Thermodynamic Modelling Approach for the Processing of Low-Temperature Belite Cement Clinker from Concrete Waste Using Na_2CO_3 & $CaCl_2$ as Mineralizers

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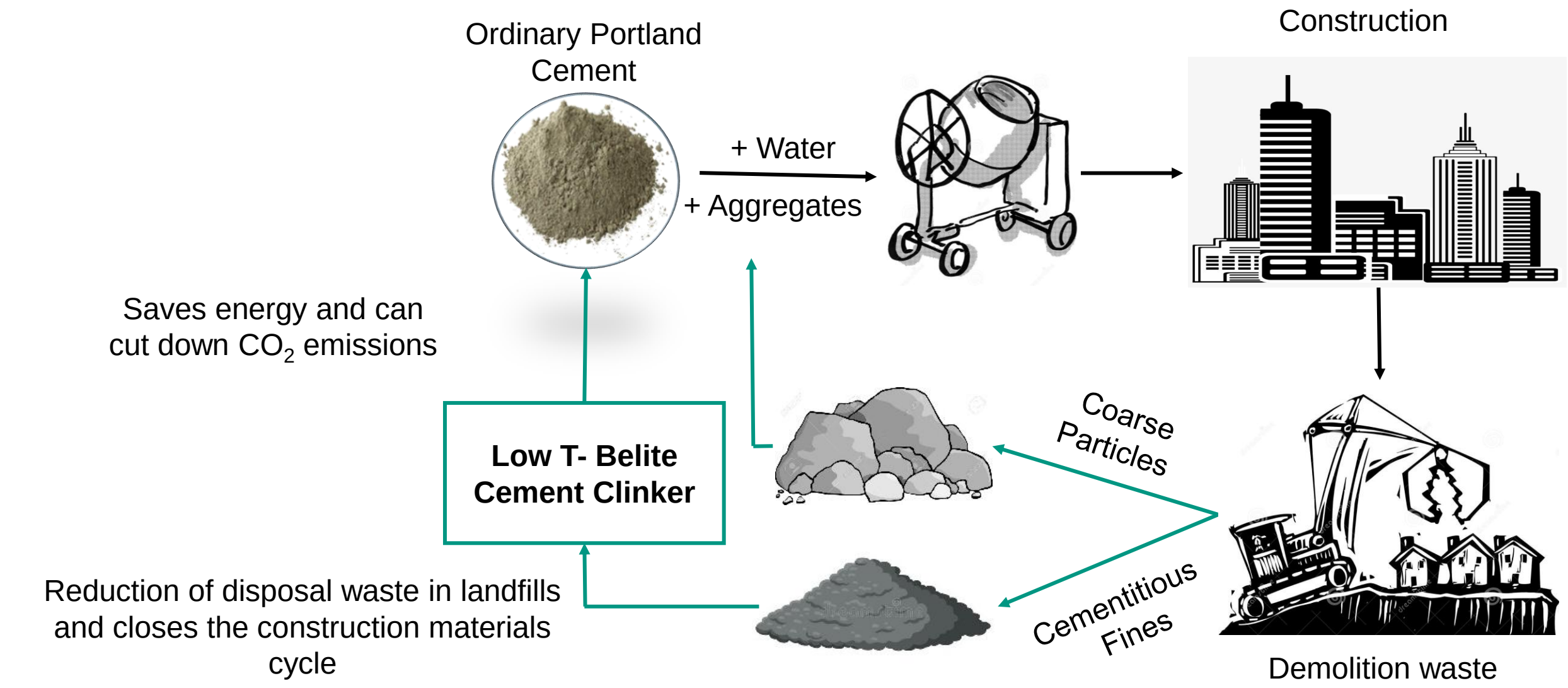
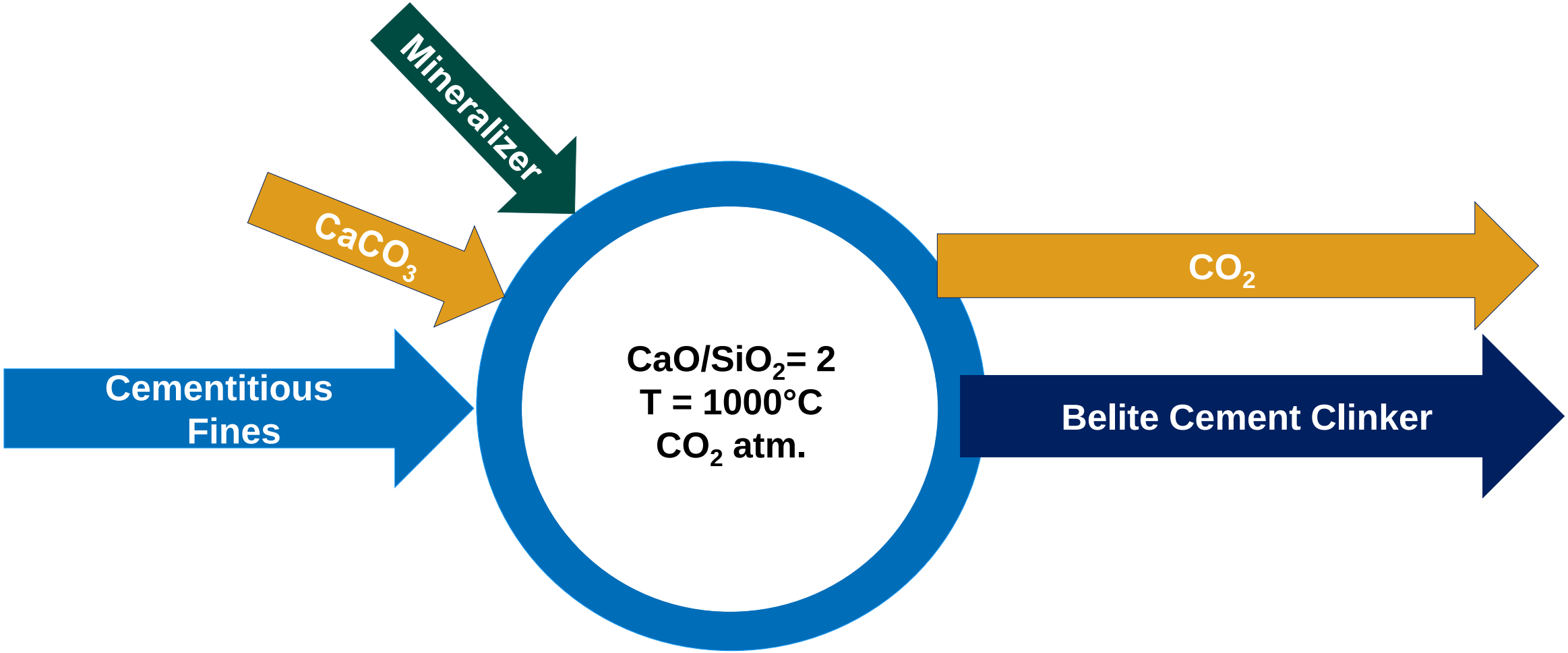
Circularity in the Cement Industry



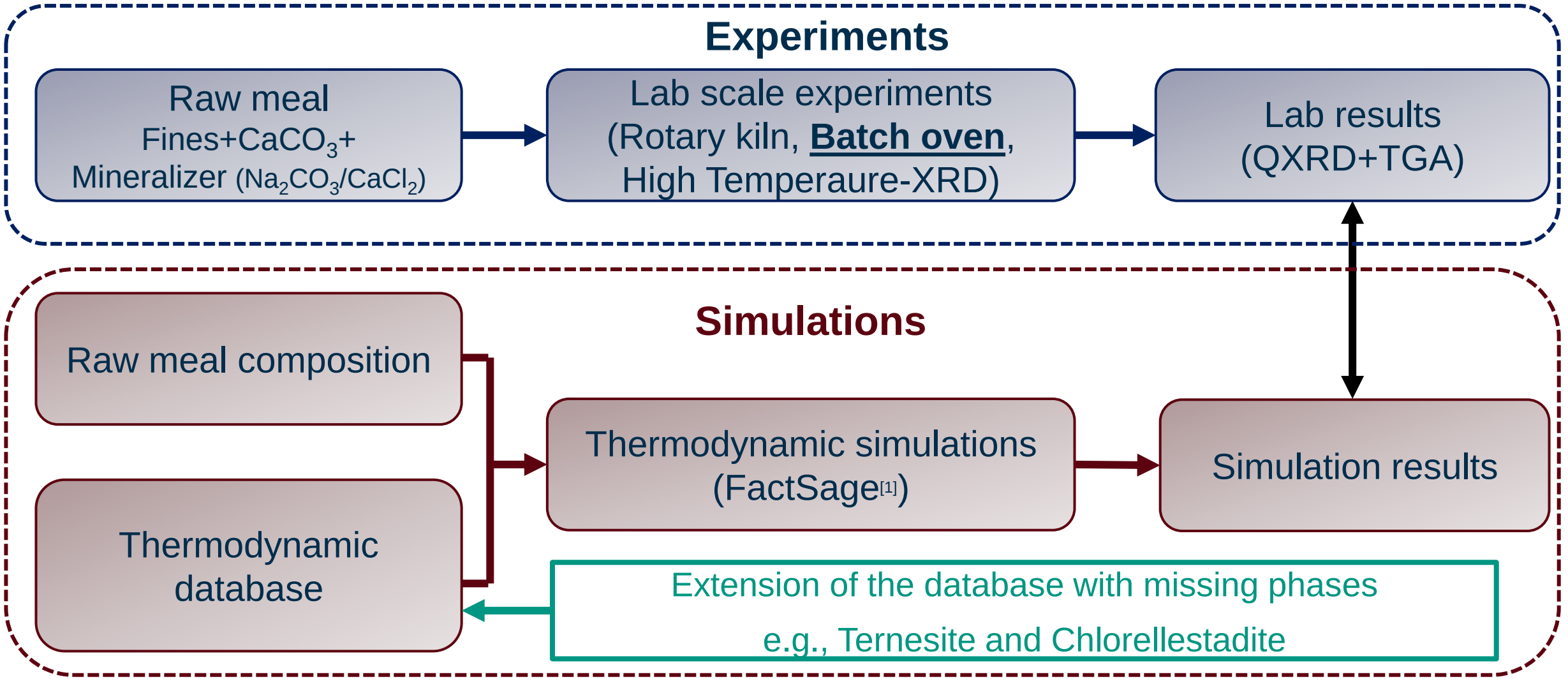
Cementitious Waste to Belite Route



Motivation

- **Composition of concrete waste**
  - Primarily composed of CaO and SiO_2
  - Minor components such as Al_2O_3, Fe_2O_3, Na_2O, K_2O and SO_3
- **Compositional variability**
  - Autoclaved Aerated Concrete (AAC) waste -> e.g SO_3 content ranging from 0.5 wt.% to 5 wt.%
- **These differences**
  - Influence clinker phase formation and stability
  - Complicate process control and process consistency
  - Increase experimental effort
- **Thermodynamic modelling**
  - Predict product phases under varying compositions
  - Reduce the need for experimental trials

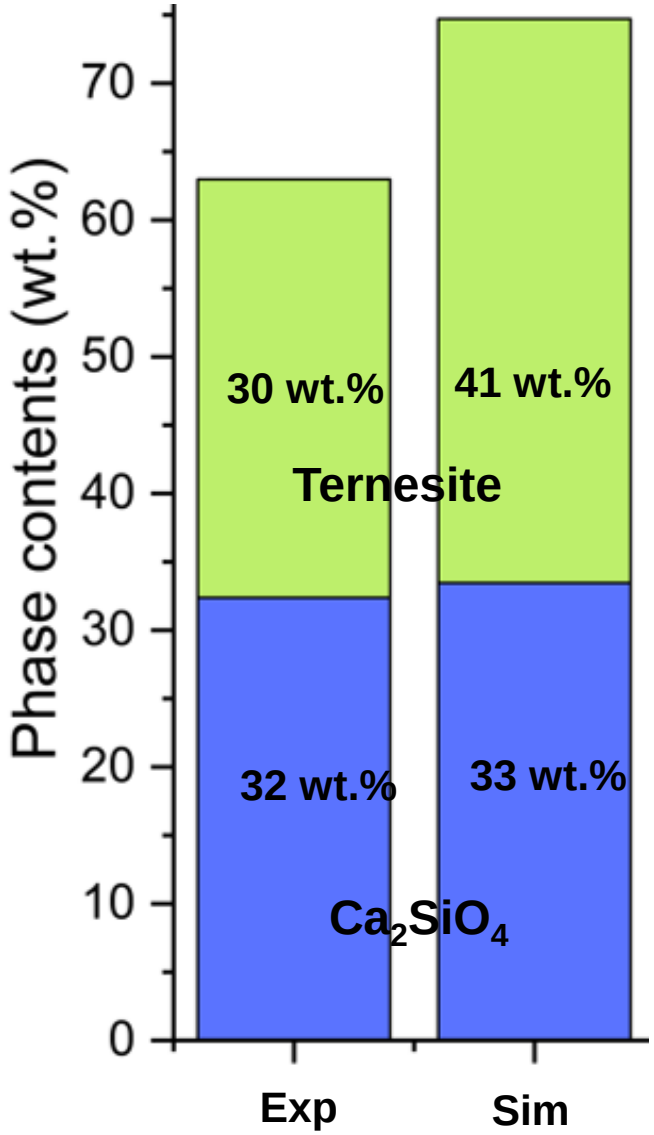
Methodology



[1] C. W. Bale, E. Bélisle, P. Chartrand, S. A. Decterov, G. Eriksson, A.E. Gheribi, K. Hack, I. H. Jung, Y. B. Kang, J. Melançon, A. D. Pelton, S. Petersen, C. Robelin. J. Sangster, P. Spencer and M-A. Van Ende, FactSage Thermochemical Software and Databases - 2010 - 2016, Calphad, vol. 54, pp 35-53, 2016 www.factsage.com

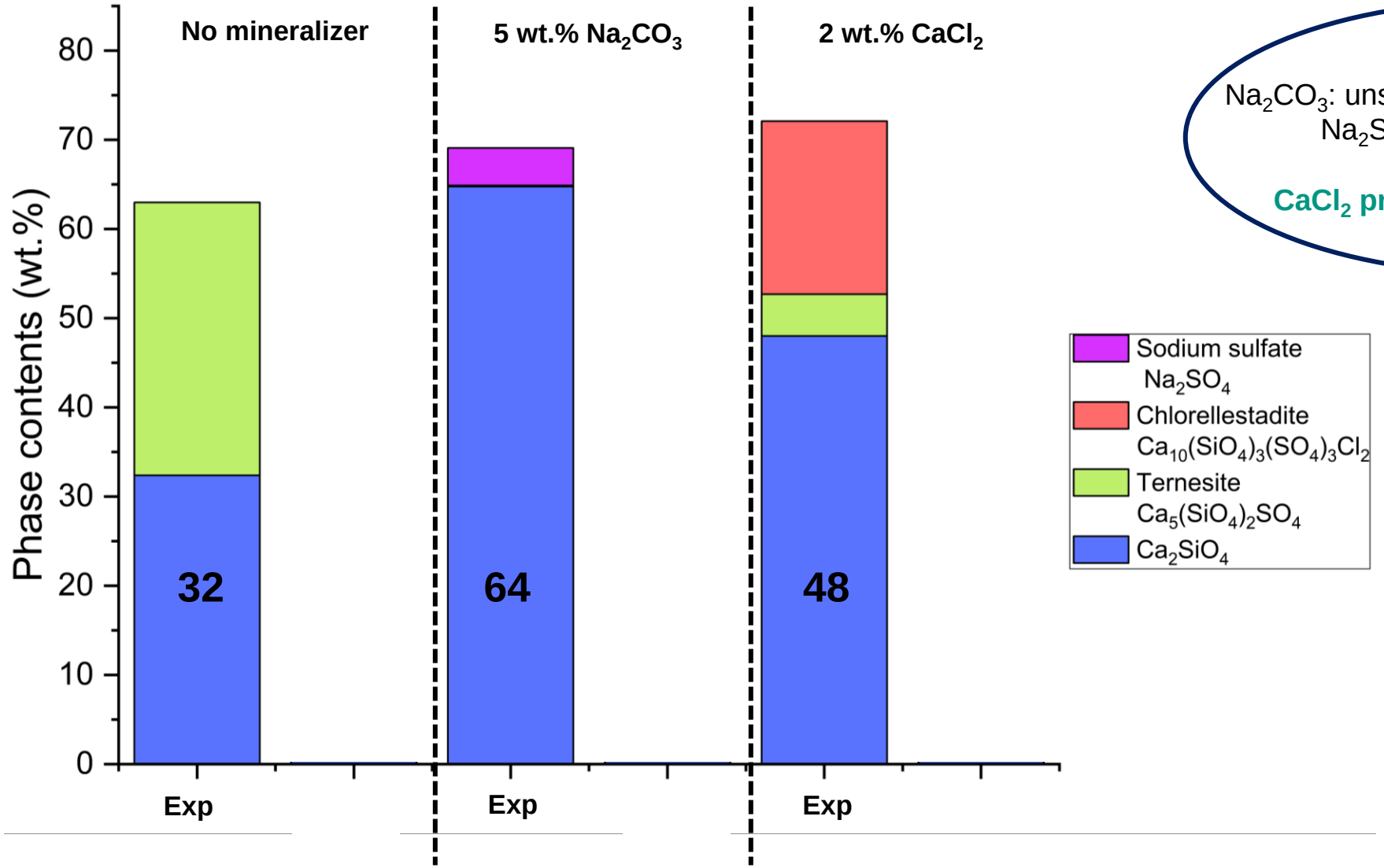
Results: Belite Cement Clinker from AAC (Exp. vs Sim.)

→ Reliable phase prediction requires a complete thermodynamic database



→ Simulation results align well with the experimental results

Results: Impact of mineralizer on AAC raw meal (High SO_3)

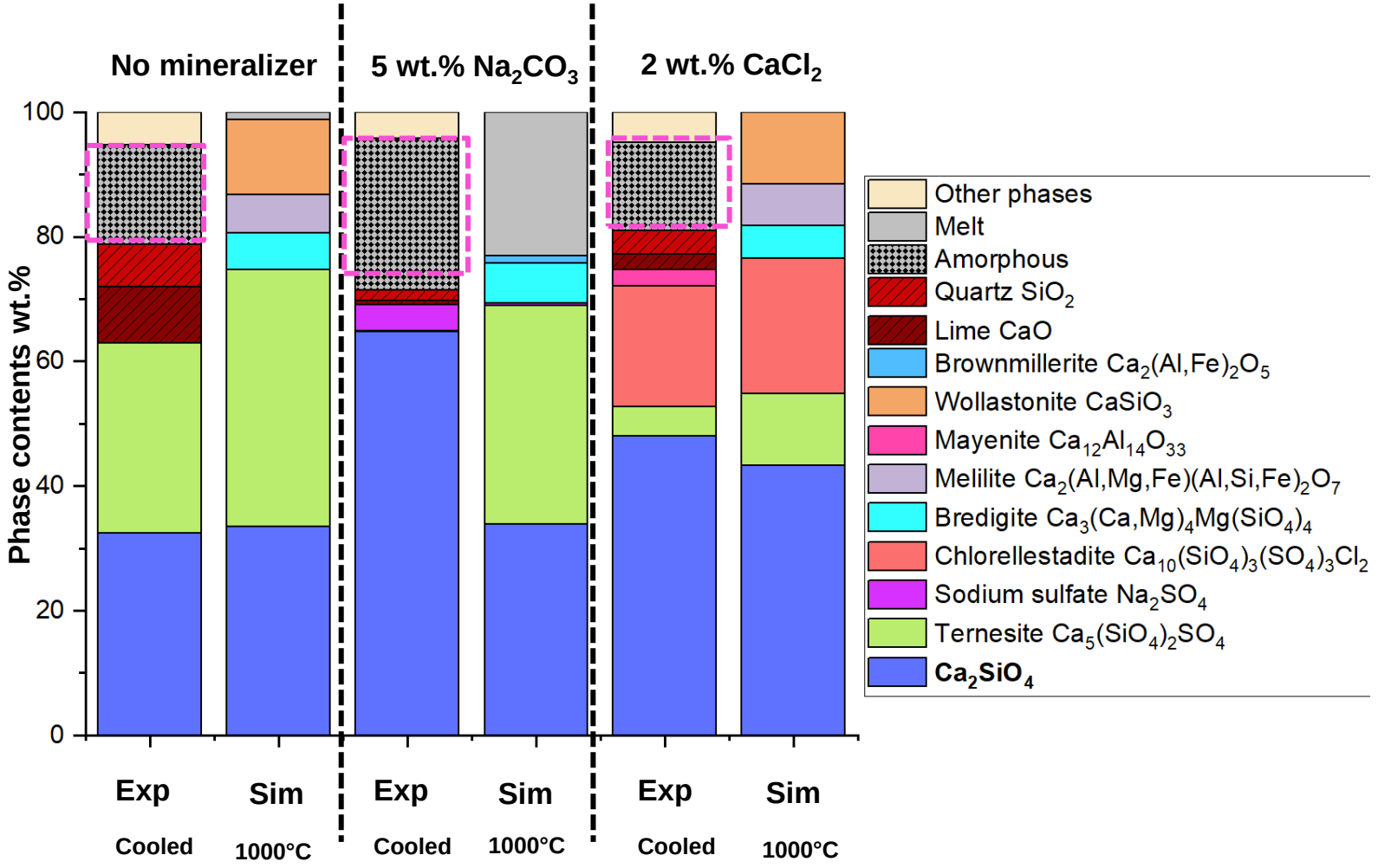


Na_2CO_3: unsuitable in high sulfate systems
Na_2SO_4 formation (highly soluble)

$CaCl_2$ prevents undesirable phases

[2] Ullrich, A.; Garbev, K.; Schweike, U.; Köhler, M.; Bergfeldt, B.; Stemmermann, P. CaCl2 as a Mineralizing Agent in Low-Temperature Recycling of Autoclaved Aerated Concrete: Cl-Immobilization by Formation of Chlorellestadite. Minerals 2022, 12, 1142.

Results: Amorphous Content, Melt Formation, Kinetic effects



Amorphous phase is observed in exp.

→ incomplete crystallization of the melt

→ grinding prior to the XRD analysis

Simulations assume equilibrium

→ Melt at high temperatures

Experiments deviate from equilibrium

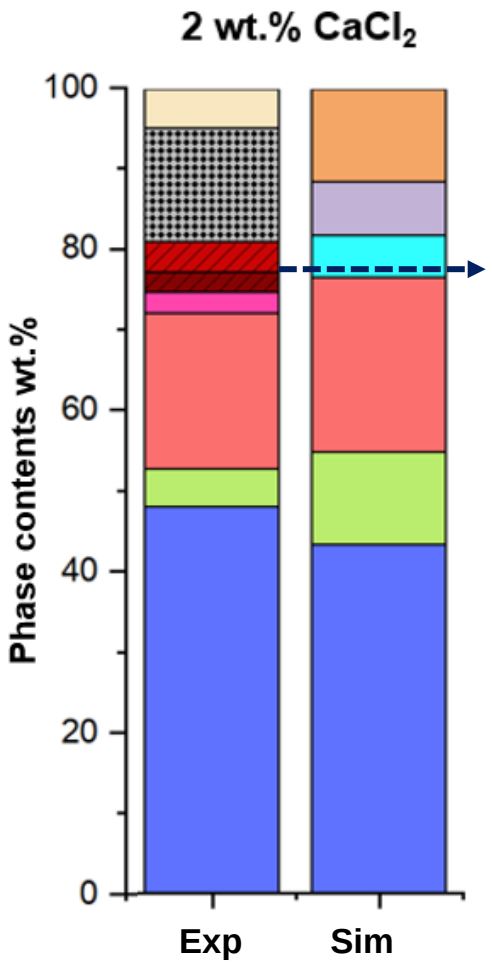
→ Likely due to inhomogeneity, grain size

→ Results in unreacted quartz and lime

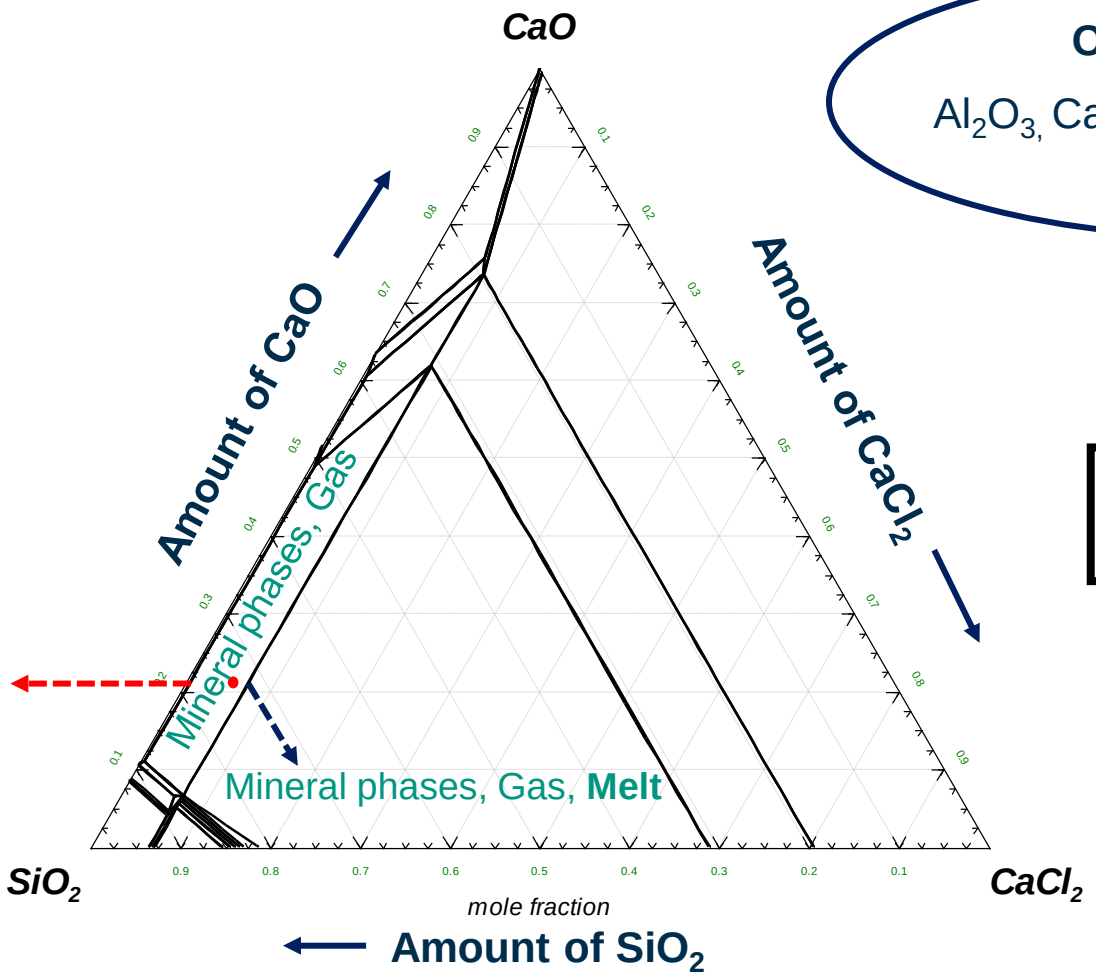
Phases stable only in simulation are

→ Bredigite: formation is sluggish in experiments

Simulation Result: Phase Diagram at 1000 °C
Belite from AAC with $CaCl_2$ as mineralizer



Unreacted
CaO, SiO_2



Raw meal
composition

Other Components

Al_2O_3, $CaSO_4$, Fe_2O_3, MgO, $CaCO_3$

Predicts phases formed due to unreacted materials

Conclusions and Outlook

- Low-temperature belite cement clinker produced from concrete waste
- Thermodynamic modelling
  - Improved database enhances prediction accuracy
  - Predicts effect of different processing conditions
- Simulation approach developed for unreacted raw materials
- Na_2CO_3 promotes higher belite formation, effective for low-sulphate systems
  - No mineralizer < Na_2CO_3 < $CaCl_2$

- Further analytical techniques will be applied to identify melt phases for model optimisation
- Thermodynamic databases will be refined in case of inconsistencies
- Future work will determine the boundaries and limitations of the belite model

Thank you for you attention!

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