FUNMIN

FUNdamental Studies of **MIN**eral Carbonation with Application to CO_2 Utilisation

Accelerating CCS Technologies

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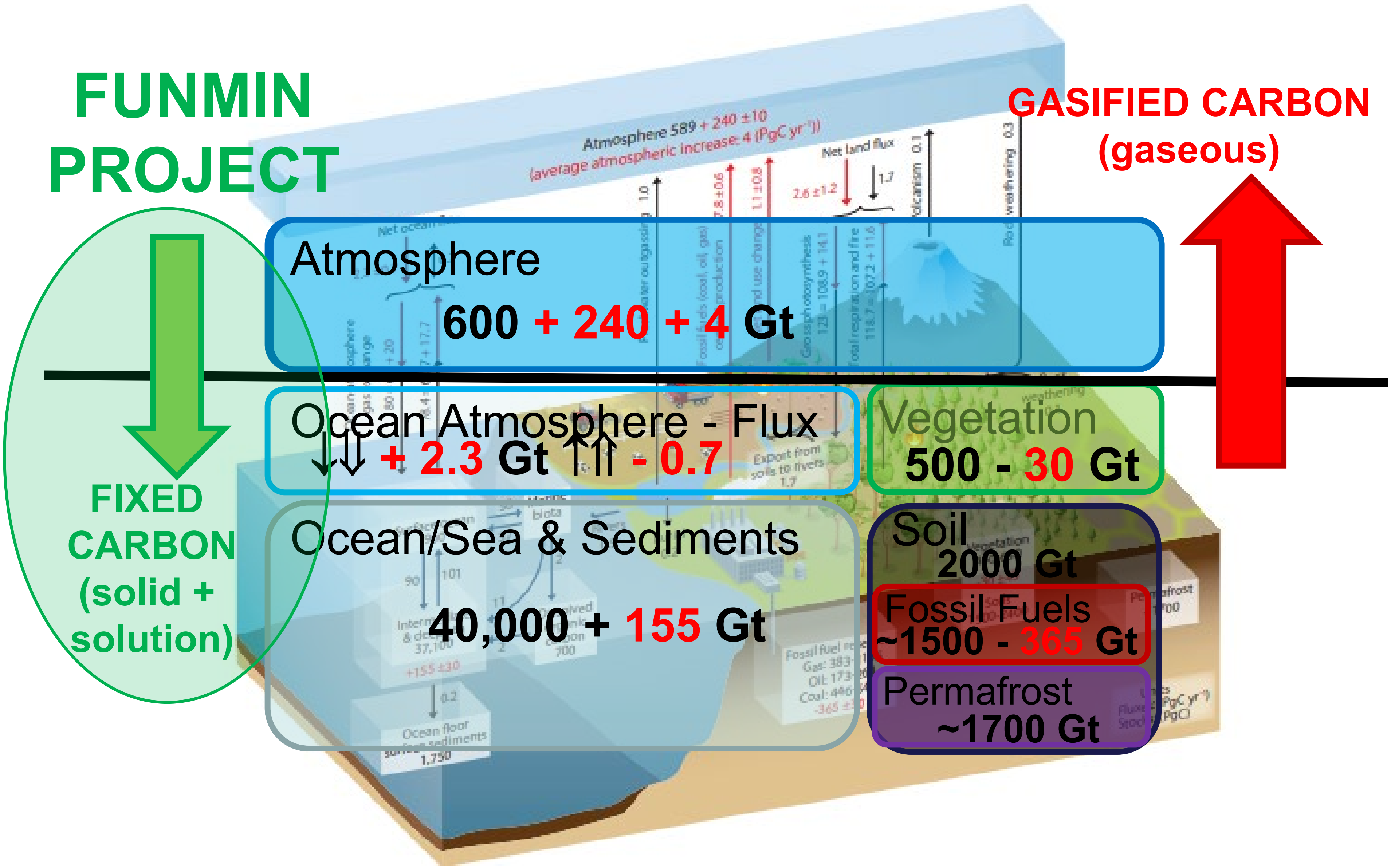
ACT knowledge sharing workshop

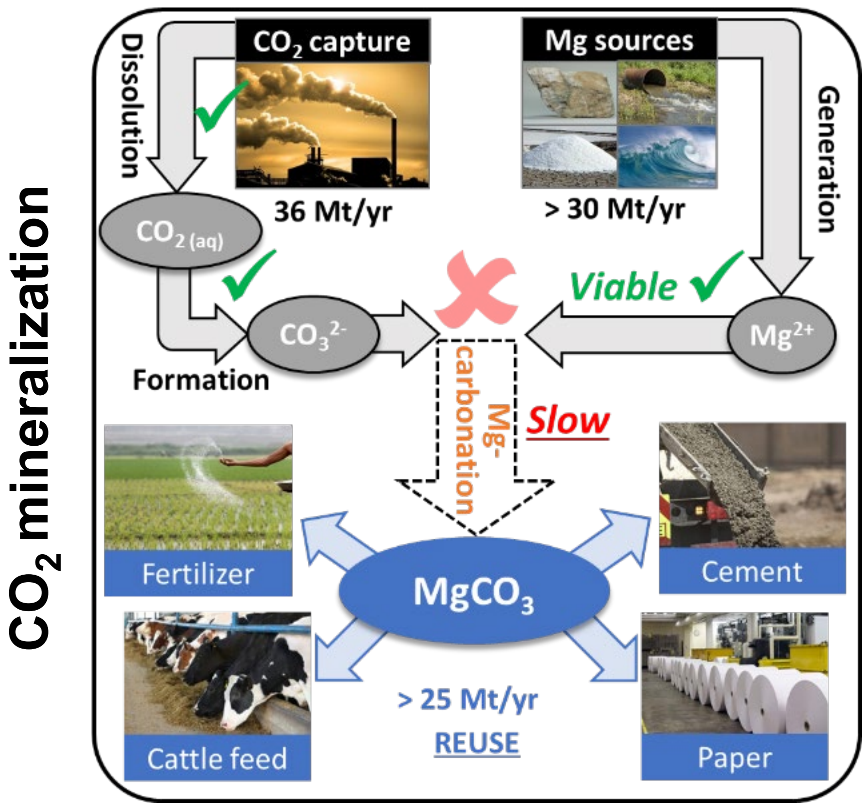
Rotterdam, 8-9 June 2022

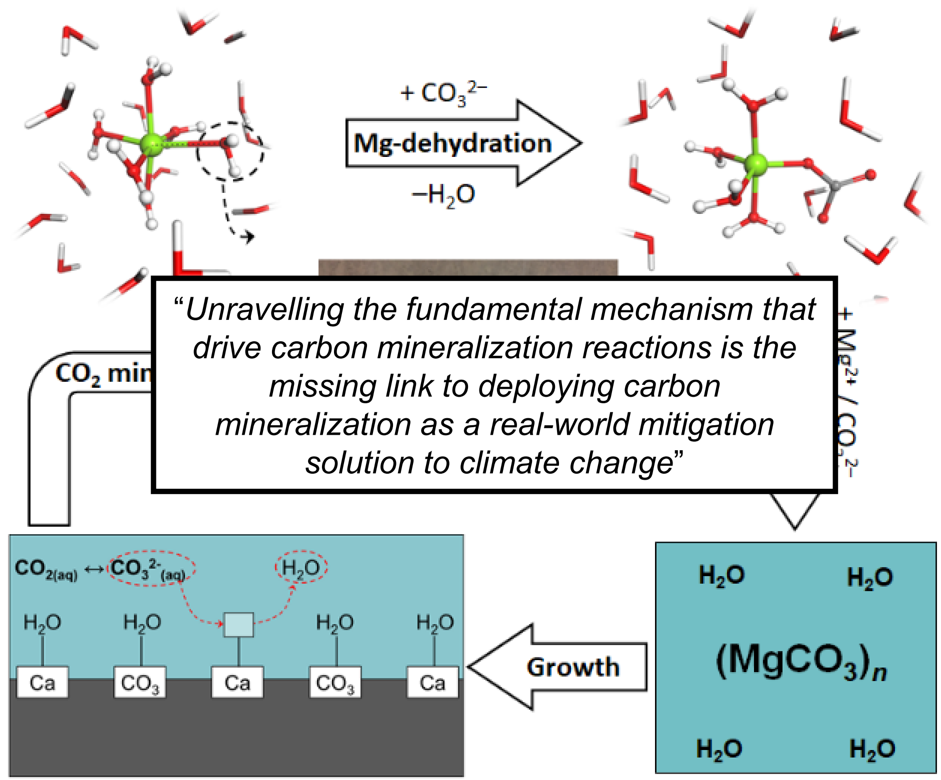
Carbon Reservoires & Fluxes + Human Fluxes



CO_2 into solid AS added-value products

"CCUS can create new industries and markets using carbon dioxide, such as chemicals, plastics, and building materials" *



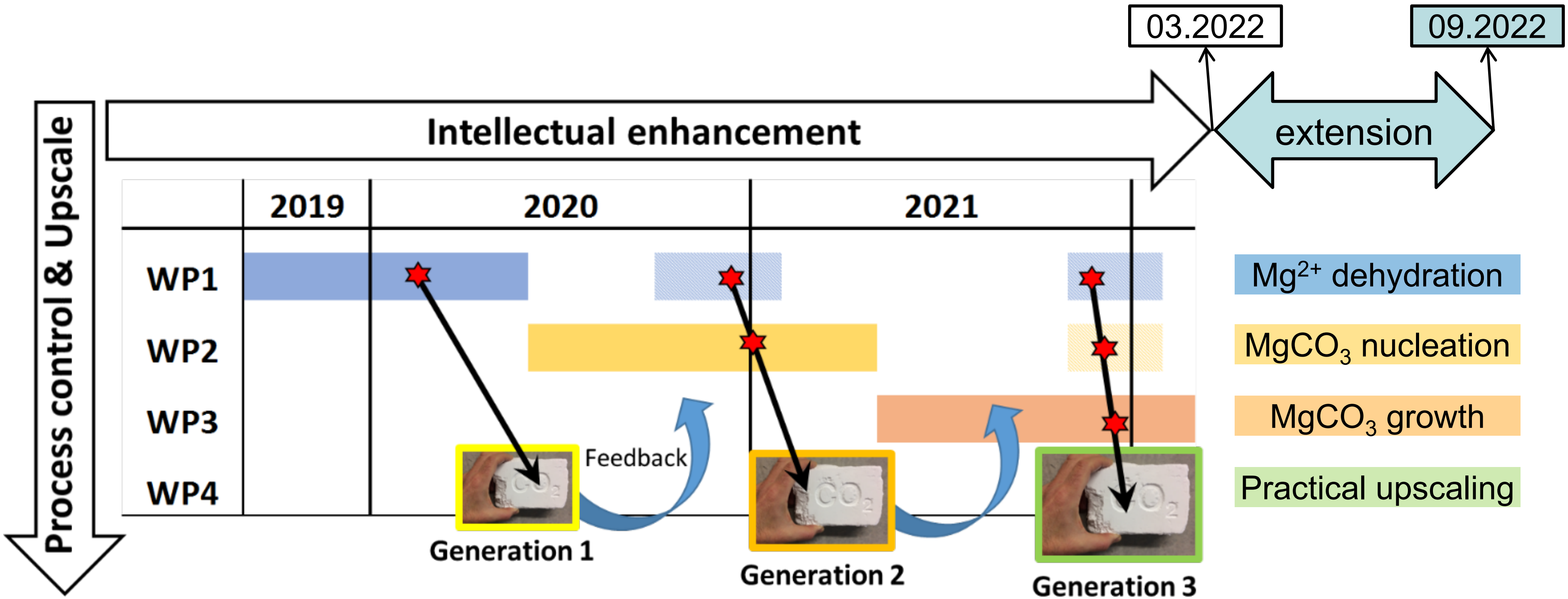


"Unravelling the fundamental mechanism that drive carbon mineralization reactions is the missing link to deploying carbon mineralization as a real-world mitigation solution to climate change"

* The UK carbon capture, usage and storage (CCUS) deployment pathway, BEIS, 2018

Project implementation

Core activities (**WP1-3**) to characterize the **molecular processes** controlling $MgCO_3$ crystallization; applied component (**WP4**) to **optimise** conditions



Interaction between the scientific (**WP1-3**) and practical (**WP4**) components of the project.
WP1: Mg-dehydration; **WP2**: $MgCO_3$ nucleation; **WP3**: Magnesite Growth; **WP4**: Upscaling

Key achievements

1. Control rate-determining Mg^{2+} dehydration

2. Database of additives promoting $MgCO_3$ formation

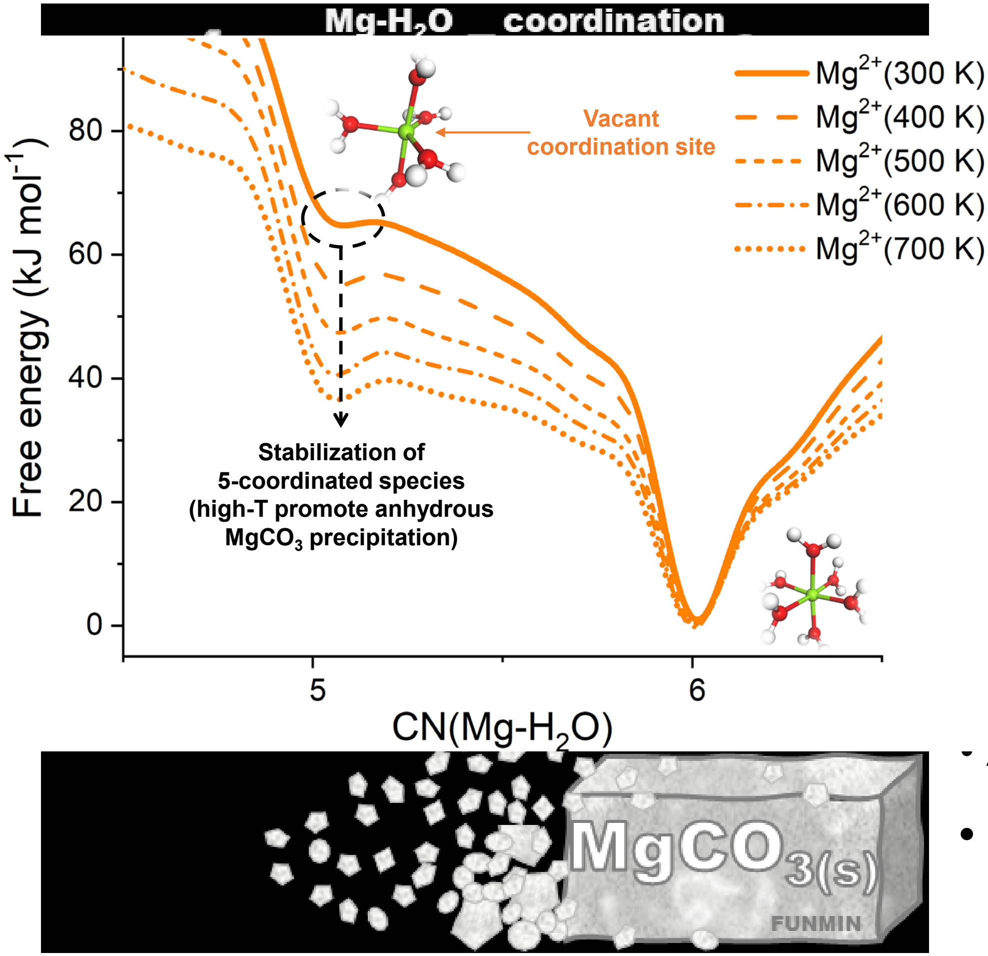
3. Empirical tracking of additives' effect on $MgCO_3$ production

4. Mechanism of $MgCO_3$ production & form
5. (amorphous-to-crystalline transition

6. Flow cell(s) for "real time" watching CO_2 mineralization

7. Pre-industrial bulk rector for generating 10s of kg of carbonates

WP1: Processes controlling Mg^{2+} dehydration



Front cover
CrystEngComm, 2021, 23, 4896-4900

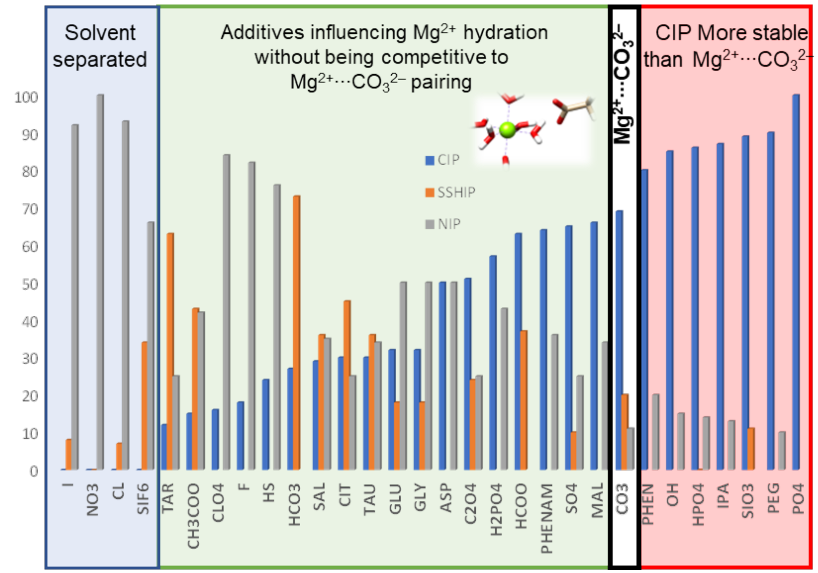
CrystEngComm HOT article:

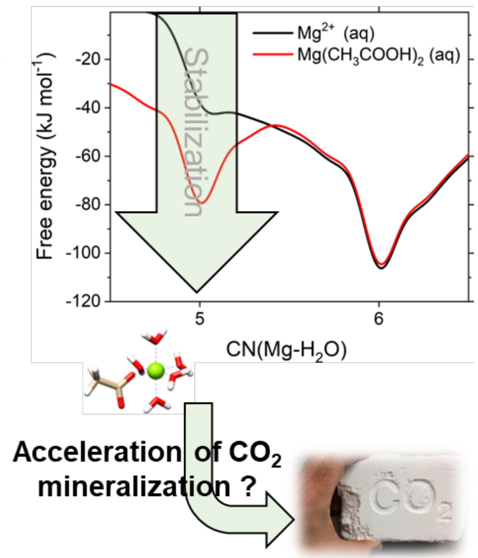
"New insights into the role of solution additive anions in Mg^{2+} dehydration: implications for mineral carbonation"

Key points:

- **$Mg(H_2O)_6^{2+}$ only stable coordination in pure water**
- **Additives help initiate mineralisation**
- **Promotion of low-temperature mineralisation**

WP1: Computational database of solution additives



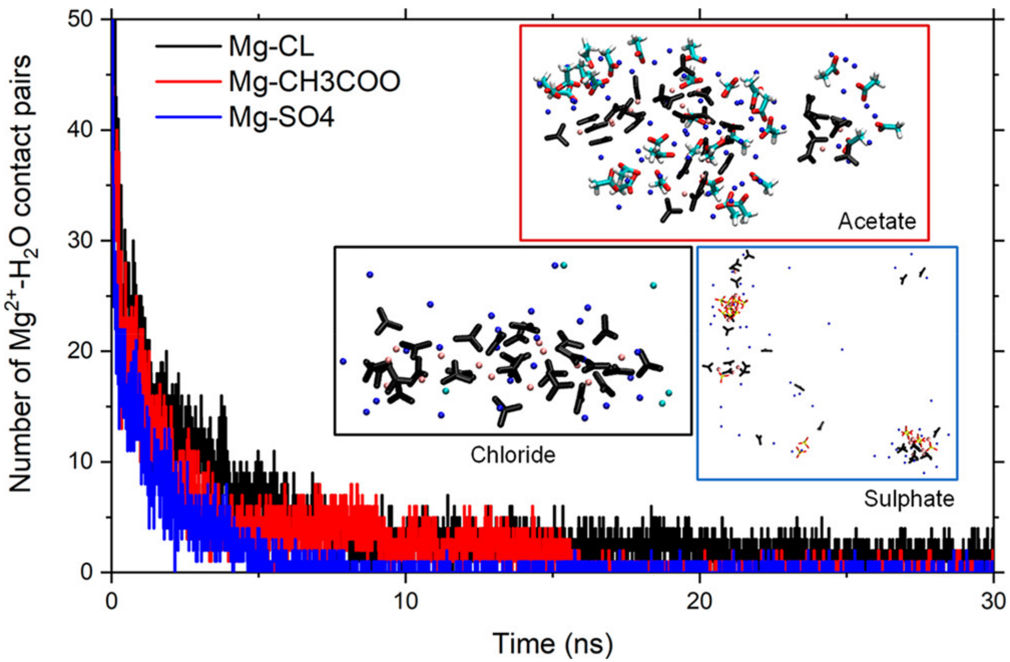


Non-competitive ions promoting Mg^{2+} dehydration

Key points:

- Extensive computer simulations of the early stages of $MgCO_3$ nucleation in the presence of solution additives
- Characterised the ability of thirty additives to promote dehydration based on well-defined molecular level criteria
- Identification of solution composition conditions catalysing the low-temperature CO_2 conversion into $MgCO_3$ → **promotion of CO_2-mineralisation at 25° C**

WP2: Effect of solution additives on $MgCO_3$ aggregation



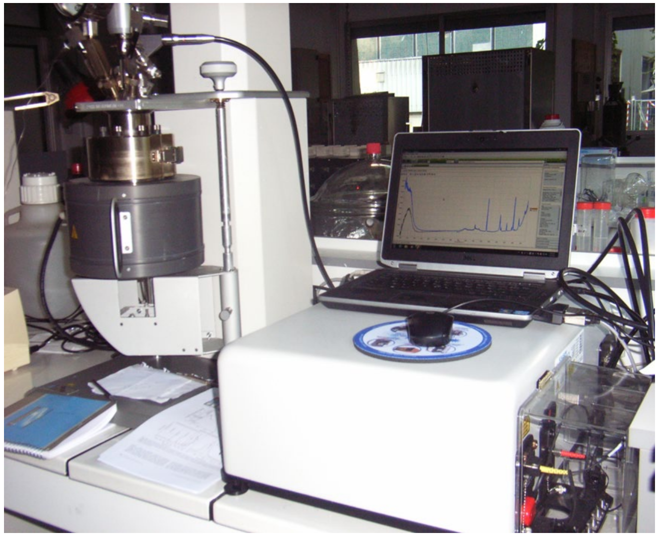
Non-competitive ions promoting $MgCO_3$ crystal nucleation

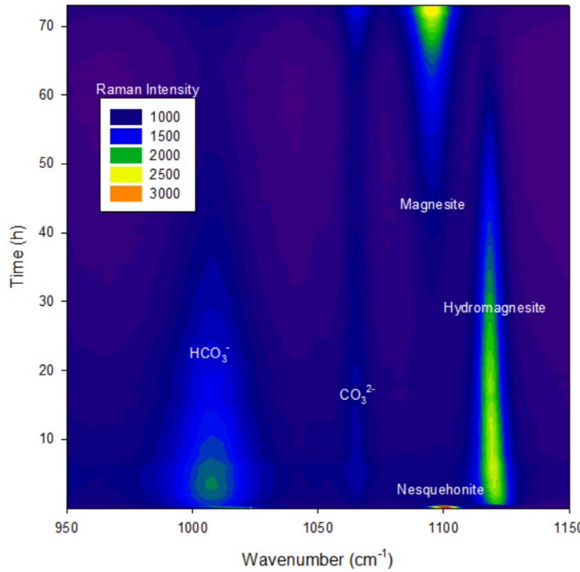
Key points:

- **Formation of stable carbonates with non-hazardous additives (**acetate, chloride, and sulphate**)**
- **Agreement between simulation ↔ experiment**

Crystal Growth & Design, 2022, 22, 3080–3089.

WP2: Experimental verification of $MgCO_3$ growth





Raman monitoring during nucleation and growth of $MgCO_3$ particles and crystals under hydrothermal conditions

Key points:

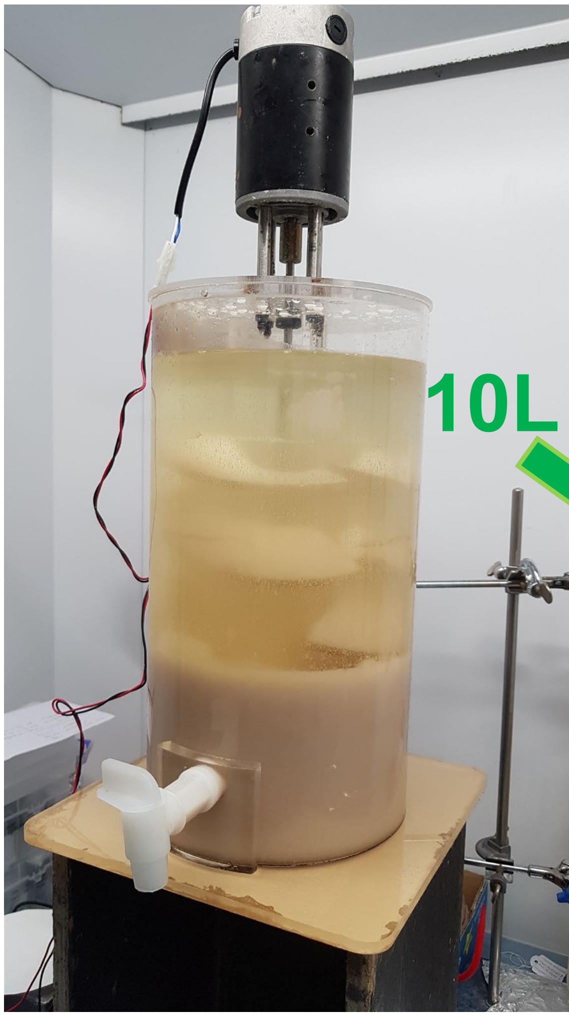
- Real-time nucleation measurements under different solution conditions (CH_3COO^- , SO_4^{2-}, NO_3^-, …)
- Classical nucleation pathway revealed
- The presence of acetate ions promotes "low" T $MgCO_3$ formation

$MgCl_2.7H_2O$ (aq) + $NaCO_3$ (aq) → $MgCO_3 \cdot 3H_2O$ (s), T = 90 ° C (stable hydrated phase)

$Mg(\mathbf{CH_3COO})_2$ (aq) + $NaCO_3$ (aq) →

$MgCO_3 \cdot 3H_2O$ (s) → $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$ (s) → $\mathbf{MgCO_3}$ (s), T = 90 ° C (fast)

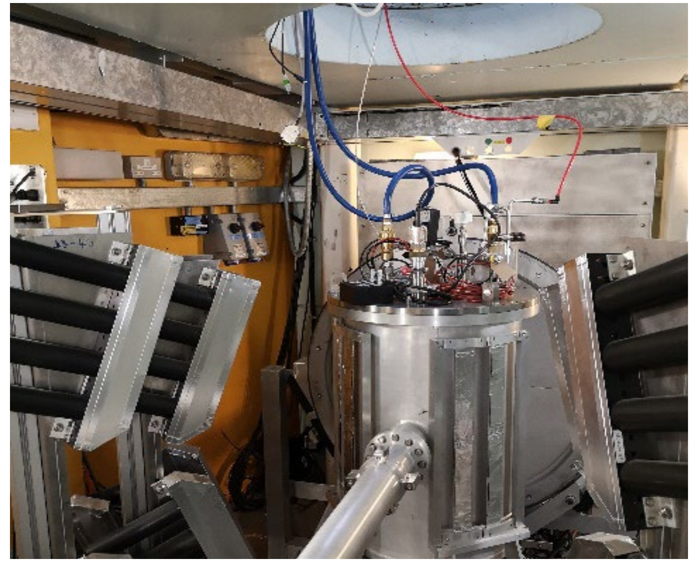
WP4: Scale-up of CO_2-mineralisation pre-industrial scale & control of Mg-carbonate growth



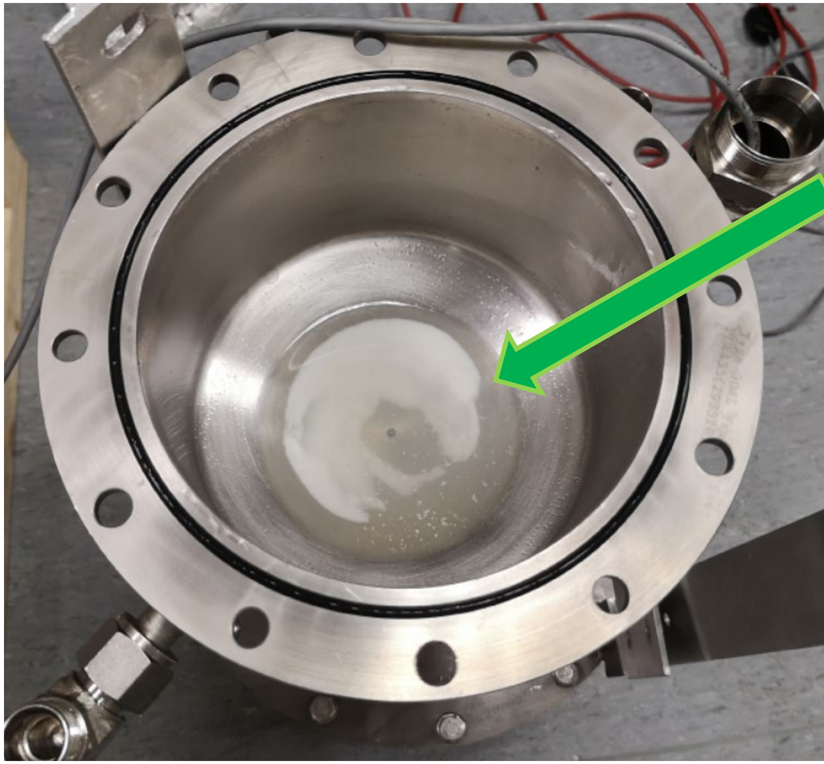
- 1st generation bulk CO2-mineralisation reactor built . Has 10L capacity, generates carbonates @ ~1-2kg / hour
- Modulating conditions and solution chemistry generates differing forms → allowing for control of particle sizing and properties

1-2kg / hr

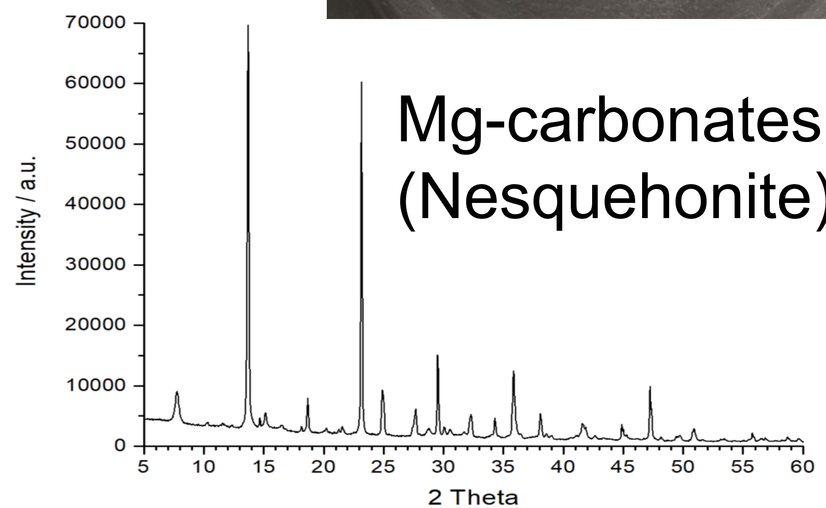
WP4: Tracking CO_2 mineralisation from nano- to bulk-scales – Neutron beam analyses in real-time



WP4: Mg-Carbonates produced @ ~50-100g scales



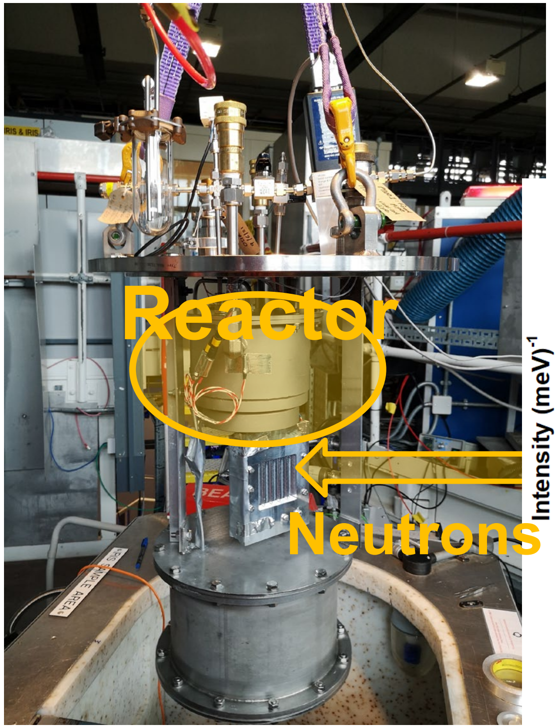
Residual Carbonates

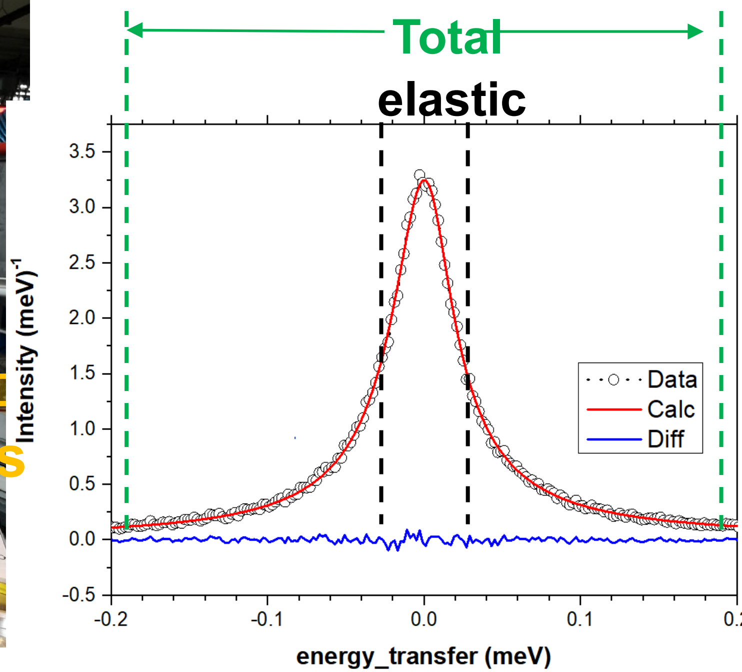


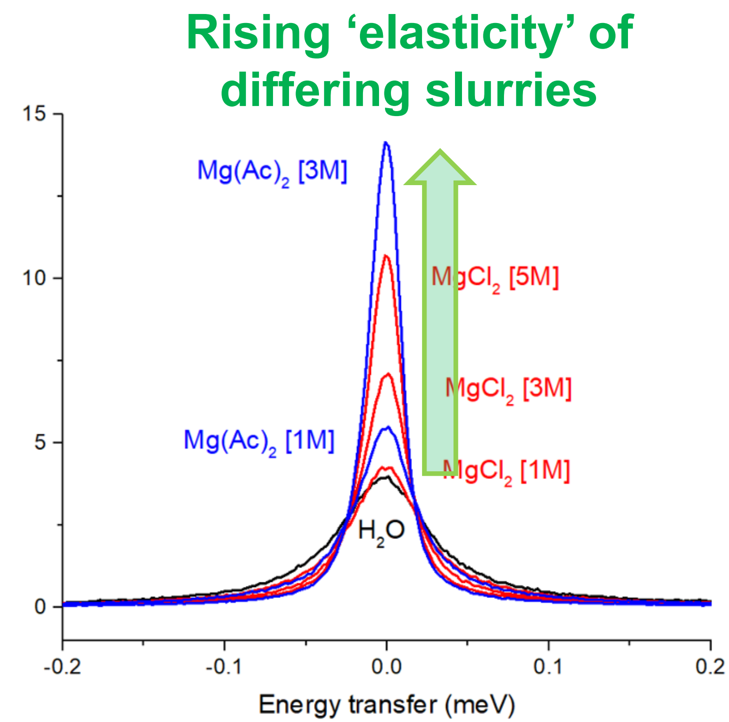
Key results:

- Mineralisation reactor retained industrial conditions and product homogeneity, residual carbonates in reactor likewise easily processed (removed) confirming reactor re-use (i.e., industrial robustness)
- Output product Mg-carbonates (i.e., nesquehonite) was confirmed as pure via XRD measurements

WP4: Determining viscosity in CO_2-mineralisation solutions with quasi-elastic neutrons



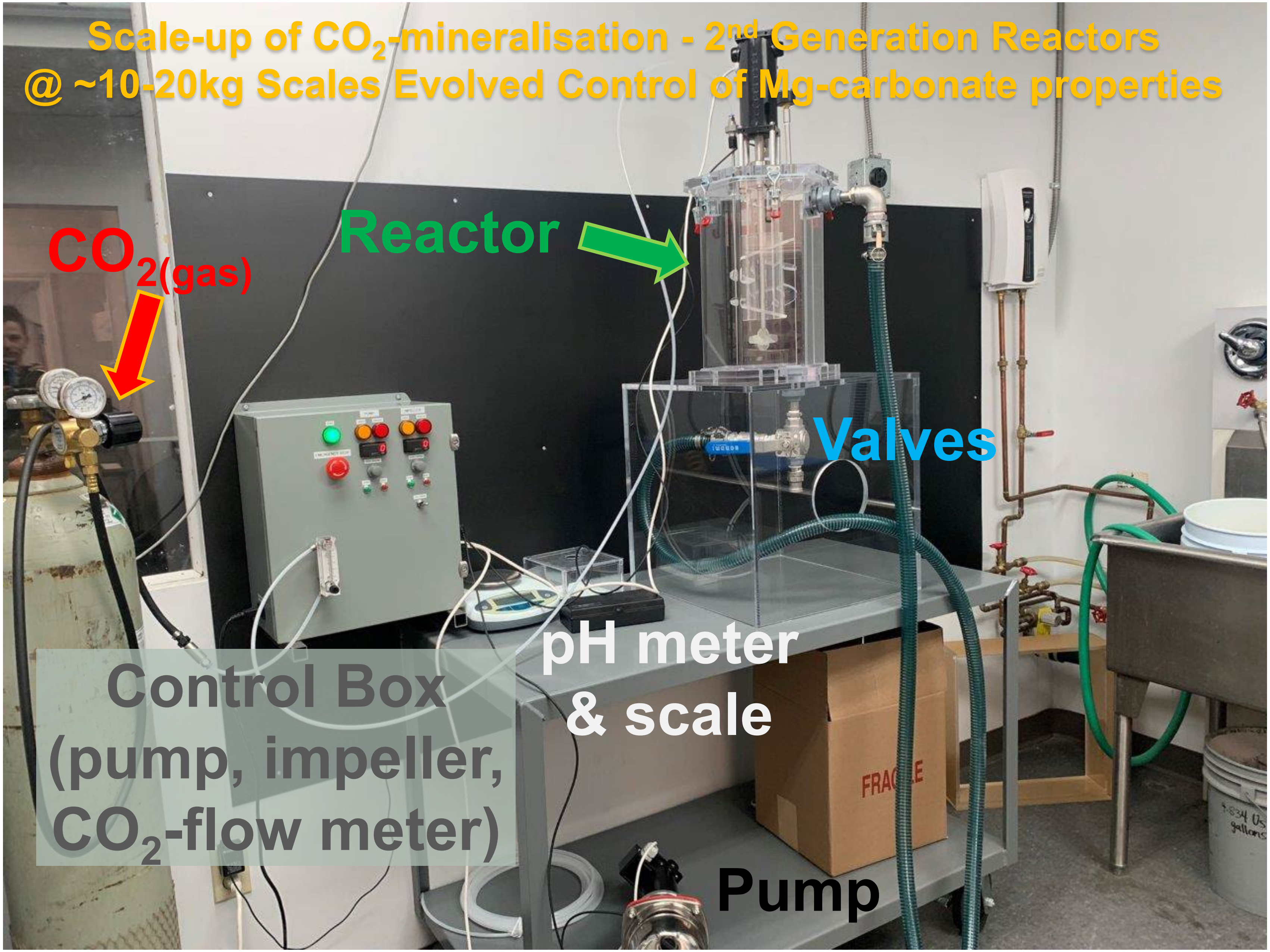




Key Points:

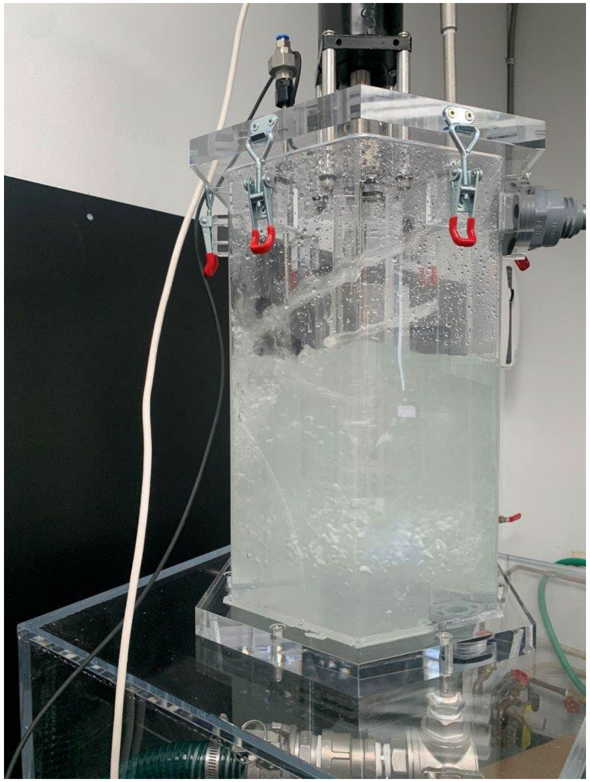
- Quasi-elastic scattering provides real-time tracking of viscosity. Changes ongoing Differing 'elasticity' values for the solutions are related to differing bulk viscosity and aggregation present and evolving...
- In this case, precise resolution of H_2O-solvent motions and differing aggregations of solutes.

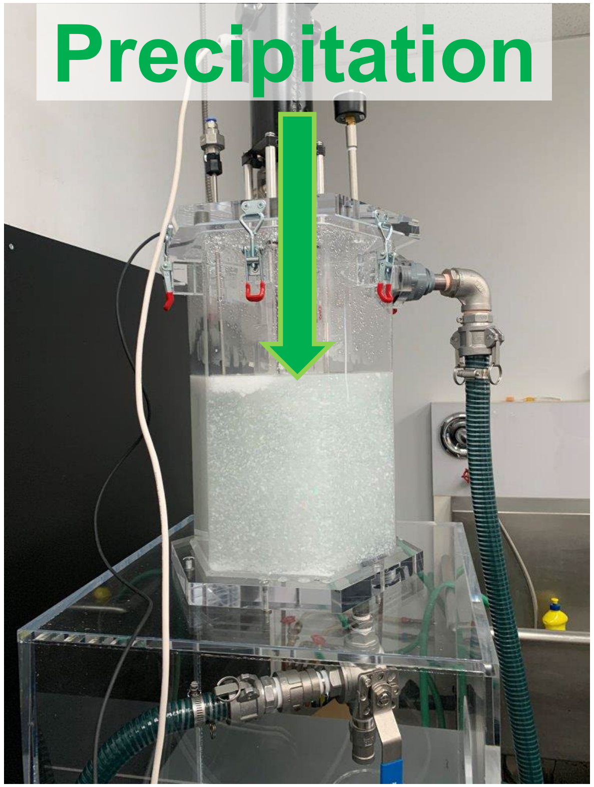
Scale-up of CO_2-mineralisation - 2nd Generation Reactors @ ~10-20kg Scales Evolved Control of Mg-carbonate properties



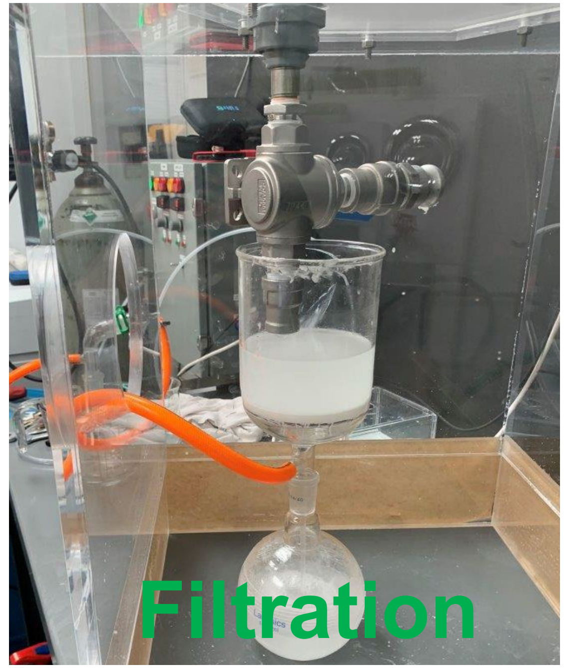
WP4: Scale-up: Here to 10+kg / hour.
Visualising Bulk Mineralisation

H_2O → Brine → Add CO_2

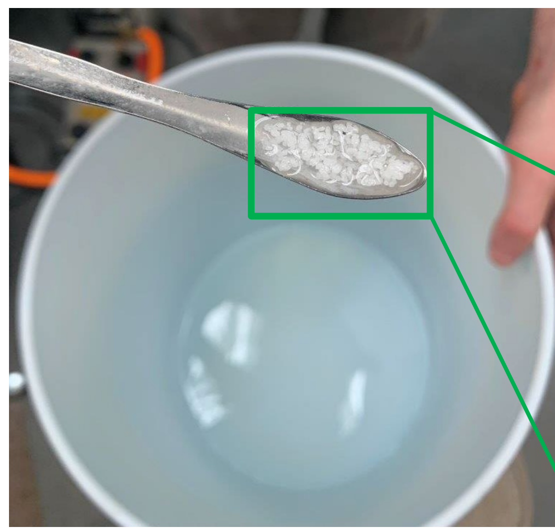


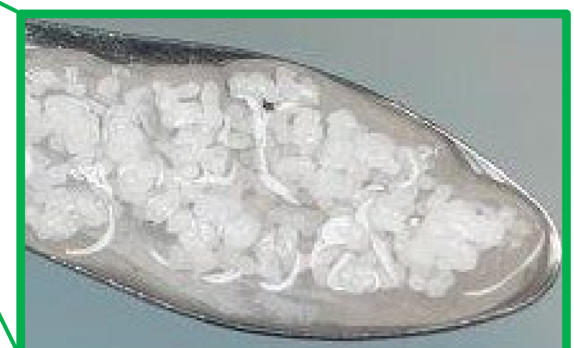


WP4: Scale-up: Precipitates form aggregates & clusters



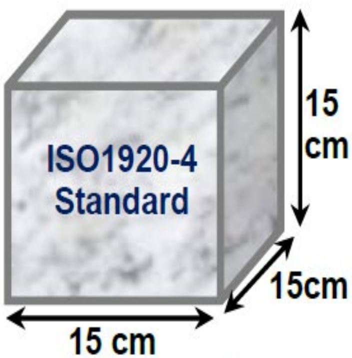
- Precipitates initially form flocculates
- Aggregates and clusters begin to form then supra- aggregate structures: stalactite like cones
- Filtration generates fine carbonate particles, which can then be dried or left as wet slurries





WP4: Scale-up: What to do with carbonates? Infrastructure

'Eurocubo'
(DRC, Srl., Italy)



Vol=3375 cm^3 ≈ 8kg

WP4: Scaling-up the Scale-Up: Compatibility with Concrete

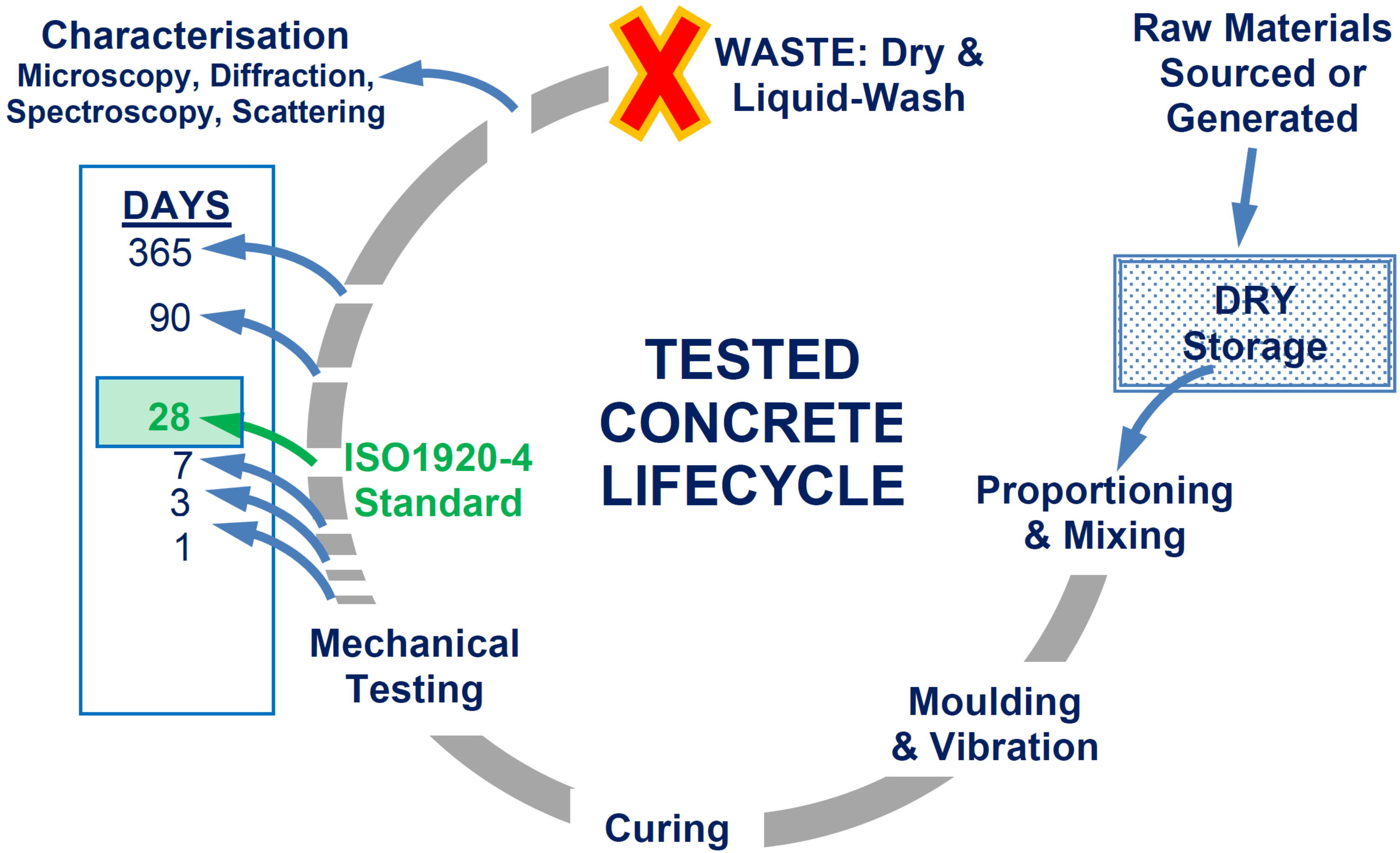
silo

direct?

compaction

- Mg-CO_3 (s) can be directly added to concrete; replacing cement (up to 30%) = € £ $ and lowers CO_2 footprint
- $MgCO_3$s ‘fixed’ carbon further reduces CO_2 budget
- We have also added agricultural wastes = preventing their degradation and release of CO_2, methane, etc.. (agriculture contributes ~9.5 gT/yr = ~1/3 of all emissions)

Sustainable Project Lifecycle



Demolition Waste – Same Fate as Fly Ash?

bbc.com/news/science-environment-61580979

Climate Change: MPs say building demolitions must be reduced

By Roger Harrabin
BBC energy and environment analyst

26 May | Comments

https://www.bbc.com/news/science-environment-61580979

26 May, 2022

Acknowledgements

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