A Framework for Self-Sufficient Reactive Transport Modeling of Concrete with Low-Carbon Foot-Print

O. Burkan Isgor and W. Jason Weis

aci CONCRETE CONVENTION

Concrete with Low-carbon footprint

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(Vector Corrosion Technologies)

Life Cycle Performance

Increase the service life of the structures

Performance-based mixture proportioning

Service life modeling

Reduced carbon footprint

Reduce Clinker

Reduce Cement Content

Increase low-carbon footprint supplementary cementitious materials (e.g., SCMs) and powder extenders (e.g., ground limestone)

New concrete mixtures

PLC

+

SCM

+

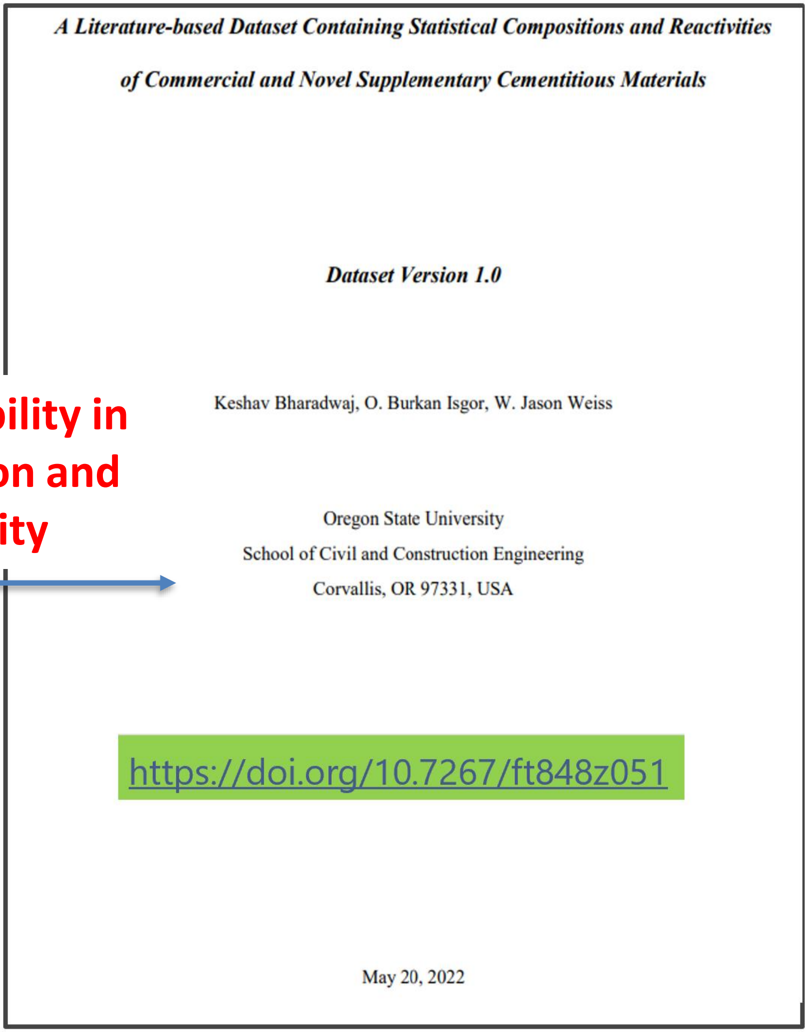
Water

Portland Limestone Cement
(OPC + Ground limestone (> 15% mass)

Novel or Underutilized SCMs

- Off-spec SCMs (off-spec fly ash, natural pozzolans, slags, etc.);
- Alternative ashes (bottom ash, reclaimed ash, agricultural ash, etc.);
- Other industrial and natural products (pumice, under-utilized clays, etc.);
- Powder extenders (limestone, biochar, etc.)

High variability in composition and reactivity



A Literature-based Dataset Containing Statistical Compositions and Reactivities of Commercial and Novel Supplementary Cementitious Materials

Dataset Version 1.0

Keshav Bharadwaj, O. Burkan Isgor, W. Jason Weiss

Oregon State University
School of Civil and Construction Engineering
Corvallis, OR 97331, USA

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Designed for specific performance such as strength, pH, transport properties, electrical properties, etc.

How will these new concretes perform under service conditions?

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- Chemical deterioration
  - – Corrosion of steel, AAR, sulfate attack, acid attack, carbonation, salt damage, etc.
- Physical deterioration
  - – Freeze/thaw damage, etc.

Water plays a major role in most deterioration mechanisms !!!

upload.wikimedia.org/wikipedia/commons/e/ea/Chungsong_bridge_04.jpg

commons.wikimedia.org/wiki/File:Figure_3_-_ASR_cracks_concrete_step_barrier_FHWA_2006.PNG

Service life modeling of concrete

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Moisture movement (e.g., wetting/drying, ponding, etc.)

+

Transport of ionic (e.g., chloride, sulfates, etc.), gaseous (e.g., CO_2,O_2) species

Diffusion + Electrical migration + Chemical activity + Advection

+

Reactions (e.g., chloride binding, sulfate attack, carbonation, etc.)

Service life modeling of concrete

Moisture movement (e.g., wetting/drying, ponding, etc.)

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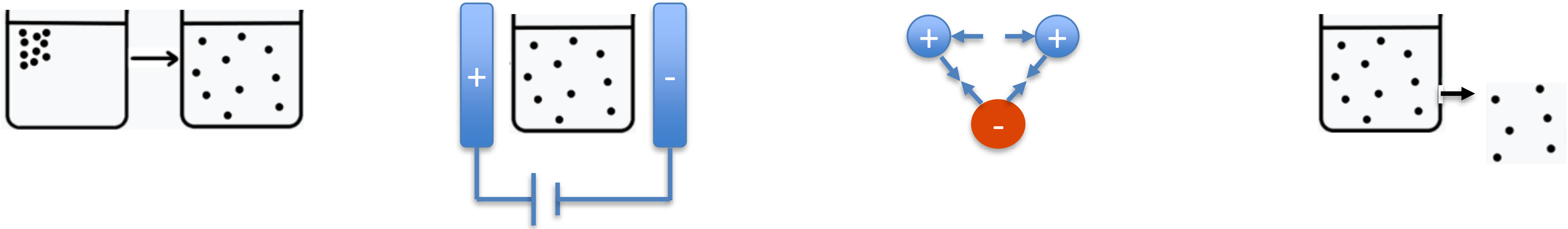
Service life modeling of concrete

Ionic flux = Diffusion + Electrical migration + Chemical activity + Advection



https://commons.wikimedia.org/wiki/File:Osmosis_and_Diffusion_CLMiller_CC_BY_SA.png

Service life modeling of concrete

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$$\underbrace{-\,D_i\,\nabla c_{aq,i}}_{}\;-\;\underbrace{D_i\,c_{aq,i}\,\frac{Fz}{RT}\,\nabla\emptyset}_{}\;-\;\underbrace{D_i\,c_{aq,i}\,\nabla\ln\gamma_i}_{}\;+\;\underbrace{c_{aq,i}\,v_L+c_{G,i}\,v_G}_{}$$

Ionic flux = Diffusion + Electrical migration + Chemical activity + Advection

Reactive-transport modeling

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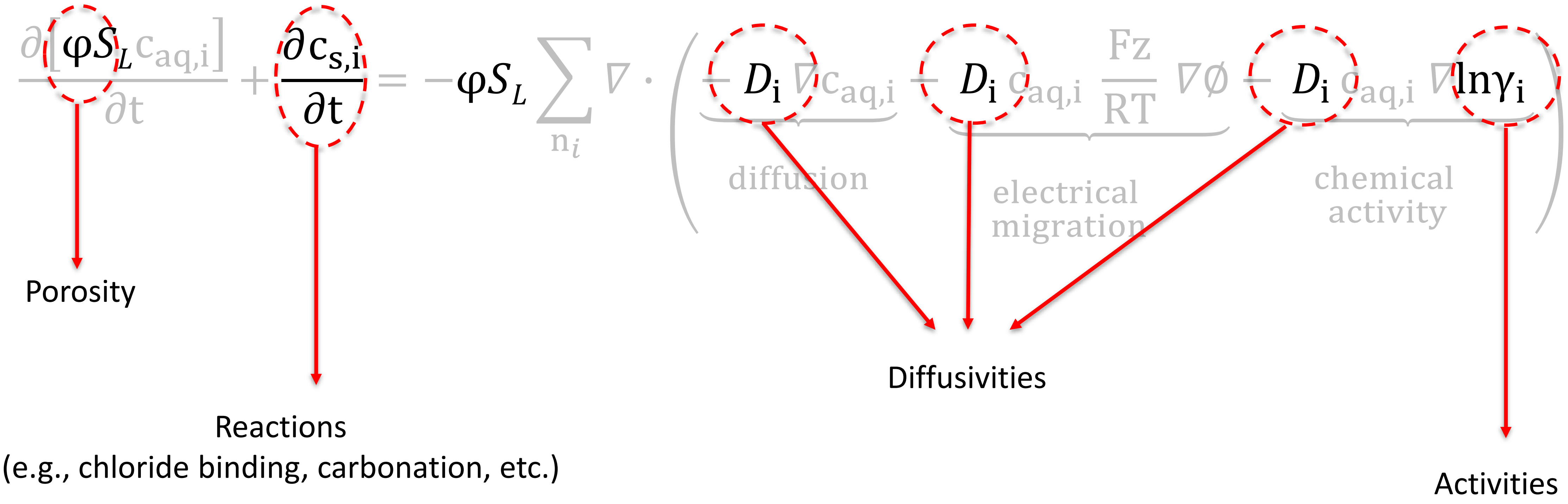
$$\frac{\partial\left[\varphi S_L c_{aq,i}\right]}{\partial t}+\frac{\partial c_{s,i}}{\partial t}=-\varphi S_L\sum_{n_i}\nabla\cdot\left(\underbrace{-D_i\nabla c_{aq,i}}_{\text{diffusion}}-\underbrace{D_i c_{aq,i}\frac{Fz}{RT}\nabla\emptyset}_{\text{electrical migration}}-\underbrace{D_i c_{aq,i}\nabla\ln\gamma_i}_{\text{chemical activity}}\right)$$

Reactive-transport modeling



$$\frac{\partial[\varphi S_L c_{aq,i}]}{\partial t} + \frac{\partial c_{s,i}}{\partial t} = -\varphi S_L \sum_{n_i} \nabla \cdot \left(\underbrace{- D_i \nabla c_{aq,i}}_{\text{diffusion}} \underbrace{- D_i c_{aq,i} \frac{Fz}{RT} \nabla \emptyset}_{\text{electrical migration}} \underbrace{- D_i c_{aq,i} \nabla \ln\gamma_i}_{\text{chemical activity}} \right)$$

Porosity

Reactions
(e.g., chloride binding, carbonation, etc.)

Diffusivities

Activities

Reactive-transport modeling

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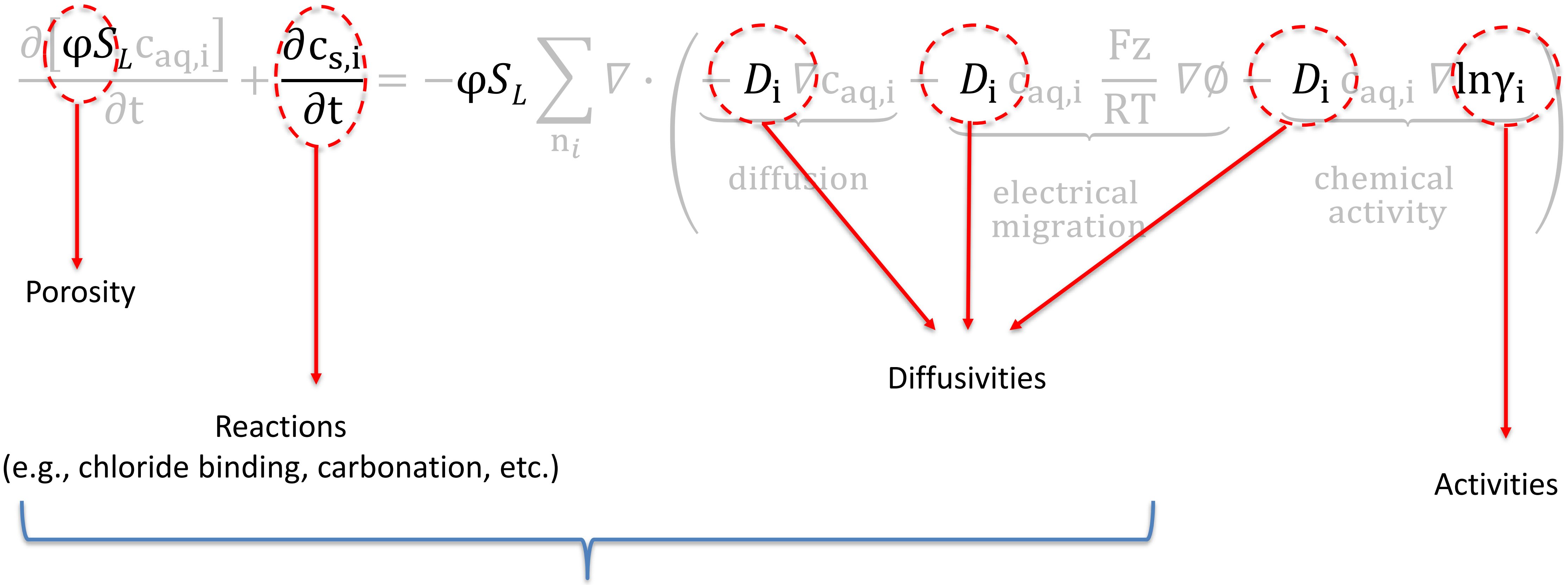

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Porosity

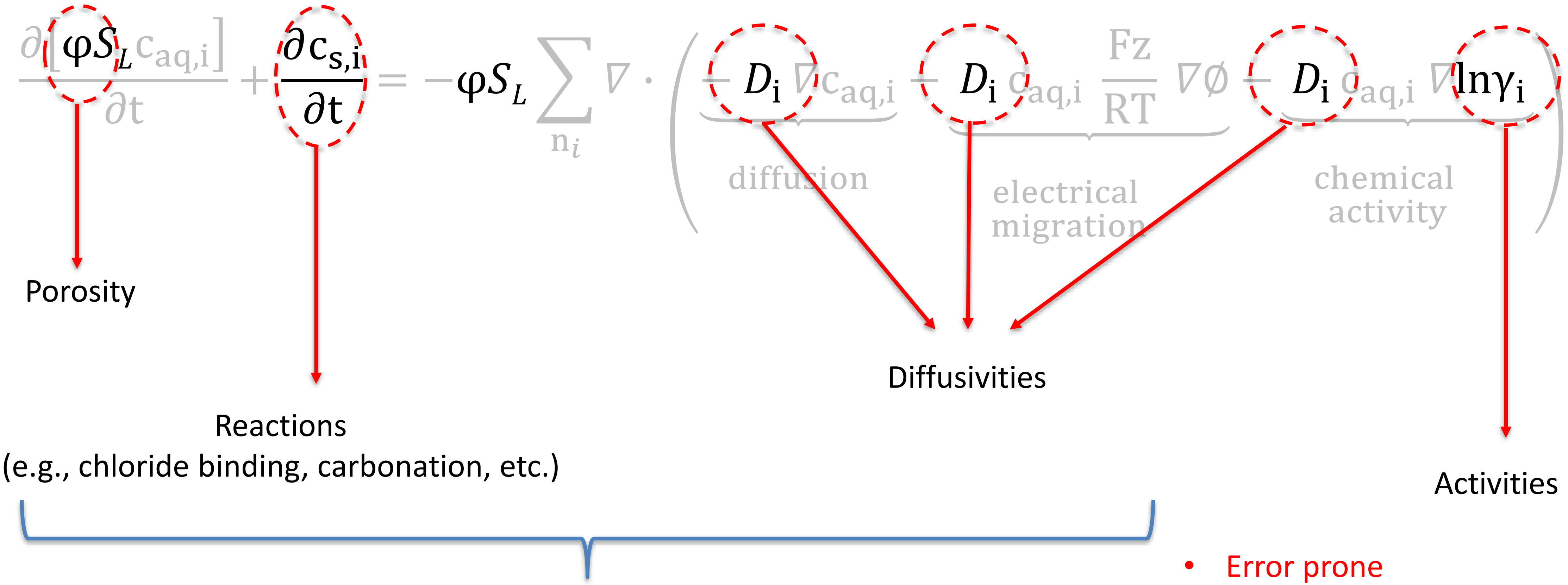
Reactions
(e.g., chloride binding, carbonation, etc.)

Diffusivities

Activities

Experimentally obtained

Reactive-transport modeling



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Porosity

Reactions
(e.g., chloride binding, carbonation, etc.)

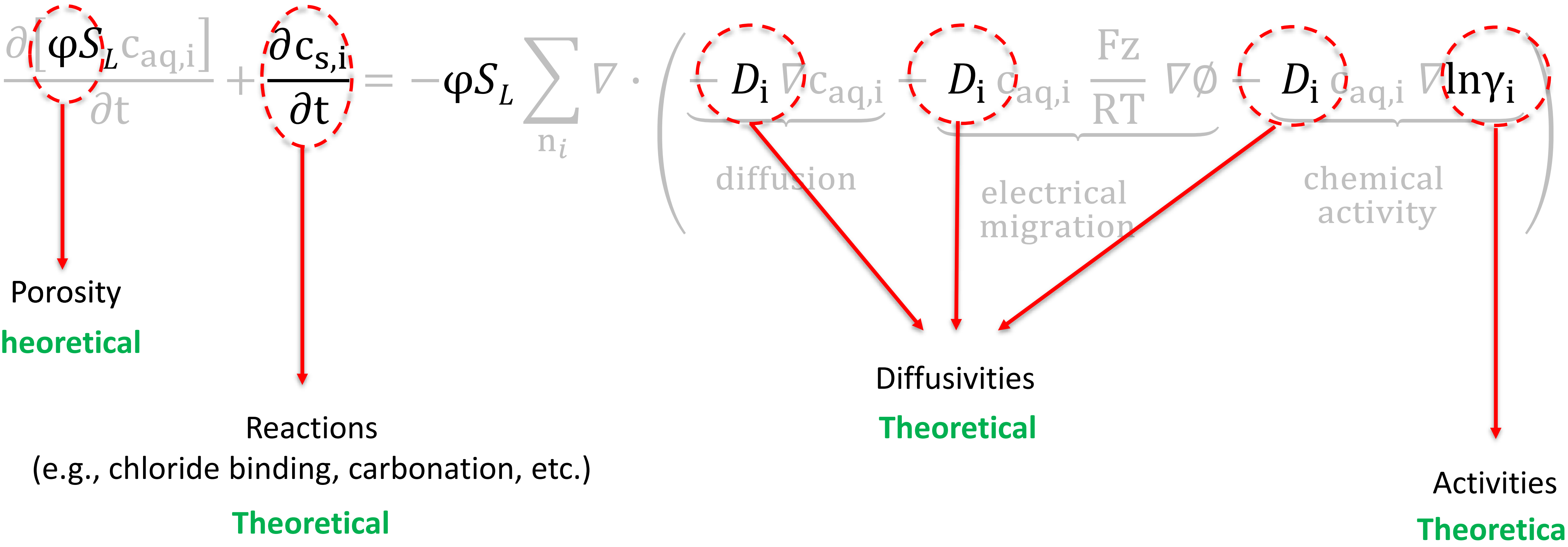
Diffusivities

Activities

Experimentally obtained →

- Error prone
- Inaccurate / unrepresentative
- Time consuming
- Expensive

“Self-sufficient” model



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Porosity

Theoretical

Reactions
(e.g., chloride binding, carbonation, etc.)

Theoretical

Diffusivities

Theoretical

Activities

Theoretical

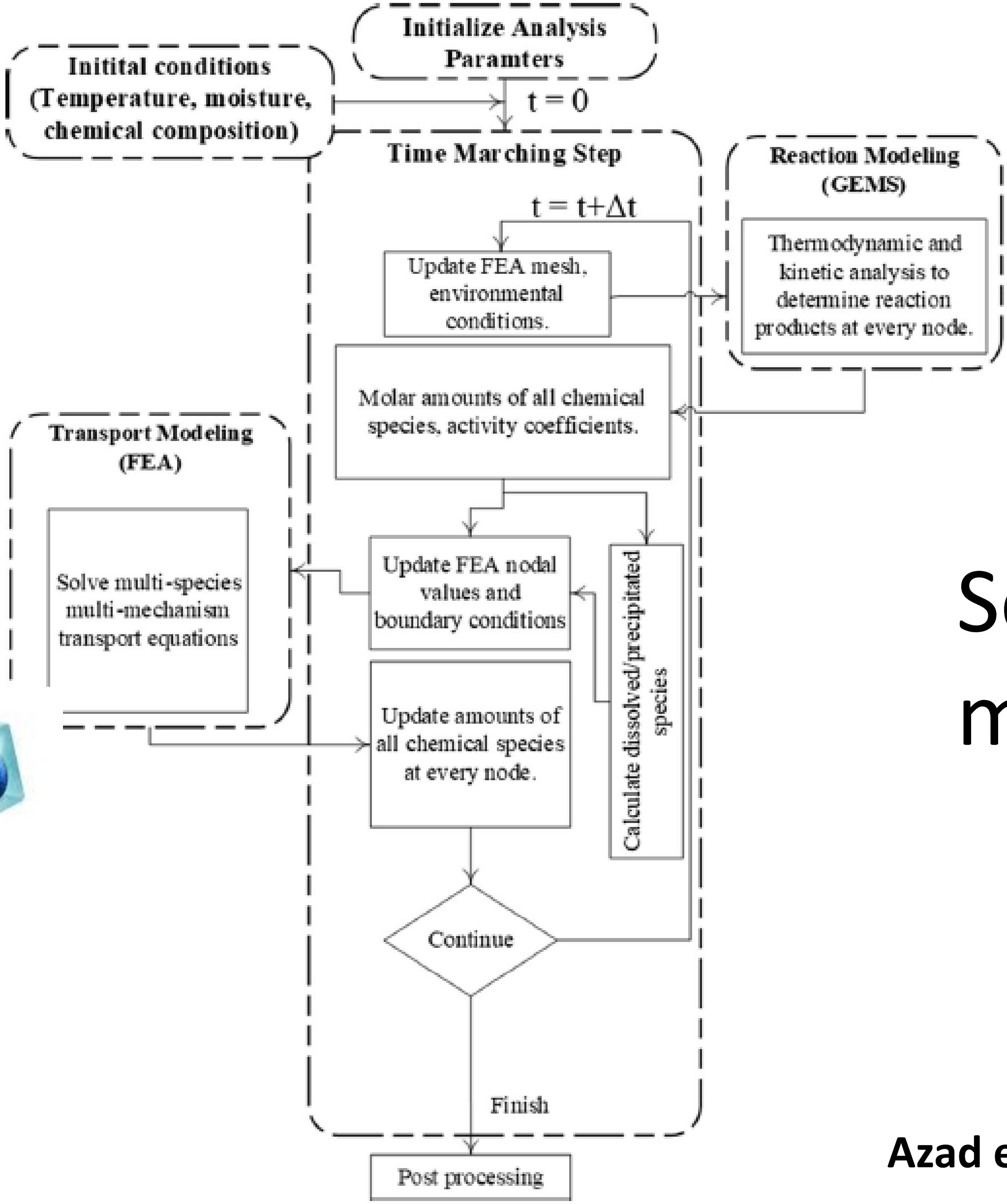
Using thermodynamical calculations…

Time marching

MOOSE

Multiphysics Object-Oriented Simulation Environment

COMSOL MULTIPHYSICS



GEMS3K

Self-sufficient modeling algorithm

Azad et al., Computer & Geosciences, 2016

How do we move from “empirical” to “self-sufficient”?

Can we predict properties we need?

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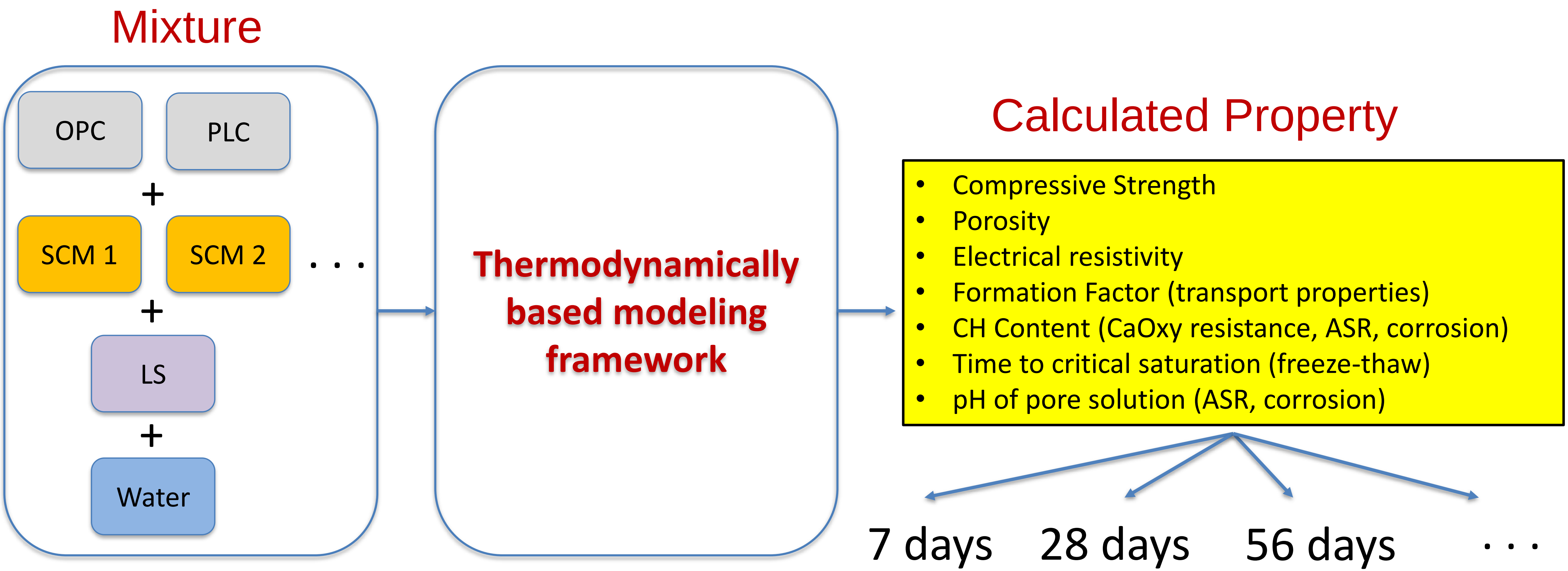


Mixture

OPC
PLC
+
SCM 1
SCM 2
. . .
+
LS
+
Water

Thermodynamically based modeling framework

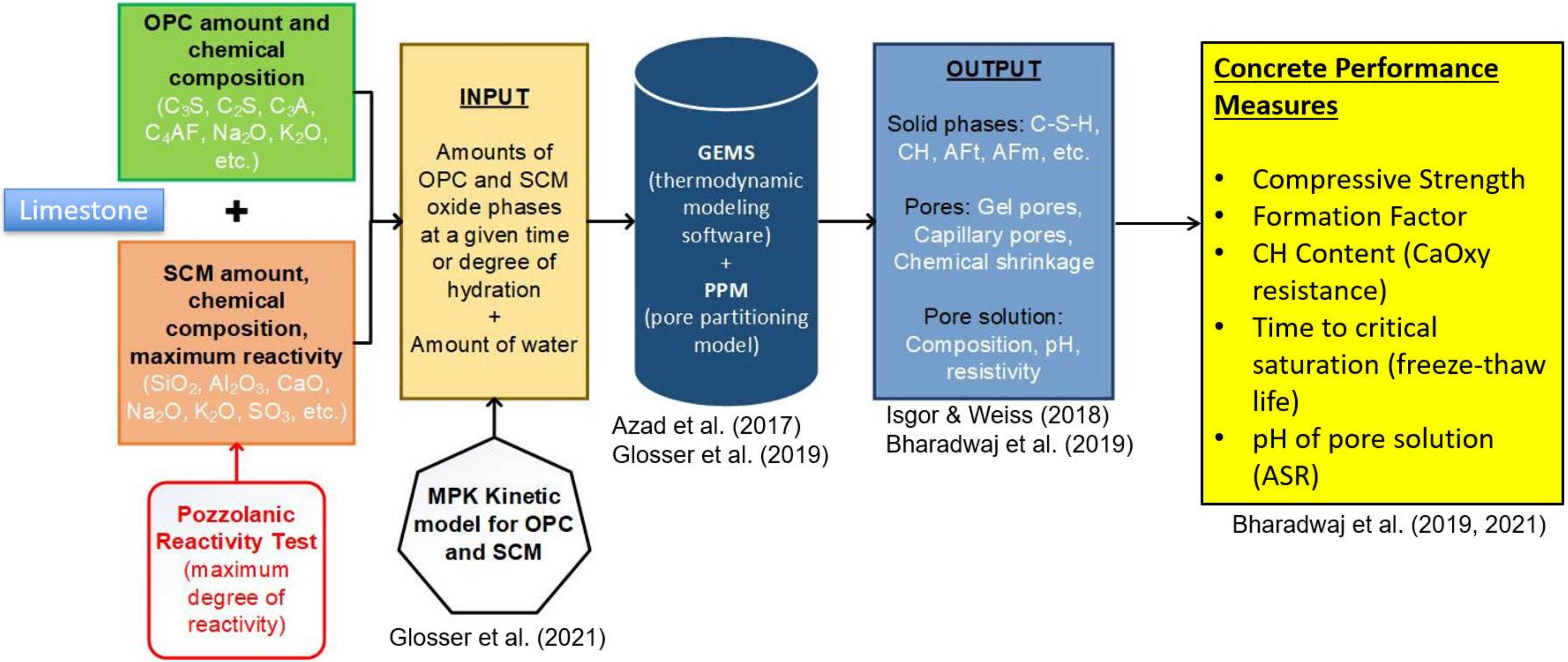
Calculated Property

- Compressive Strength
- Porosity
- Electrical resistivity
- Formation Factor (transport properties)
- CH Content (CaOxy resistance, ASR, corrosion)
- Time to critical saturation (freeze-thaw)
- pH of pore solution (ASR, corrosion)

7 days
28 days
56 days
. . .

Azad et al (2017); Isgor and Weiss (2018); Bharadwaj et al. (2019, 2021); Glosser et al. (2019, 2021)

Modeling framework



OPC amount and chemical composition (C_3S, C_2S, C_3A, C_4AF, Na_2O, K_2O, etc.)

Limestone

+

SCM amount, chemical composition, maximum reactivity (SiO_2, Al_2O_3, CaO, Na_2O, K_2O, SO_3, etc.)

Pozzolanic Reactivity Test (maximum degree of reactivity)

INPUT

Amounts of OPC and SCM oxide phases at a given time or degree of hydration + Amount of water

MPK Kinetic model for OPC and SCM

Glosser et al. (2021)

GEMS (thermodynamic modeling software) + **PPM** (pore partitioning model)

Azad et al. (2017)
Glosser et al. (2019)

OUTPUT

Solid phases: C-S-H, CH, AFt, AFm, etc.

Pores: Gel pores, Capillary pores, Chemical shrinkage

Pore solution: Composition, pH, resistivity

Isgor & Weiss (2018)
Bharadwaj et al. (2019)

Concrete Performance Measures

- Compressive Strength
- Formation Factor
- CH Content (CaOxy resistance)
- Time to critical saturation (freeze-thaw life)
- pH of pore solution (ASR)

Bharadwaj et al. (2019, 2021)

Modeling framework – SCM reactivity

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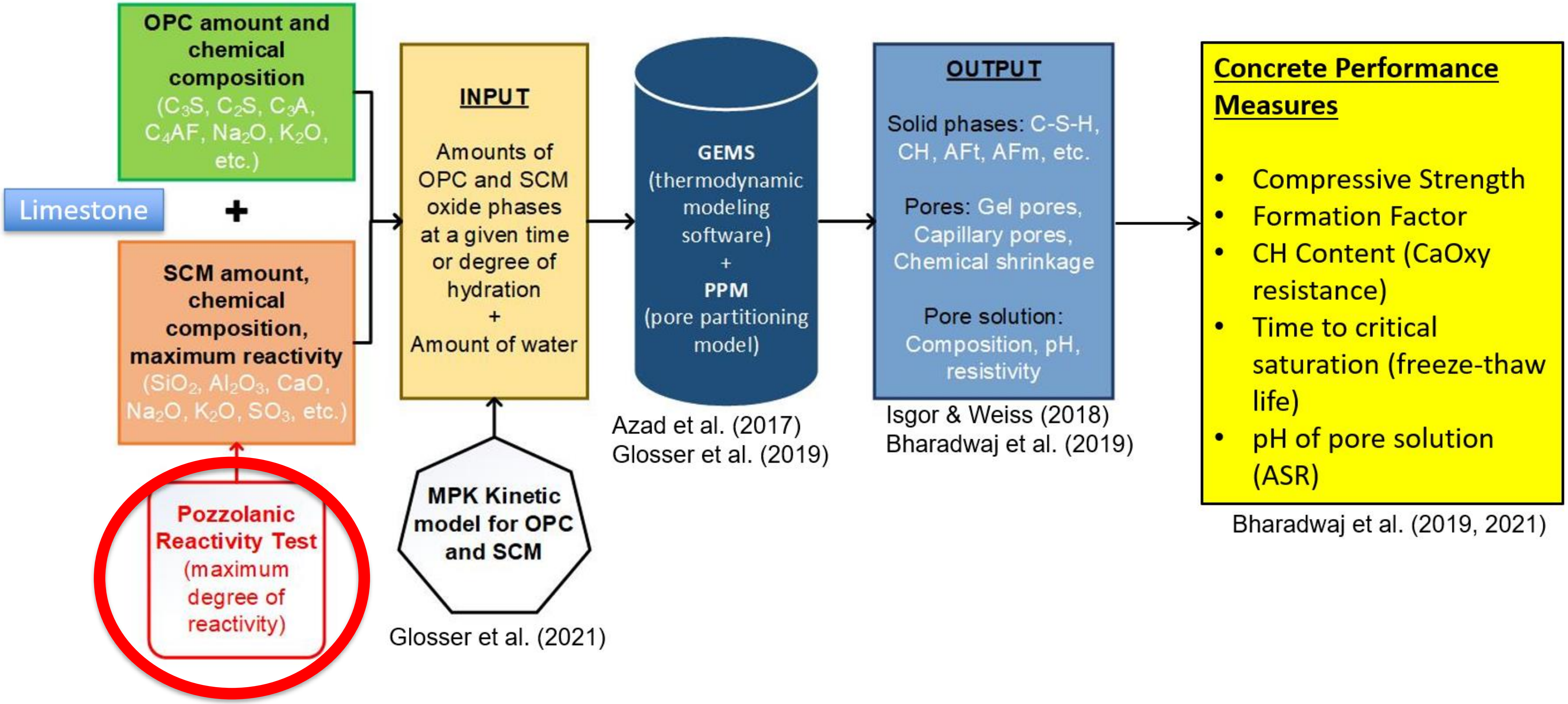

OPC amount and chemical composition
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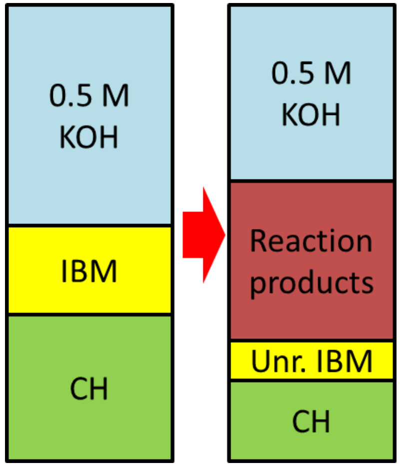
Bharadwaj et al. (2019, 2021)

Pozzolanic reactivity test (PRT)

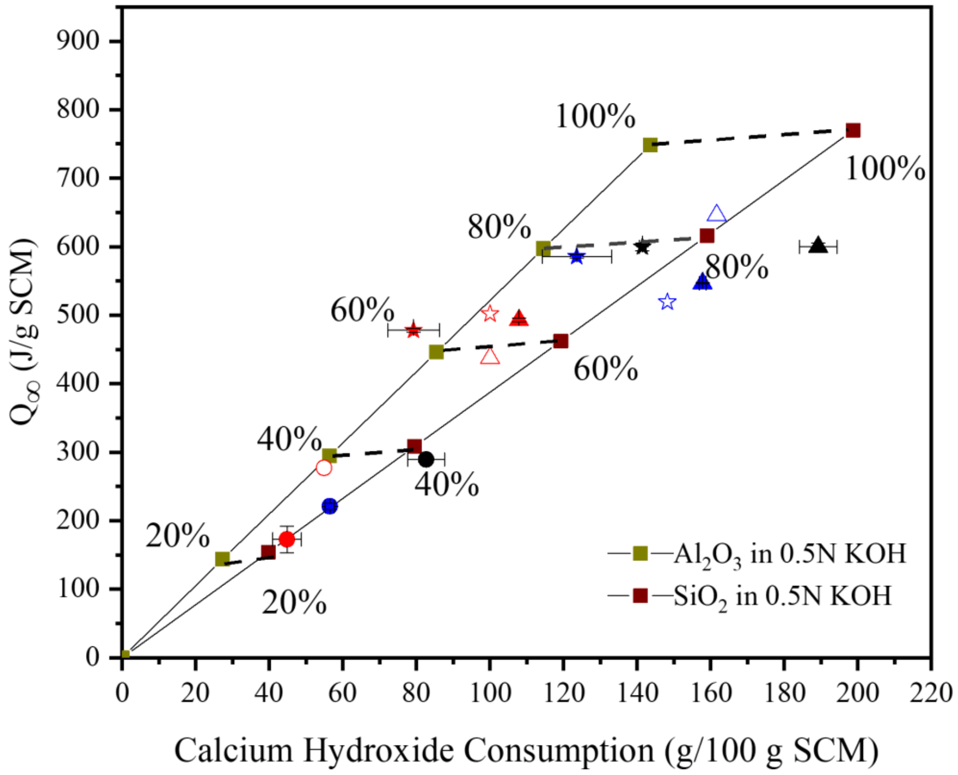
Pozzolanic reactivity test ("PRT") can determine maximum degree of reactivity (DoR*)



$$\mathrm{SCM} + \mathrm{CH} + \mathrm{H_2O} \xrightarrow{50^{o}C} \text{reaction products} + Q$$

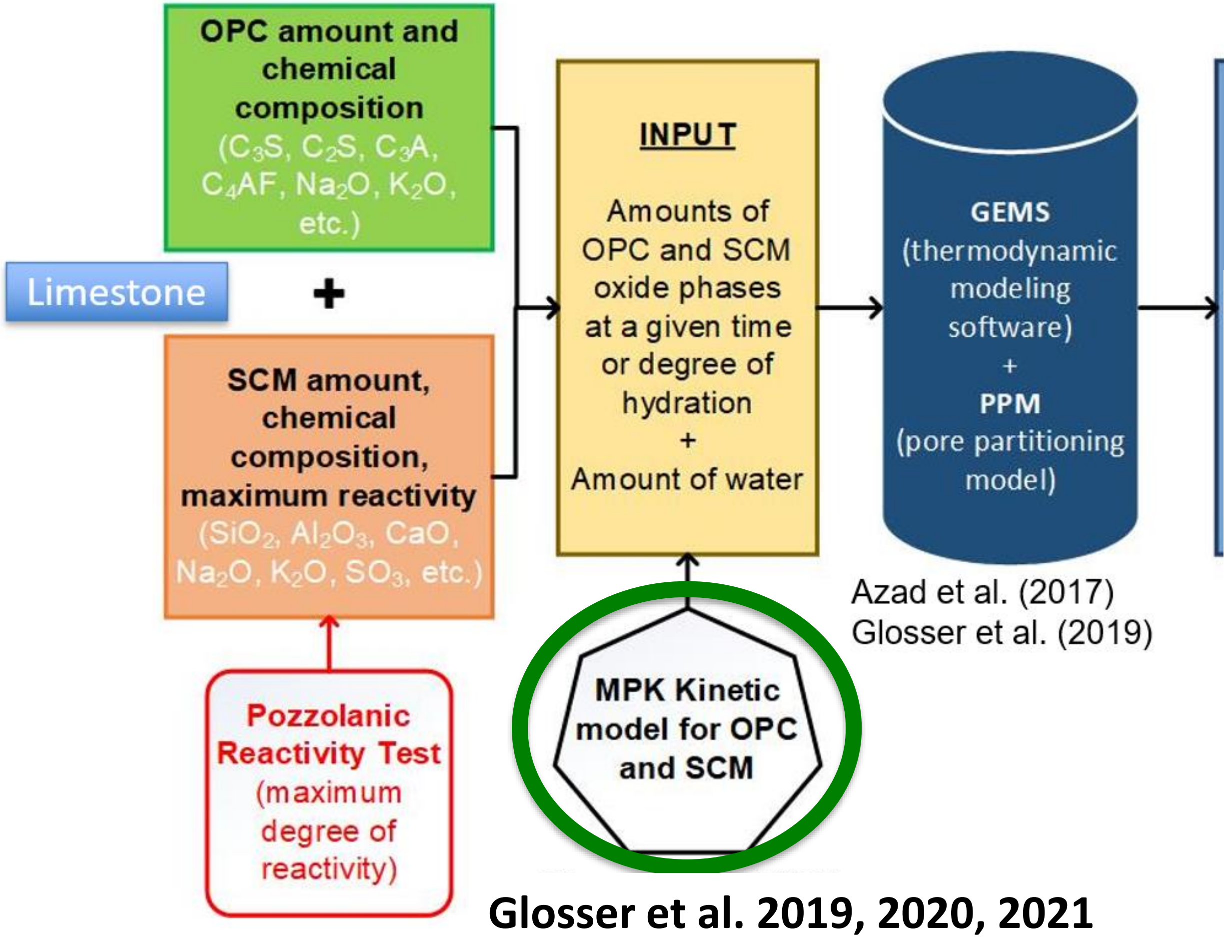
Measure CH consumption

Measure heat release



$$DOR^* = \frac{Q_\infty - c_1 \cdot CH_{consumed}}{c_2}$$

Modeling framework - kinetics



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OUTPUT

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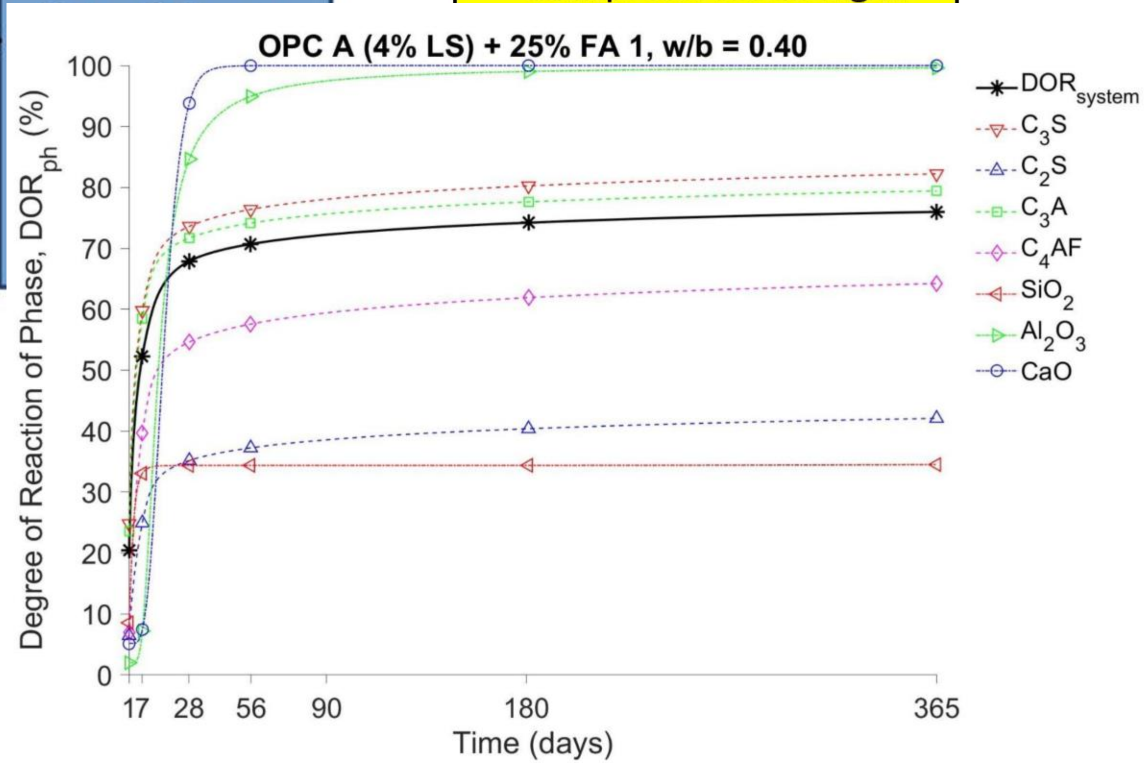
Concrete Performance Measures

- Compressive Strength



Glosser et al. 2019, 2020, 2021

Modeling framework - thermodynamics

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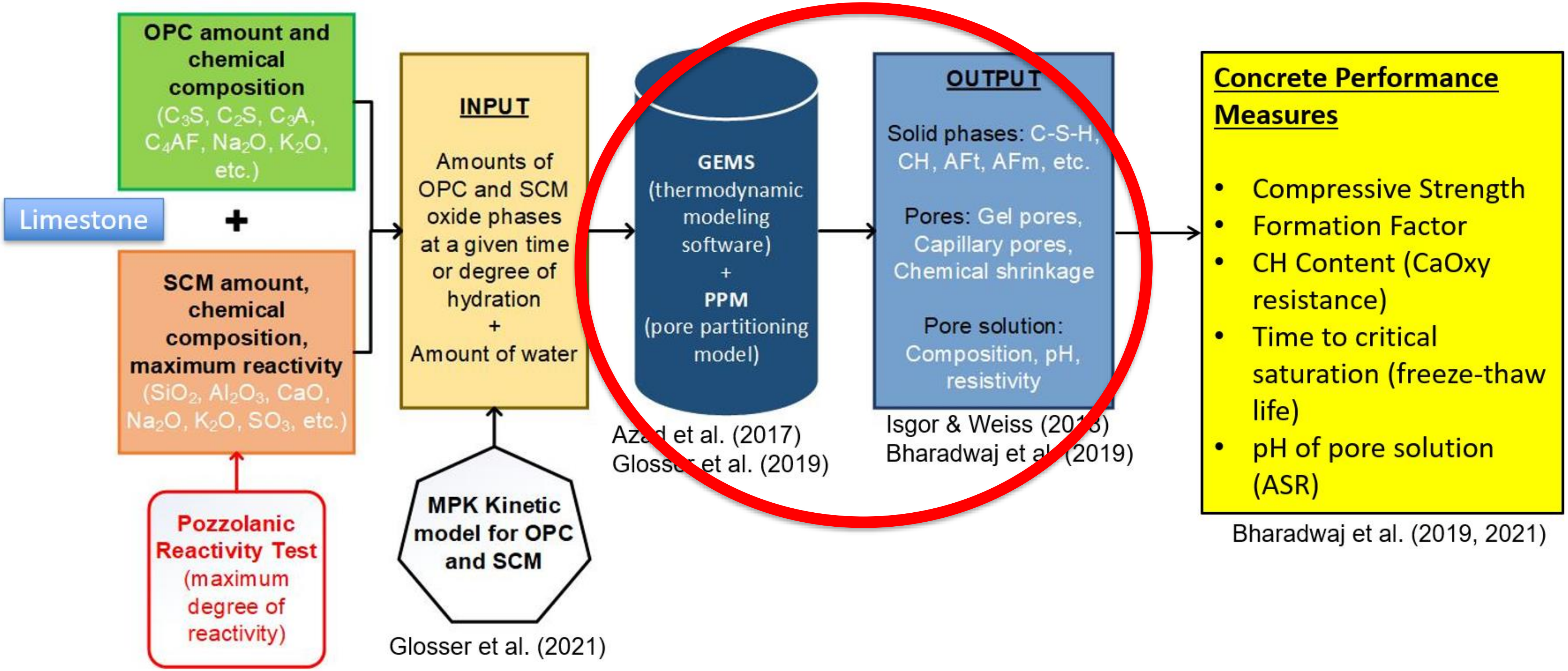

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- Formation Factor
- CH Content (CaOxy resistance)
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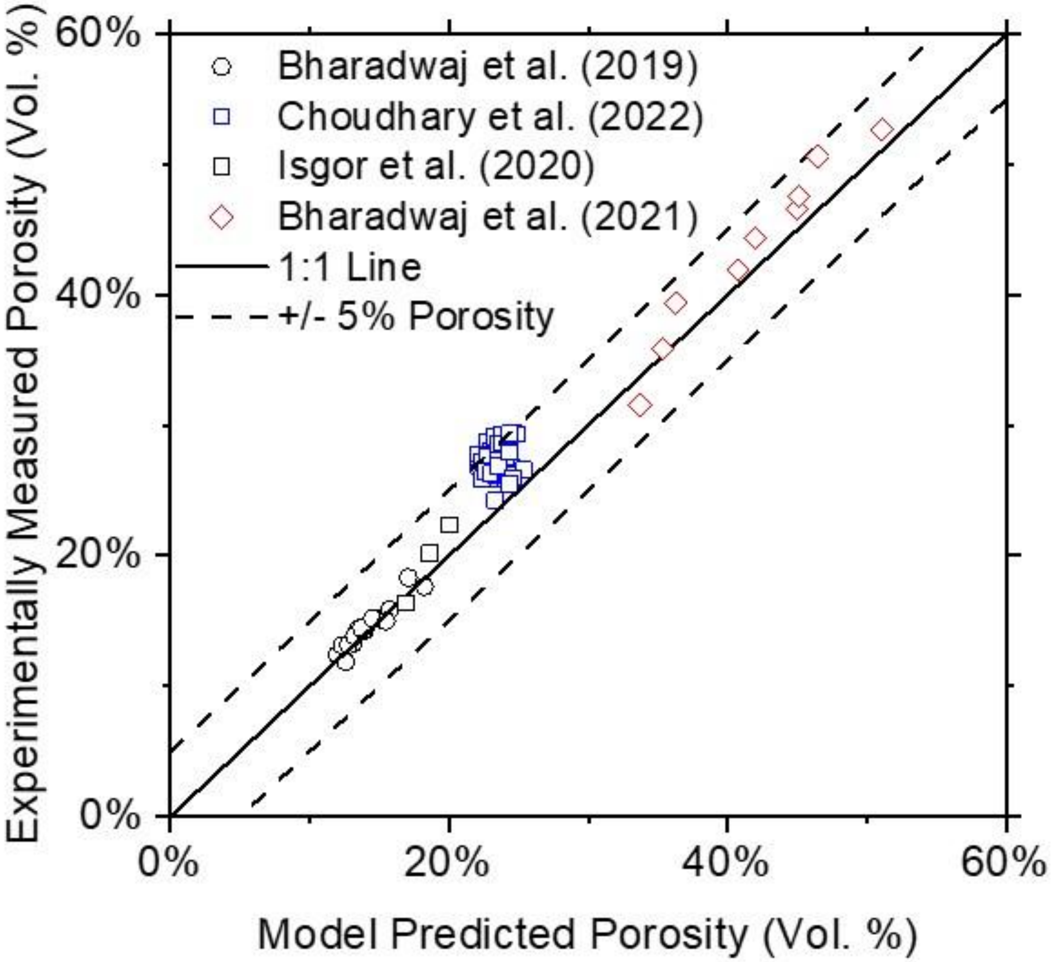
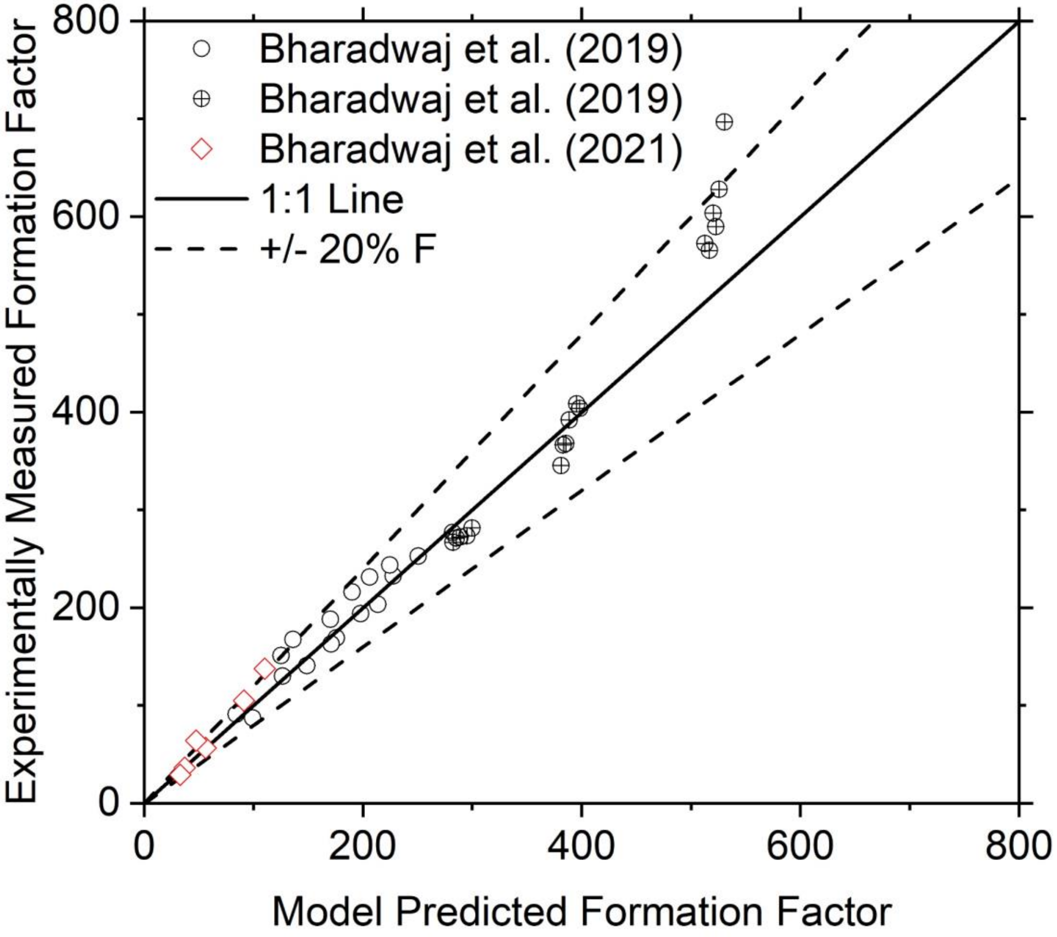
Bharadwaj et al. (2019, 2021)

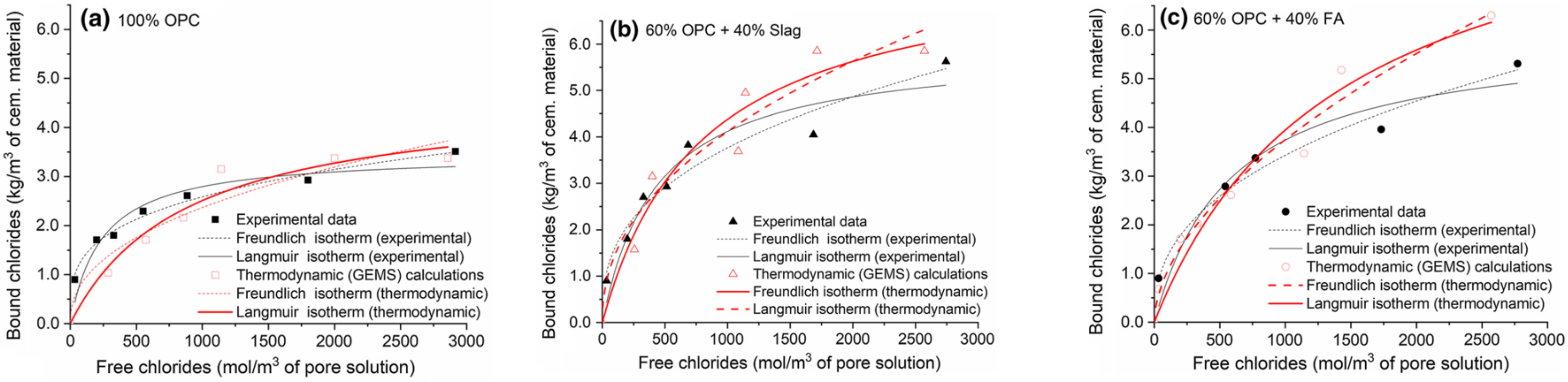
Does this framework work?





Does this framework work?

Thermodynamically calculated chloride binding isotherms:



(Isgor and Weiss, Materials and Structures, 2019)

(Azad et al., Computer & Geosciences, 2016)

So, we can model any mixture...

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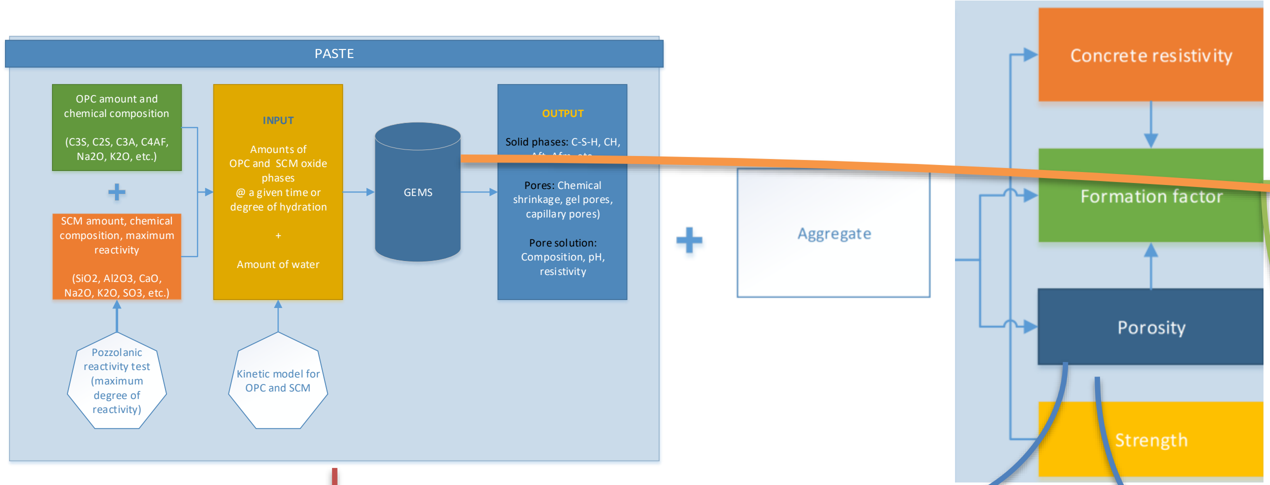
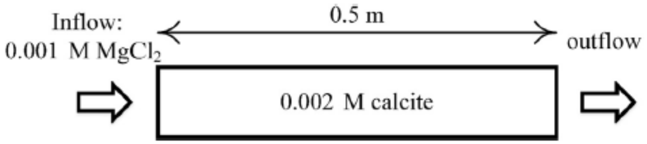
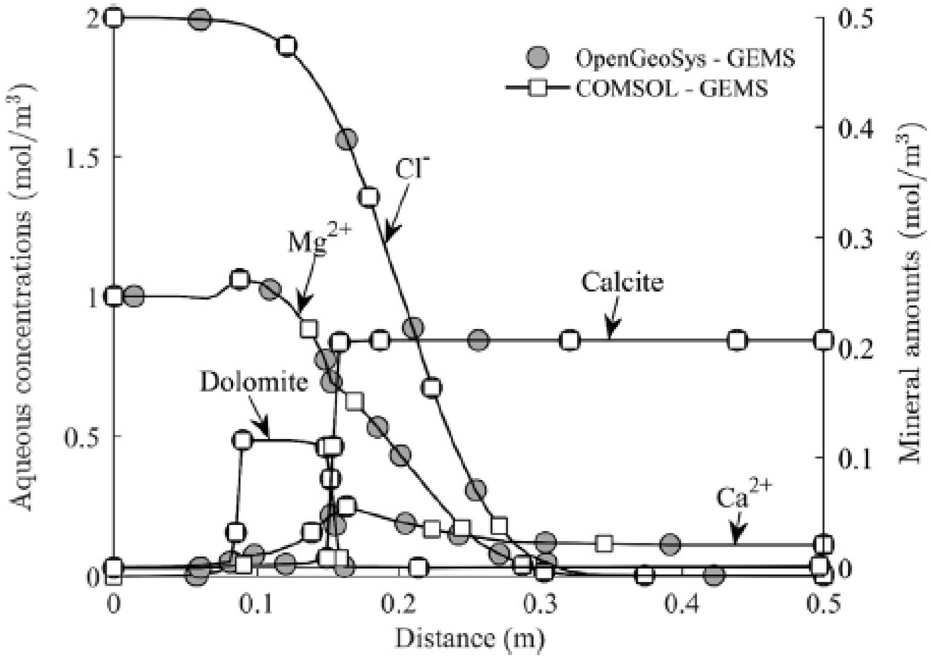


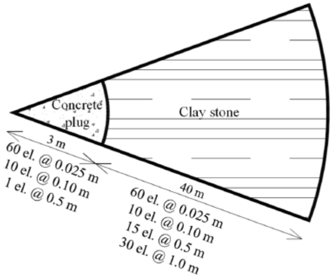
$$\frac{\partial\left[\varphi S_L c_{aq,i}\right]}{\partial t}+\frac{\partial c_{s,i}}{\partial t}=-\varphi S_L\sum_{n_i}\nabla\cdot\left(\underbrace{-D_i\,\nabla c_{aq,i}}_{\text{diffusion}}-\underbrace{D_i\,c_{aq,i}\,\frac{Fz}{RT}\,\nabla\emptyset}_{\text{electrical migration}}-\underbrace{D_i\,c_{aq,i}\,\nabla\ln\gamma_i}_{\text{chemical activity}}\right)$$

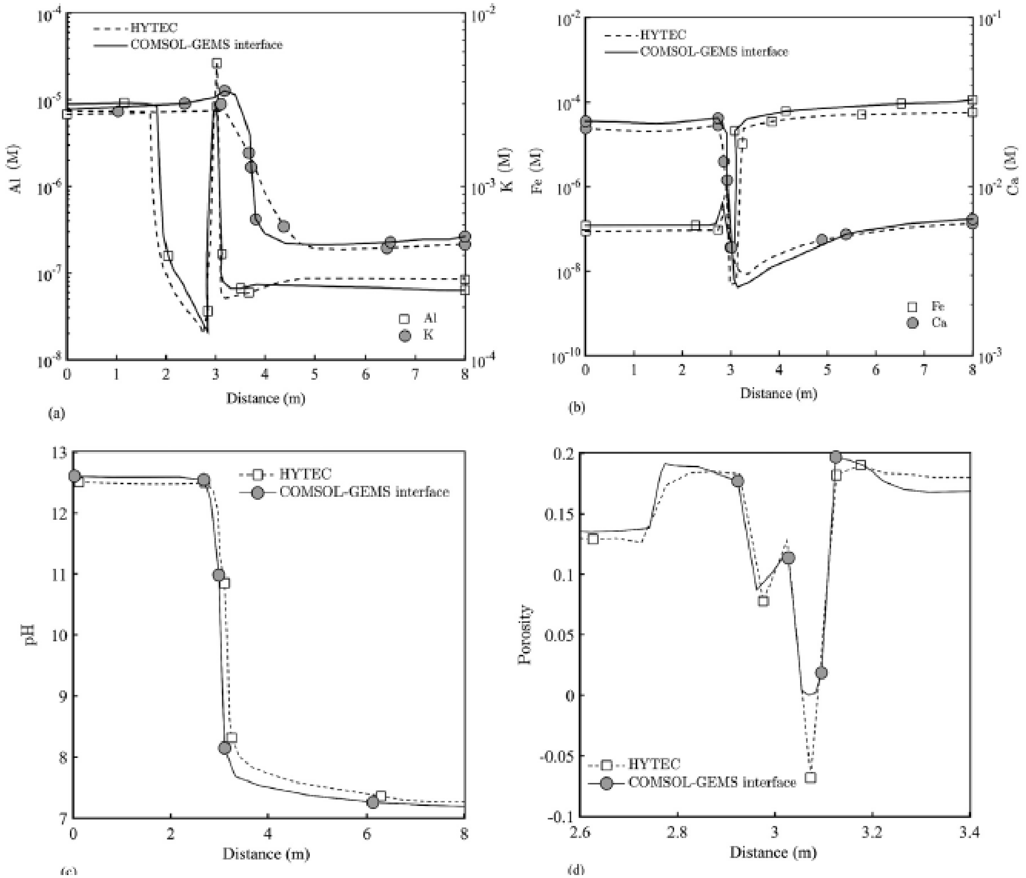
Validation / benchmarking





Azad et al., Computer & Geosciences, 2016





Conclusion

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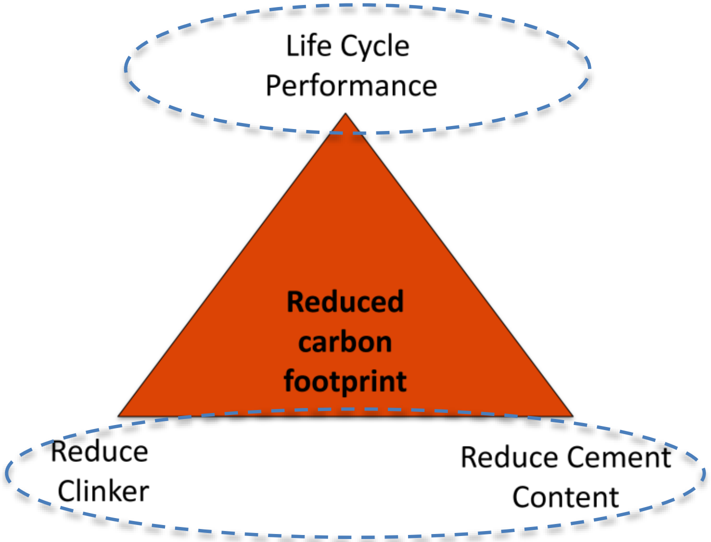

Increase the use of low-carbon footprint cementitious materials and powder extenders

- Modeling reactive transport processes in concrete for predicting service life is possible irrespective of
  - Chemical composition of the materials
  - Reactivity of the materials
- We can do this using a coupled approach in which we model reactive processes using thermodynamic / kinetic algorithms and transport processes using finite element analysis.
- This approach eliminates the need to experimentally characterize every concrete mixture for modeling, hence it is dubbed “self-sufficient”.
- This approach allows the modeling of concrete produced with underutilized, novel, low-carbon footprint binders and powder extenders.

Acknowledgements

Oregon State University
College of Engineering

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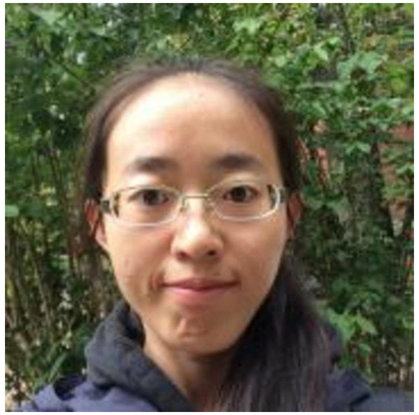
Post-doctoral researcher
(currently, Senior Engineer at WSP)



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Dr. Keshav Bharadwaj
Ph.D. student, Post-doctoral researcher
(currently, Assistant Professor at IIT, Delhi)

Thank you

Oregon State University
College of Engineering

O. Burkan Isgor
Burkan.Isgor@oregonstate.edu