of the liquid \((\text{kg} / \text{m}^3)\), \(N\) is the rotational speed of the impeller \((\text{s}^{-1})\), \(D_I\) is the diameter of the impeller
(m), \(\mu_L\) is the dynamic viscosity of the liquid \((\text{Pa} \cdot \text{s})\), and \(D_L\) is the diffusion coefficient of the chosen
species in the liquid phase \((\text{m}^2 / \text{s})\).

The actual value of \(Sh\) must be determined using empirical correlations. Many experimental studies
of mass transfer from a particle to a fluid exist, some of which concern the dissolution of solid
particles. The choice of a suitable equation should be based on the one that best fits experimental
observations for the system in question. In the absence of prior experience, an equation that has been
found to fit a variety of data reasonable well is the Frössling Equation (Eq. 8), which is valid for a
wide range of \(Sc\) and \(Re\) up to 1000 \([8]\).

\[
Sh = 2 + 0.6 \cdot Re^{1/2} \cdot Sc^{1/3} \quad (8)
\]

To calculate \(Sh\), you may start with the Frössling Equation, which requires calculation of \(Re\) and
\(Sc\). Confirm if the range of \(Re\)'s used matches the validity range of the equation. If not, search the
literature for a more appropriate equation. Once you have determined values of \(Sh\) for the different
mixing rates, and for the difference CO\(_2\) partial pressure series, comment on the results. Can you tell
what the rate limiting step is, or is further investigation needed? Does the effect of mixing differ at
different CO\(_2\) partial pressures, and if so why? How can this mass transfer analysis aid in process
design to reduce the energy demand of the process? Are there other benefits that mixing may bring
that were not assessed? Are there other mixing methods or reactor designs that could improve mixing or reduce the energy demand of mixing?

3. Report requirements

1. The report should contain the following sections: cover page, table of contents, table of figures, table of tables, energetic analysis (as per below), reaction rate law (as per below), mass transfer analysis (as per below), conclusions and recommendations (as per below), references, appendix (as per below).

2. Energetic analysis: (a) explain how you adapted the proposed procedure to reach the energy consumption and net CO$_2$ sequestration results (what assumptions had to be made, what changes you made, if any, to the proposed procedure, etc.); (b) show values (and sources) of all parameters used in the equations; (c) show the energy consumption value of each individual process/equipment; (d) show the calculation procedure of converting energy consumption to CO$_2$ emissions (footprint) and the compare the CO$_2$ emissions rate to the CO$_2$ sequestration rate to determine if net CO$_2$ sequestration is achieved; (e) discuss what process changes you may make, if more experimental or modelling information, to improve the efficiency of the process; (f) write conclusions and recommendations on whether accelerated mineral carbonation can become an industrially feasible process for CO$_2$ sequestration.

3. Reaction rate law: (a) explain the procedure used to develop the rate law(s), including data and graphs used; (b) explain assumptions taken and any limitation of the applicability of the rate law(s); (c) comment on what you learned about the mineral carbonation reaction based on the rate law(s) obtained; (d) comment on how the rate law(s) can aid in improving the process design and energy consumption presented earlier.

4. Mass transfer analysis: (a) explain the procedure used in the analysis, including data and graphs used; (b) explain assumptions taken and any limitation on validity of the analysis results; (c) comment on what you learned about the mineral carbonation reaction based on the results obtained; (d) comment on how the analysis can aid in improving the process design and energy consumption presented earlier.

5. Appendix: include any graph, figure or table that supports the design and analysis results, but that is not central to the report discussions. Add captions for each appendix entry.

4. Conclusions

The ultimate objective of the proposed design project is to better train chemical engineering students given their future careers. Graduates with experience in mineral carbonation investigation and design would potentially be better trained to develop engineering solutions that take into account sustainability criteria. Also, having gone through a memorable undergraduate exercise in mineral carbonation investigation and design would potentially reinforce learned concepts of chemical engineering fundamentals, and make it more likely that graduate would recall those fundamental concepts in their future careers.

5. References

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6. Appendix

Table A. Assumptions, mathematical equations and values of parameters adopted for the energetic evaluation (adapted from Costa et al. [3]). Re-used from Fantucci et al. [4], CC BY.

| Unit operation                     | Assumptions and equations adopted                                                                 | Definition and units of symbols and some numerical value suggestions |
|------------------------------------|-----------------------------------------------------------------------------------------------------|---------------------------------------------------------------------|
| Size reduction                     | $E_{SR} = 10 \cdot W_i \cdot \left( \frac{1}{\sqrt{d_{fin}}} \right)$                                    | $E_{SR}$ = milling energy (kWh/tonne,woll)                           |
|                                    |                                                                                                    | $W_i$ = Bond’s work index (= 12.16 kWh/tonne) [9]                   |
|                                    |                                                                                                    | $d_{in}$ = initial particle size (80% passing) (μm)                  |
|                                    |                                                                                                    | $d_{fin}$ = final particle size (80% passing) (μm)                  |
| Reactor mixing                     | $E_{RM} = G^2 \times m \times V_{slurry} \times J_H$                                                | $E_{RM}$ = mixing energy (Wh)                                       |
|                                    |                                                                                                    | $V_{slurry}$ = slurry volume (m³)                                   |
|                                    |                                                                                                    | $G$ = velocity gradient (s⁻¹)                                      |
|                                    |                                                                                                    | $m$ = dynamic viscosity of the slurry (Pa·s)                        |
|                                    |                                                                                                    | $J_H$ = hydraulic residence time (h)                               |
| Slurry heating                      | $E_{SH} = V_{slurry} \times r_{slurry} \times c_p,slurry \times DT$                                 | $E_{SH}$ = heating energy (J)                                       |
|                                    |                                                                                                    | $r_{slurry}$ = slurry density (kg/m³)                               |
|                                    |                                                                                                    | $c_p,slurry$ = specific heat of the slurry (J·kg⁻¹·K⁻¹) (for wollastonite $c_p,woll$ = 1.1125·10² + 1.4373·10⁻²·T + 16.936·T₀.5 - 2.7779·10⁶·T⁻² (J·mol⁻¹·K⁻¹) [10] |
|                                    |                                                                                                    | $DT$ = temperature difference (assumed to be 30 K [10], the remaining heat to be supplied being recovered from the slurry recycled from the carbonation reactor) |
| CO₂ compression                     | Multi-stage compressor used (maximum number of stages = 5) [11]. For each stage:                   | $E_{c,i}$ = compression energy per stage (J/kg,CO₂)                 |
|                                    | $E_{c,i} = \frac{Z \cdot R \cdot T_{in}}{M \cdot \eta_{IS}} \cdot \frac{k_x}{k_x - 1} \cdot \left( \frac{k_x - 1}{C^R \cdot k_x - 1} \right)$ | $E_c$ = total compression energy (J/kg,CO₂)                         |
|                                    |                                                                                                    | $CR$ = compression ratio = $(P_{fin}/P_{in})^{1/N}$                |
|                                    |                                                                                                    | $P_{fin}$ = final pressure (end of stage) (Pa)                     |
|                                    |                                                                                                    | $P_{in}$ = initial pressure (start of stage) (Pa)                  |
|                                    |                                                                                                    | $N$ = number of compression stages                                 |
|                                    |                                                                                                    | $Z$ = average CO₂ compressibility factor for each stage (e.g. $Z = 0.99435$ at 1.013 bar and 15 °C) [12] |
|                                    |                                                                                                    | $R$ = universal gas constant (8.314 J·mol⁻¹·K⁻¹)                   |
|                                    |                                                                                                    | $T_{in}$ = CO₂ temperature at the compressor inlet (K)             |
|                                    |                                                                                                    | $M$ = molecular weight of CO₂ (0.044 kg·mol⁻¹)                     |
|                                    |                                                                                                    | $\eta_{IS}$ = isentropic efficiency of the compressor              |
|                                    |                                                                                                    | $k_x = (Cp/C_v)$ = average ratio of the specific heats of CO₂ for each stage. |
| Heat released by the reaction      | Calculated from the enthalpy of reaction of wollastonite with CO₂ [13].                            | $DH_{calc} = \approx -86.99$ kJ/mol,CO₂                            |
| Heat loss from the carbonation     | Heat transfer assumed by natural convection on the exterior ambient-air side.                      | $Q_{conv} = h \cdot A_s \cdot (T_s - T_0)$                         |
| reactor                            |                                                                                                    | $h$ = average heat transfer coefficient (W·m⁻¹·K⁻¹) (calculated from Nusselt number expression for natural convection from reactor surface) |
|                                    |                                                                                                    | $A_s$ = surface area of the reactor (m²)                           |
|                                    |                                                                                                    | $T_s$ = temperature at the outer surface of reactor (K)            |
|                                    |                                                                                                    | $T_0$ = ambient temperature (K)                                   |
| Solid/liquid separation            | $E_{SH} = G^2 \times m \times V_{slurry} \times J_H$                                               | Same as for rapid mixing, except assume $G = 60$ s⁻¹               |
| CO₂ capture [14]                   | $E_{Capt} = 4000$ kJ/kg CO₂ captured                                                                | Amount of energy required to capture (concentrate) CO₂ from emission source. |