

# **Sustainability in cement industry: Thermodynamic modelling of belite cement clinker**

**Conference: Transforming towards a sustainable society – challenges and solutions**

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# Outline

- Introduction
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- Approach
- Results
- Summary and Outlook

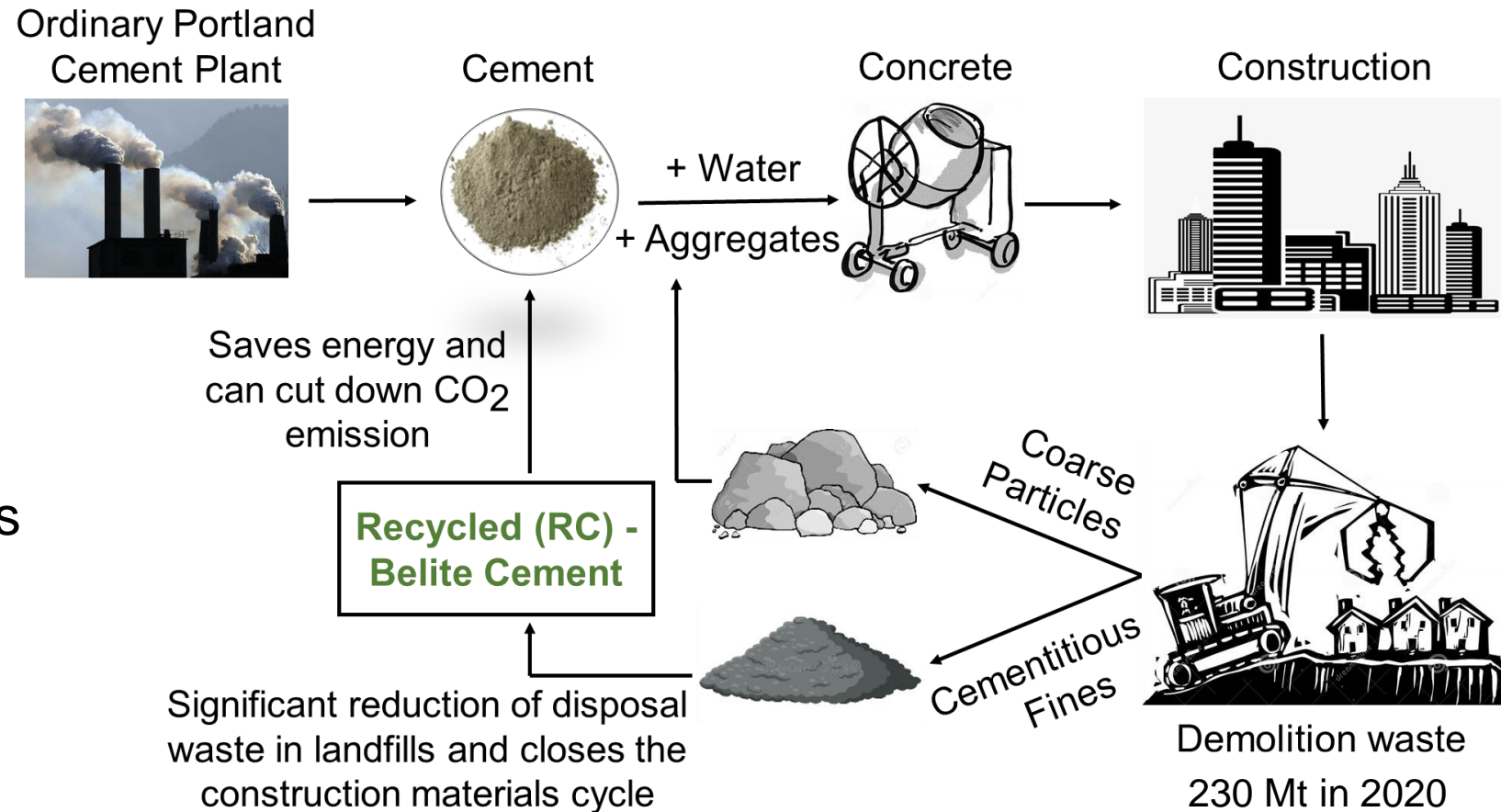
# Introduction: Zero Emission Circular Concrete

## Cement:

- > Hydraulic binder
- > Energy intensive process
- > Responsible for 8% of the global CO<sub>2</sub> emissions [1]

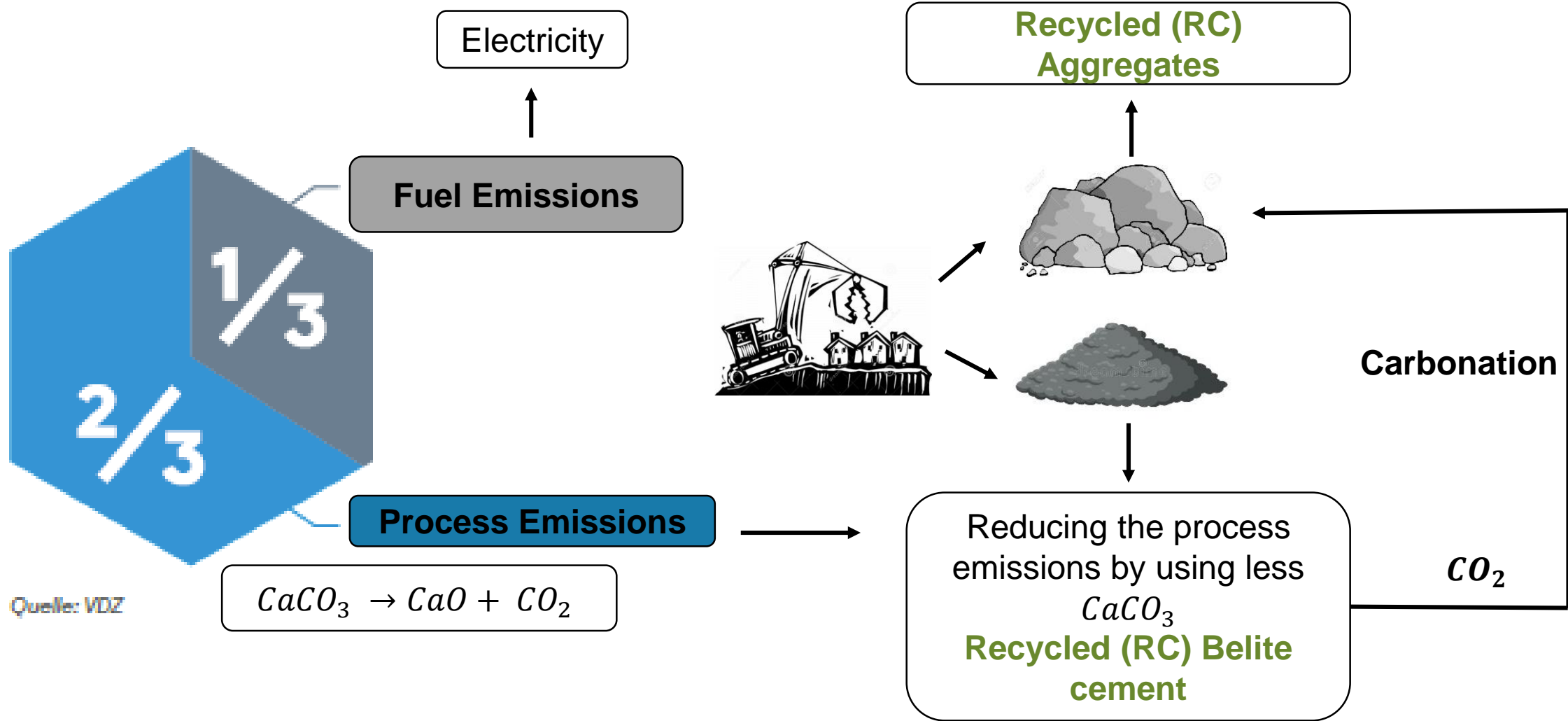
## Objectives:

- > Reuse of cementitious fines
- > Optimization of RC – belite cement process using thermodynamic modelling



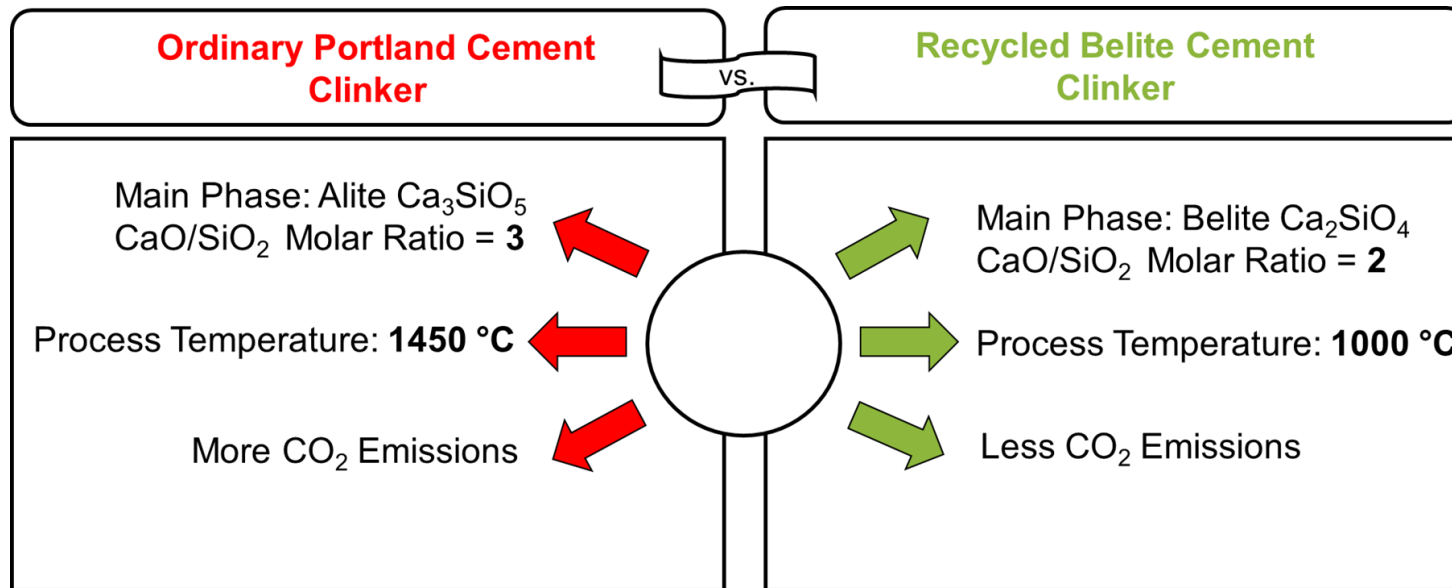
[1]: Robbie, M.A. Global CO<sub>2</sub> emissions from cement production, 1928-2018. Earth Syst. Sci. Data 2019, 11, 1675-1710

# Introduction: Zero Emission Circular Concrete RC-Cement + RC-Aggregates



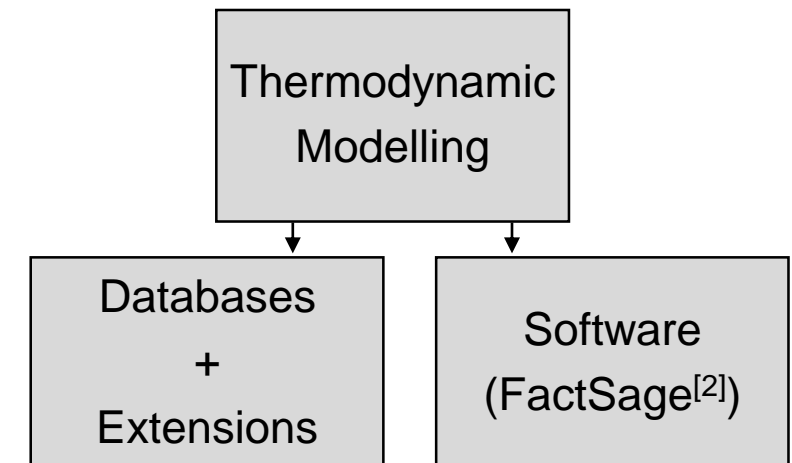
Quelle: VDZ

# Theoretical Background



## Thermodynamic Modelling

- > Prediction of phase composition and reaction path
- > Search for optimal conditions

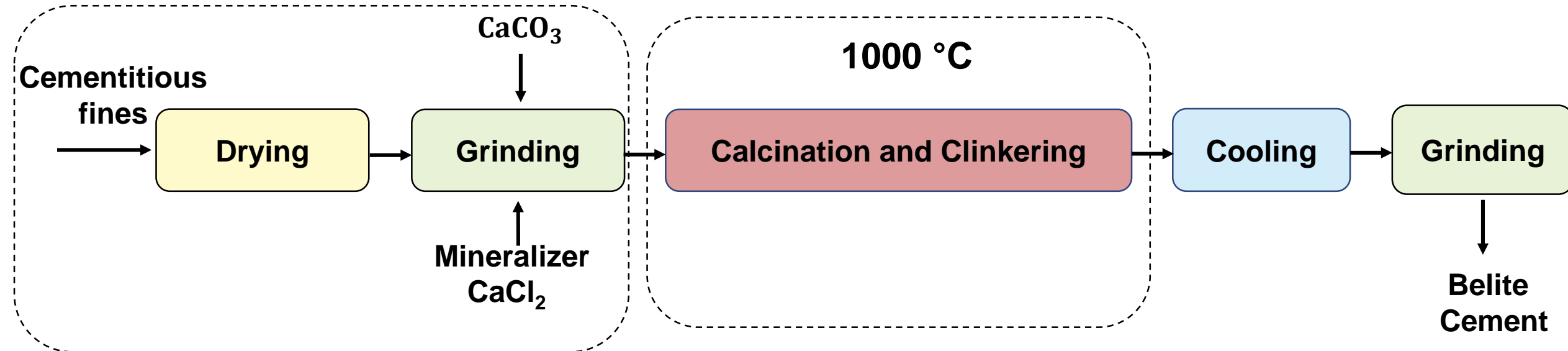


[2]: <https://www.factsage.com/>

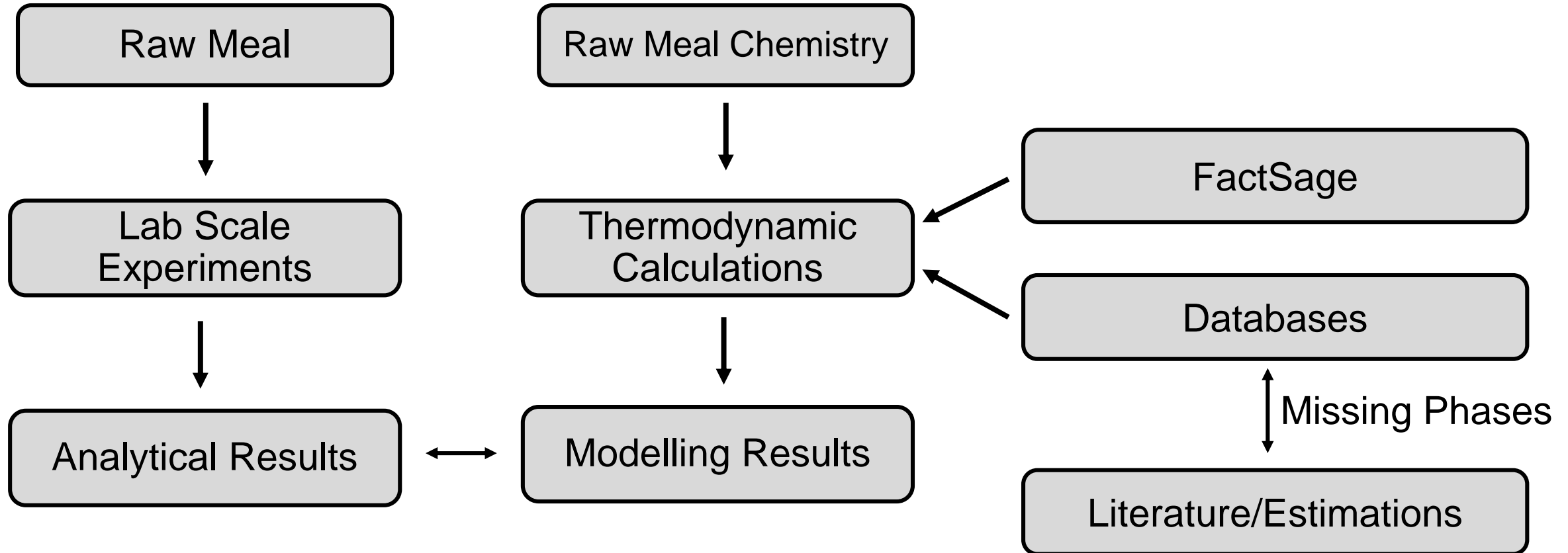
# KIT Belite Process

## Raw Meal Preparation

## Thermodynamic Modelling



# Modelling Approach



# Results: Simulation

Raw Meal with  $\text{CaCl}_2$   
as mineralizer

## Extensions (Implemented Phases):

- Chlorellestadite  $\text{Ca}_{10}(\text{SiO}_4)_3(\text{SO}_4)_3(\text{Cl})_2$
- Chlormayenite  $\text{Ca}_{12}\text{Al}_{14}\text{Cl}_2\text{O}_{32}$
- Ternesite  $\text{Ca}_5(\text{SiO}_4)_2\text{SO}_4$
- Yeelimite  $\text{Ca}_4\text{Al}_6(\text{SO}_4)\text{O}_{12}$
- Mayenit  $\text{Ca}_{12}\text{Al}_{14}\text{O}_{33}$

## Input

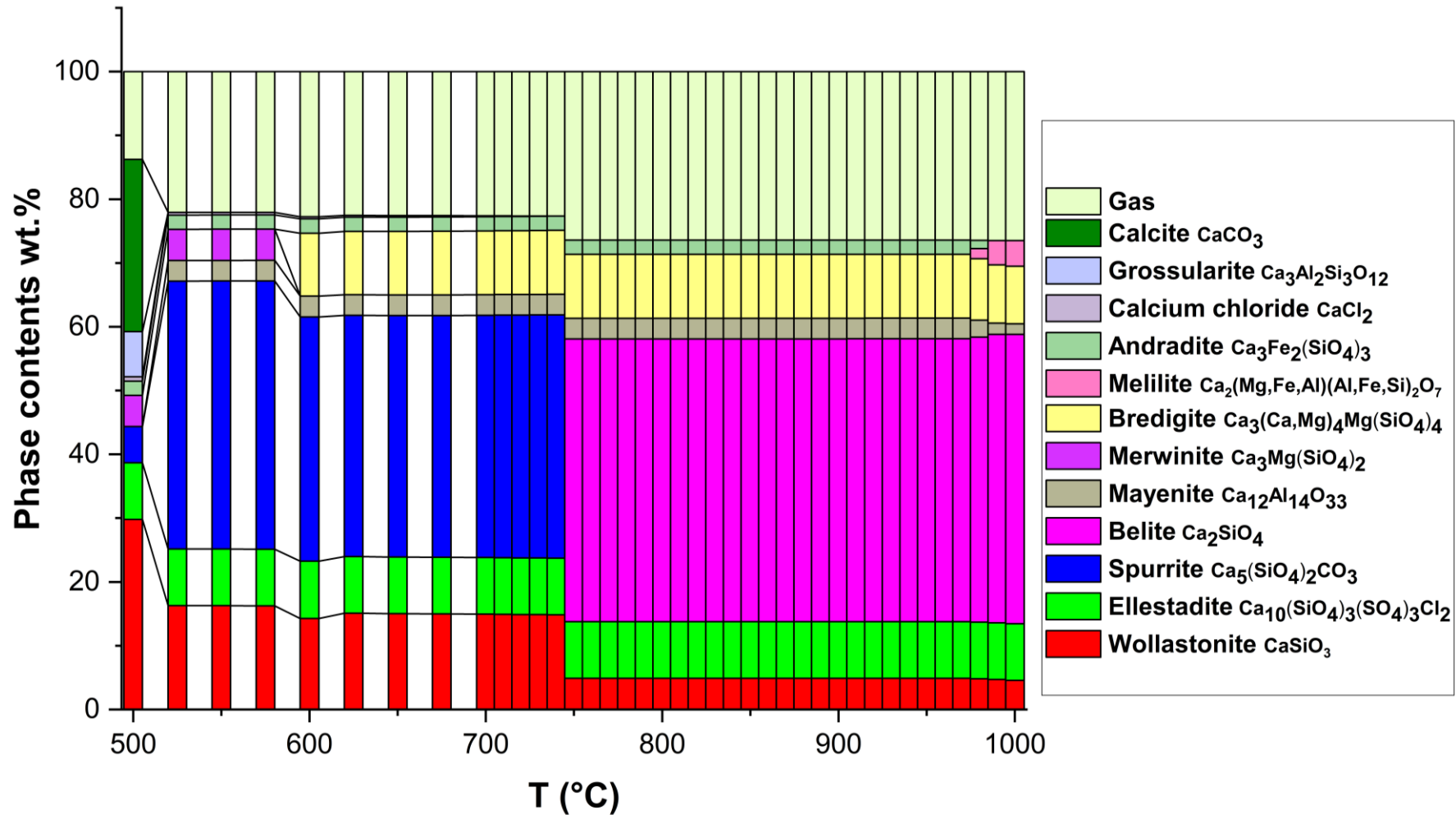
Input	wt. %
$\text{CaCO}_3$	50.9
$\text{SiO}_2$	23.9
$\text{CaO}$	13.3
$\text{CaSO}_4$	3.5
$\text{CaCl}_2$	1.7
$\text{Al}_2\text{O}_3$	1.6
$\text{Fe}_2\text{O}_3$	0.7
$\text{MgO}$	0.6
$\text{H}_2\text{O}$	3.8
Total	100

## Output Equilibrium Result at 1000°C

Phases	wt. %
Belite $\text{Ca}_2\text{SiO}_4$	45.4
Bredigite $\text{Ca}_3(\text{Ca}, \text{Mg})_4\text{Mg}(\text{SiO}_4)_4$	9.0
Chlorellestadite $\text{Ca}_{10}(\text{SiO}_4)_3(\text{SO}_4)_3\text{Cl}_2$	8.9
Wollastonite $\text{CaSiO}_3$	4.6
Melilite $\text{Ca}_2(\text{Mg}, \text{Fe}, \text{Al})(\text{Al}, \text{Fe}, \text{Si})_2\text{O}_7$	4.0
Chlormayenite $\text{Ca}_{12}\text{Al}_{14}\text{Cl}_2\text{O}_{32}$	1.7
Gas ( $\text{CO}_2$ and $\text{H}_2\text{O}$ )	26.4
Total	100



# Results: Simulation



# Results: Simulation Vs. Experiments

Phases	wt. % Simulations	wt. % Experiments	
Belite $\text{Ca}_2\text{SiO}_4$	61.7	63.8	-> Product is 60% of solid
Bredigite $\text{Ca}_3(\text{Ca}, \text{Mg})_4\text{Mg}(\text{SiO}_4)_4$	12.3	0	-> Mg
Chlorellestadite $\text{Ca}_{10}(\text{SiO}_4)_3(\text{SO}_4)_3\text{Cl}_2$	12.1	9.9	-> $\text{SO}_4$ , Cl
Wollastonite $\text{CaSiO}_3$	6.2	0.6	
Melilite $\text{Ca}_2(\text{Mg}, \text{Fe}, \text{Al})(\text{Al}, \text{Fe}, \text{Si})_2\text{O}_7$	5.4	0	-> Mg, Fe, Al
Chlormayenite $\text{Ca}_{12}\text{Al}_{14}\text{Cl}_2\text{O}_{32}$	2.3	3.9	-> Al, Cl
Ternesite $\text{Ca}_5(\text{SiO}_4)_2\text{SO}_4$	0	0.1	
Lime $\text{CaO}$	0	0.1	} -> Grain size, kinetics, inhomogeneity
Quartz $\text{SiO}_2$	0	2.1	
Amorphous content	0	15.0	-> Real product contains amorphous content
Other phases	0	4.5	
Total	100	100	

# Summary and Outlook

## ■ Cementious Fines to Recycled Belite Cement :

- Saves resources
- Emits less CO<sub>2</sub>
- Avoids Landfill

■ Pilot Plant

## ■ Thermodynamic Modelling:

- Prediction of optimal conditions - > for eg. important temperature range for belite formation
- Identification of the reaction path
- Limitations: kinetics, grain size

■ Adjust modelling to real cases

■ Link HT-process model with factsage

■ Assessment of the thermodynamic model

# Thank you for your attention!

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