Karlsruher Institut für Technologie

Institut für Technische Chemie

Circular Zero Emission Concrete: Thermodynamic Modelling of Belite Cement Clinker

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P. Yarka Reddy, G. Beuchle, P. Stemmermann, D. Stapf

Outline

- Introduction
- Theoretical Background
- Approach
- Results
- Summary and Outlook

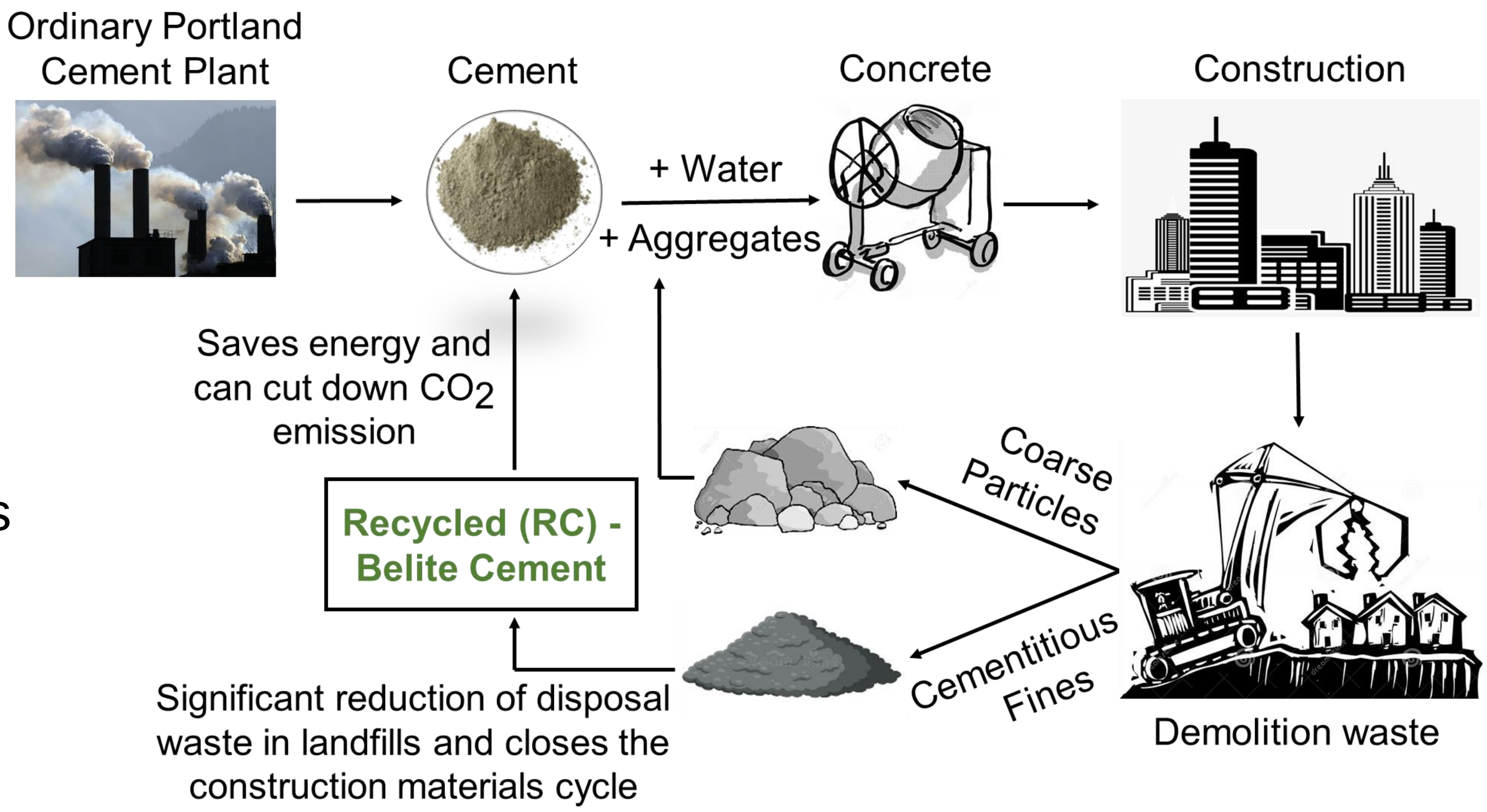
Introduction

Cement:

- > Hydraulic binder
- > Energy intensive process
- > Responsible for 8% of the global CO_2 emissions [1]

Objectives:

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



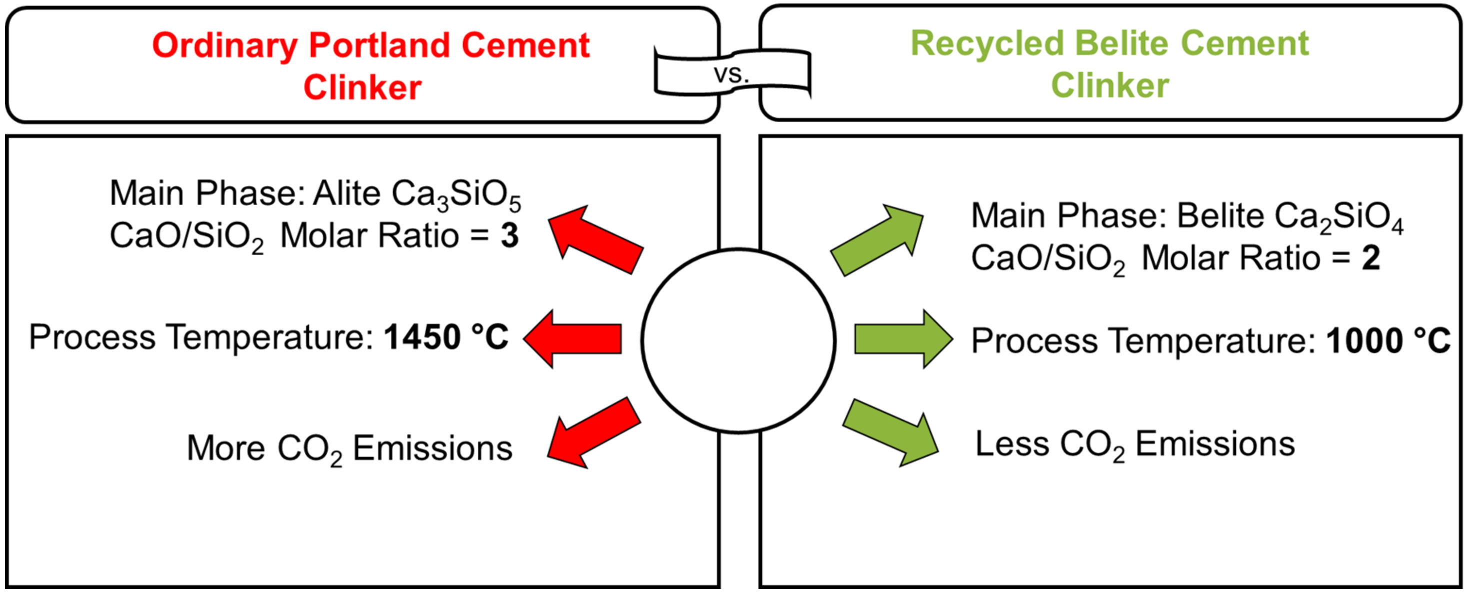
[1]: Robbie, M.A. Global CO_2 emissions from cement production,1928-2018. Earth Syst. Sci. Data 2019,11, 1675-1710

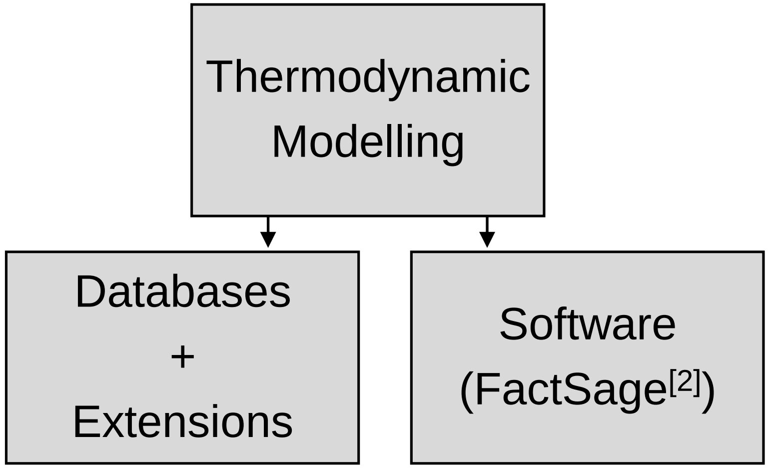
Theoretical Background

Thermodynamic Modelling

-> Prediction of phase composition and reaction path

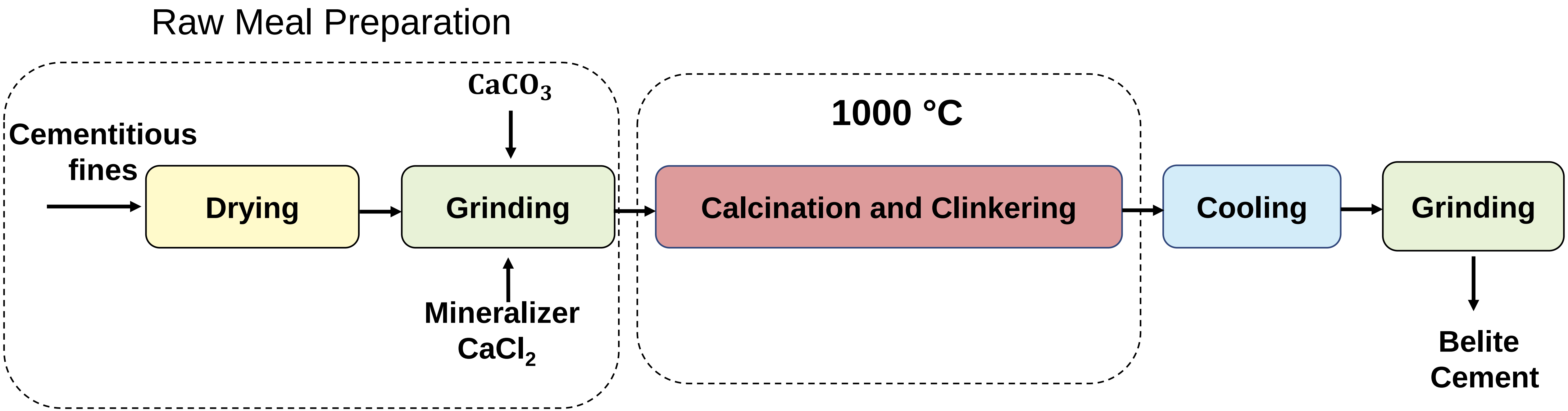
-> Search for optimal conditions



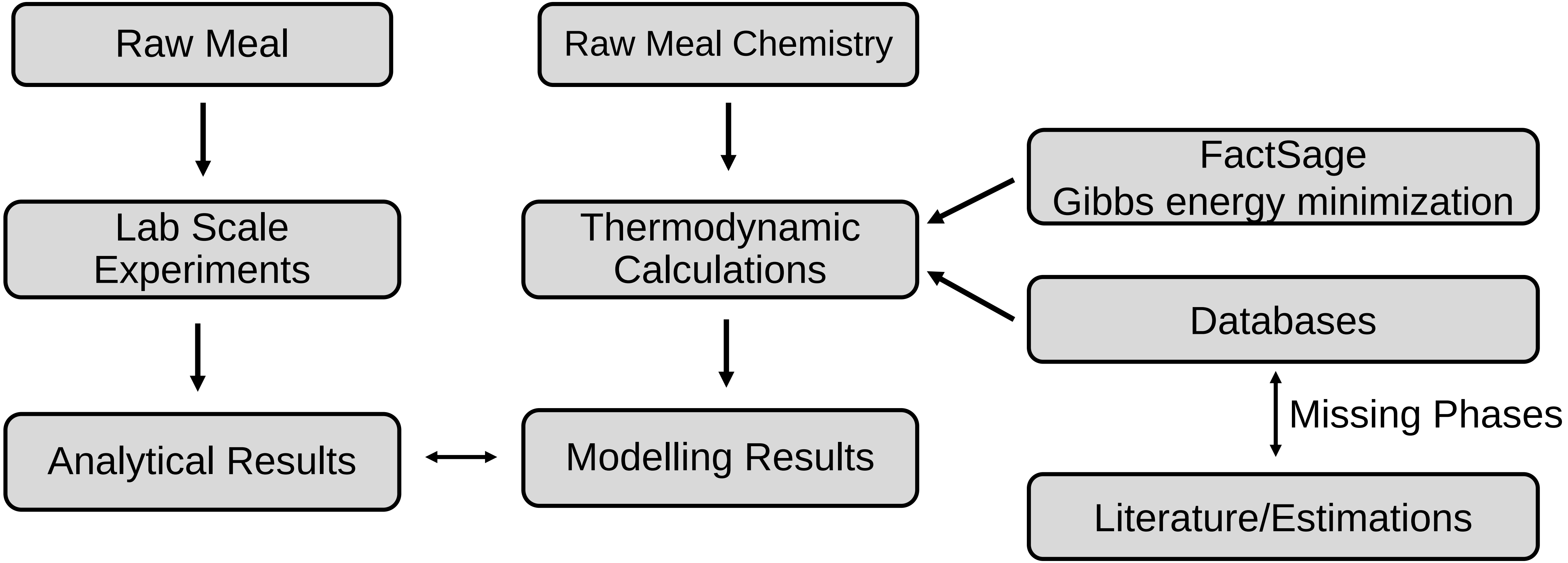


[2]: https://www.factsage.com/

KIT Belite Process



Modelling Approach



Results: Simulation

Raw Meal with $CaCl_2$ as mineralizer

Extensions (Implemented Phases):

- Chlorellestadite $Ca_{10}(SiO_4)_3(SO_4)_3(Cl)_2$
- Chlormayenite $Ca_{12}Al_{14}Cl_2O_{32}$
- Ternesite $Ca_5(SiO_4)_2SO_4$

- Yeelimite $Ca_4Al_6(SO_4)O_{12}$
- Mayenit $Ca_{12}Al_{14}O_{33}$

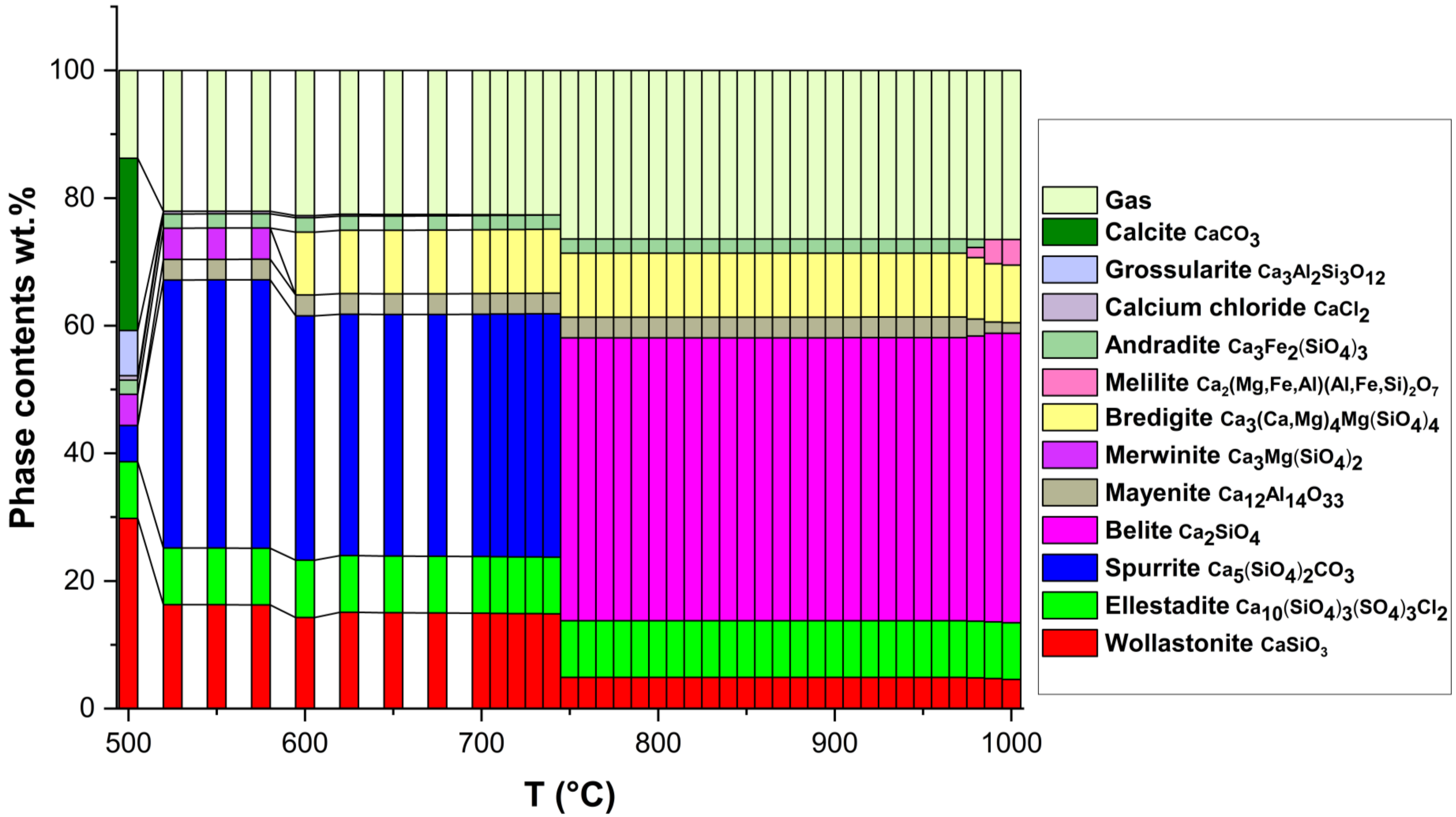
Input

Input	wt.%
$CaCO_3$	50.9
SiO_2	23.9
CaO	13.3
$CaSO_4$	3.5
$CaCl_2$	1.7
Al_2O_3	1.6
Fe_2O_3	0.7
MgO	0.6
H_2O	3.8
Total	100

Output
Equilibrium Result at 1000℃

Phases	wt. %
Belite Ca_2SiO_4	45.4
Bredigite $Ca_3(Ca,Mg)_4Mg(SiO_4)_4$	9.0
Chlorellestadite $Ca_{10}(SiO_4)_3(SO_4)_3Cl_2$	8.9
Wollastonite $CaSiO_3$	4.6
Melilite $Ca_2(Mg,Fe,Al)(Al,Fe,Si)_2O_7$	4.0
Chlormayenite $Ca_{12}Al_{14}Cl_2O_{32}$	1.7
Gas (CO_2 and H_2O)	26.4
Total	100

Results: Simulation



Results: Simulation Vs. Experiments

Phases	wt. % Simulations	wt. % Experiments
Belite Ca_2SiO_4	61.7	63.8
Bredigite $Ca_3(Ca,Mg)_4Mg(SiO_4)_4$	12.3	0
Chlorellestadite $Ca_{10}(SiO_4)_3(SO_4)_3Cl_2$	12.1	9.9
Wollastonite $CaSiO_3$	6.2	0.6
Melilite $Ca_2(Mg,Fe,Al)(Al,Fe,Si)_2O_7$	5.4	0
Chlormayenite $Ca_{12}Al_{14}Cl_2O_{32}$	2.3	3.9
Ternesite $Ca_5(SiO_4)_2SO_4$	0	0.1
Lime CaO	0	0.1
Quartz SiO_2	0	2.1
Amorphous content	0	15.0
Other phases	0	4.5
Total	100	100

-> Product is 60% of solid

-> Mg

-> SO_4, Cl

-> Mg, Fe, Al

-> Al, Cl

-> Grain size, kinetics, inhomogeneity (Lime, Quartz)

-> Real product contains amorphous content

Summary and Outlook

- Cementious Fines to Recycled Belite Cement :
  - Saves resources
  - Emits less CO_2
  - Avoids Landfill

- 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!

Pallavi Reddy Yarka Reddy M.Sc.

Karlsruhe Institute of Technology (KIT)
Institute for Technical Chemistry (ITC)

Hermann-von-Helmholtz-Platz 1
76344, Eggenstein Leopoldshafen, Germany

E-mail: pallavi.reddy@kit.edu