Thermodynamic Study of Carbon Mineralization with Recycled Concrete Fines for Carbon Capture and Utilization Applications

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I. Introduction

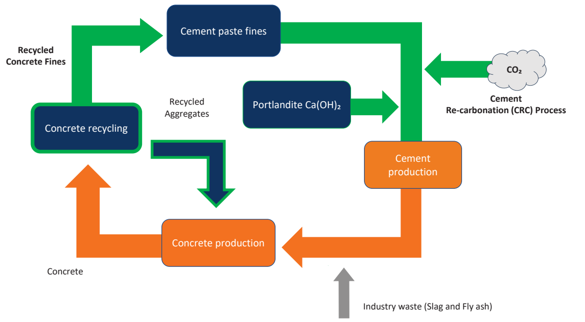
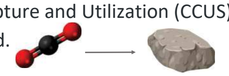


Figure 1.1: Concrete life cycle with lower CO_2 emissions. The green coloring represents the cycle improvements on the original orange process.

Motivation

- Over 30 billion tonnes of concrete are produced each year contributing to almost 10% of global CO_2 emissions.
- Although recycled concrete aggregates are more frequently used in practice, recycled concrete fines are mostly wasted.
- Carbon Mineralization is the process that occurs when concrete is exposed to carbon dioxide in the atmosphere or synthetically.
- Using the concrete as a form of Carbon Capture and Utilization (CCUS) will reduce the net CO_2 emissions produced.



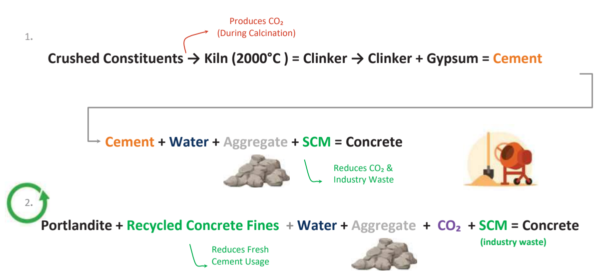
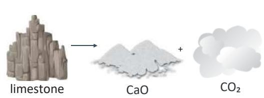


Figure 1.2 : Comparison of current concrete production process (1) with novel concrete process (2)

- Calcination of Limestone is the largest contributor to CO_2 emissions.



- The addition of cementitious supplementary materials (SCM) and CO_2 as a part of the cement mixture provides a pathway to use industry waste.
- Portlandite is an alkali activator that improves the reaction environment.

II. Materials and Methods

Modified Parrot-Killoh (MPK)

- Takes the non equilibrium inputs of the clinker phases and a few oxides and computes the mass of each at a given time based on their dissolution rates

5 Parameter Logistic (5PL)

- The 5PL fit is used to model the dissolution of the recycle concrete fines based on the degree of reaction (DoR).
- 5PL parameters are traditionally calculated based on time-variant QXRD data.

$$y = d + \frac{(a-d)}{\left[1+(x/c)^{b}\right]^{g}}$$

Figure 2.1: 5PL Equation

CemGEMS

- Thermodynamic modeling using the Parrot-Killoh method for plots describing the evolution of hydration product volumes with respect to time. [1]

Recycled Concrete Fines

- The composition of recycled concrete is dependent on the location and construction practices of that region.
- For this study, the average of three Dutch concrete plants were used:

Averaged Mass %	SiO2	CaO	Al2O3	Fe2O3	Na2O	MgO	SO3	K2O	TiO2	Cl
	62.17	24.51	5.38	2.64	0.57	1.54	1.29	1.44	0.4	0.06

Figure 2.2: Average oxide compositions for recycled concrete fines constituents [2]

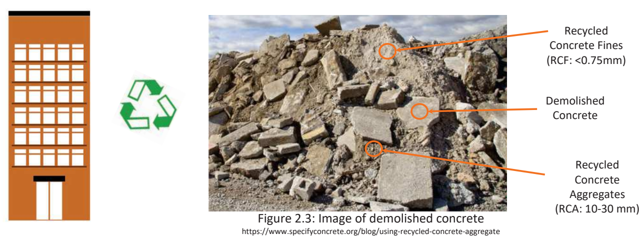


Figure 2.3: Image of demolished concrete
https://www.specifyconcrete.org/blog/using-recycled-concrete-aggregate

III. Discussion

RCF 4PL/5PL Parameters

- Due to a lack of QXRD data for RCF to fit the parameters, we used heat of reaction data over a span of 24 hours to contrive the reaction extent trend.
- Finding a range of plausible values based off of the rules that govern the 4PL/5PL fit provided us with a reasonable set of parameters to model the hydration of RCF.
- Using CemGEMS, we are able to visually represent the reactants consumed and the products formed as a function of time.

IV. Preliminary Results

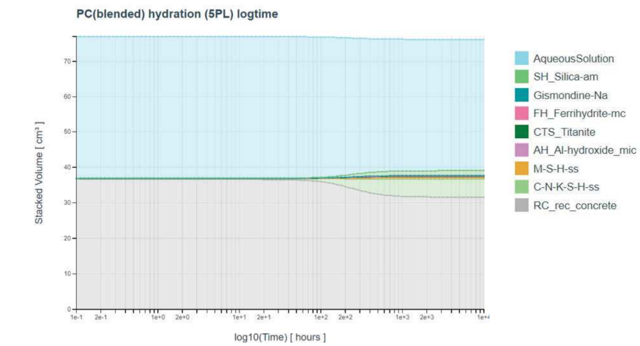


Figure 4.1: Stacked volume plot for 100g RCF & 0.4 w/b ratio
C-N-K-S-H-ss is the main hydration product that contributes to a stronger cement paste.

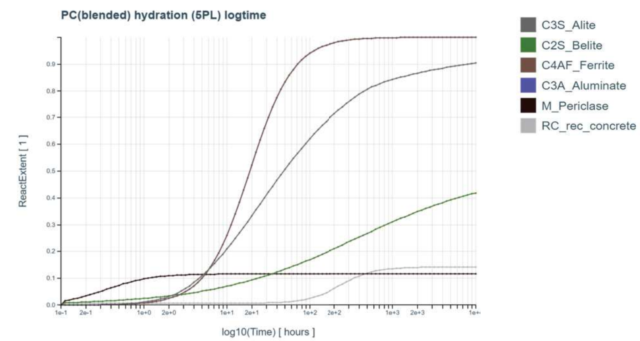


Figure 4.2: Plot containing the hydration reaction extent of clinker phases (alite, belite, ferrite, aluminate) and the extent of the recycled concrete fines. Up to 15% of the RCF is able to react to form hydration products.

V. Conclusion/ Future Work

- Substituting cement for RCF produces the main hydration products necessary.
- How much CO2 and portlandite at what temperature allows for the optimal process kinetics and products?
- What SCM will benefit the hydration process and concrete properties?
- How well do the experimental results match with the simulated data?

VI. Acknowledgements and References

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Thank you to Dr. Rick Ubic for this opportunity

[1] Kulik, D.A.; Winnefeld, F.; Kulik, A.; Miron, G.D.; Lothenbach, B. CemGEMS – an easy-to-use web application for thermodynamic modelling of cementitious materials. RILEM Tech Lett 2021, 6, 36-52; https://doi.org/10.21809/rilemtechlett.2021.140.

[2] Marija Nedeljković, Jeanette Visser, Timo G. Nijland, Siska Valcke, Erik Schlangen, Physical, chemical and mineralogical characterization of Dutch fine recycled concrete aggregates: A comparative study, Construction and Building Materials, Volume 270, 2021, 121475, ISSN 0950-0618, https://doi.org/10.1016/j.conbuildmat.2020.121475.