FROM EXPERIMENTAL SILICA FUME DISSOLUTION TO MICROSTRUCTURE MODELING AND HYDRATION KINETICS SIMULATION





[1a]Mine G. Ucak-Astarlioglu, [1b]Serdar Astarlioglu, [1a]Jedadiah Burroughs

[2]Yoonjung Han, [2]Jonathan Lapeyre, [2]Umme Zakira, and [2]Jeffrey W. Bullard

[1]US Army Engineer Research and Development Center, Geotechnical and Structures Laboratory, 1[a]Concrete and Materials Branch, [1b]Structural Mechanics Branch

[2]Zachry Department of Civil and Environmental Engineering Texas A&M University

American Concrete Institute, Fall 2023, Boston, USA

ERDC Locations

SEVEN LABORATORIES MAKING AN IMPACT ON THE NATION AND WARFIGHTERS

ERDC Headquarters
Vicksburg, Mississippi

Coastal and Hydraulics Laboratory (CHL)

Environmental Laboratory (EL)

Geotechnical and Structures Laboratory (GSL)

Information Technology Laboratory (ITL)

ERDC Laboratories

Cold Regions Research and Engineering Laboratory (CRREL)
Hanover, New Hampshire

Geospatial Research Laboratory (GRL)
Alexandria, Virginia

Construction Engineering Research Laboratory (CERL)
Champaign, Illinois

Field Offices

Permafrost Tunnel Research Facility
Fox, Alaska

Alaska Research Office
Fairbanks, Alaska

Lewisville Aquatic Ecosystem Research Facility
Lewisville, Texas

Contingency Base Integration Technology Evaluation Center (CBITEC)
Fort Leonard Wood, Missouri

Field Research Facility
Duck, North Carolina

Corbin Field Station
Woodford, Virginia

Extreme Exposure Station
Treat Island, Maine

ERDC International Research Office
London, England

US Army Corps of Engineers • Engineer Research and Development Center

Drive:

1) Understand the cement-silica fume (SF) mixtures particle packing behavior and hydration kinetics through SF dissolution kinetics in cementitious mixtures and their comparison to simulation models.

2) Accurate *simulation* of the hydration reaction and the microstructure development of cement-SF blends in UHPC.

3) Integrate SF dissolution kinetics in cementitious mixtures into the Virtual Cement and Concrete Testing Laboratory (VCCTL) model and comparison to the Thermodynamically Assisted Microstructure Evolution Simulator (THAMES).

Silica Fume Sample Characteristics Investigated*

Designation	Type	SiO_2 (wt%)	LOI (wt%)	BET (m^2/g)
SF2	Undensified	95.9	0.9	29.3
SF4	Undensified	97.8	0.9	29.4
SF5	Densified	70.0	5.1	25.7
SF6	Densified	90.4	2.5	24.0
SF7	Densified	94.3	2.0	22.8

*Burroughs, J. F. (2019). *Influence of Chemical and Physical Properties of Poorly-Ordered Silica on Reactivity and Rheology of Cementitious Materials.* PhD Thesis, Purdue University.

Why VCCTL?

- VCCTL predicts the cement hydration and its respective three-dimensional microstructure.

Why THAMES?

- THAMES interconnects thermodynamics, microstructure, and kinetics investigation under one model.

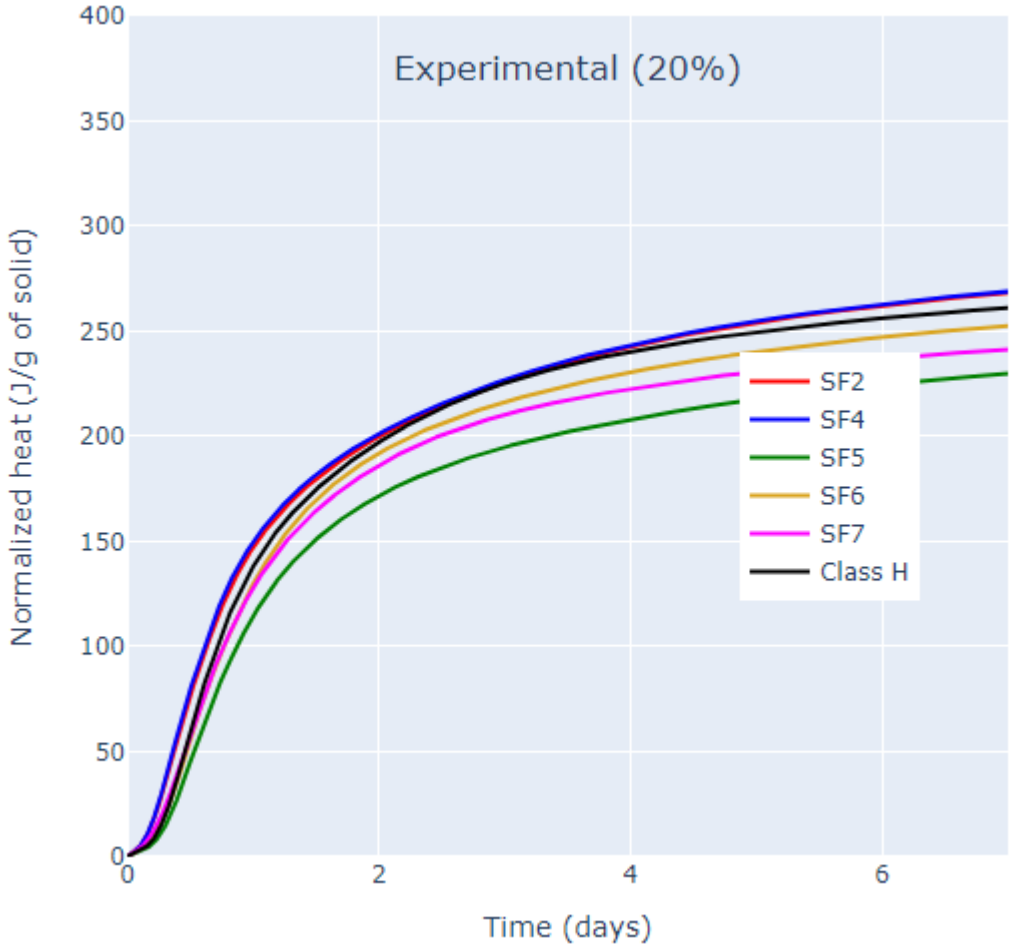
- THAMES has advanced simulation capability not only for only portland cement but also for other material structures.

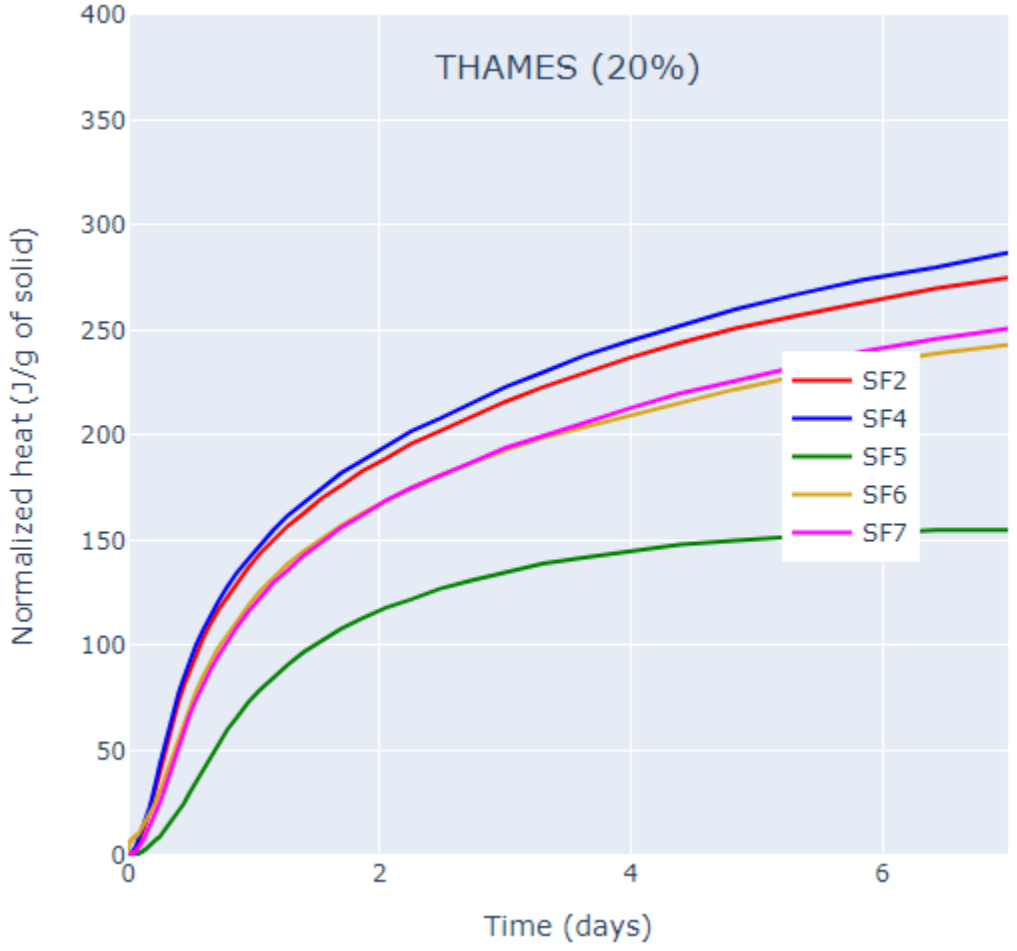
THAMES Modifications:

Wider range of materials and simulation conditions
(by Jeffrey Bullard Group at TAMU):

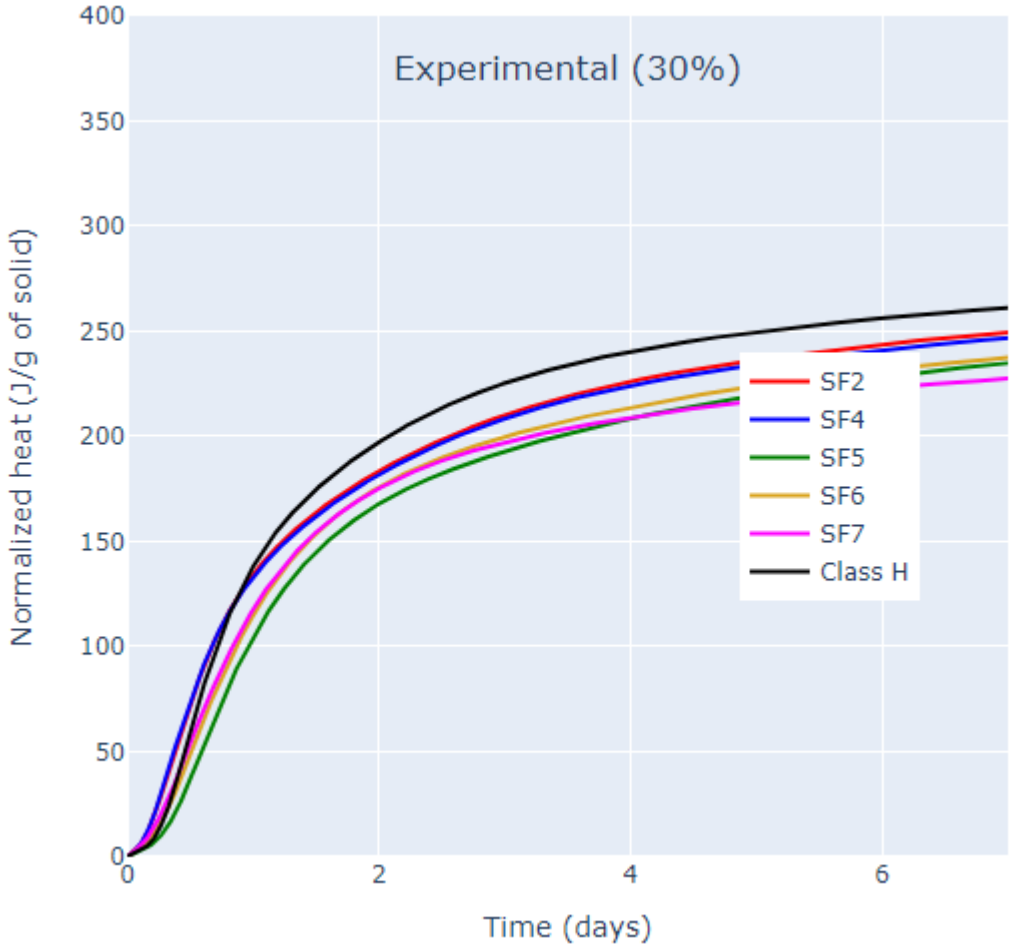
- Simulate saturated or sealed moisture conditions.
- Produce the empty porosity from the largest capillary pores, under sealed conditions, keeping 27% of C-S-H gel porosity saturated. The remaining is consistent with the chemical shrinkage predicted by the thermodynamic calculations.
- Prescribe the water-solid ratio of the material without requiring new thermodynamic input files.

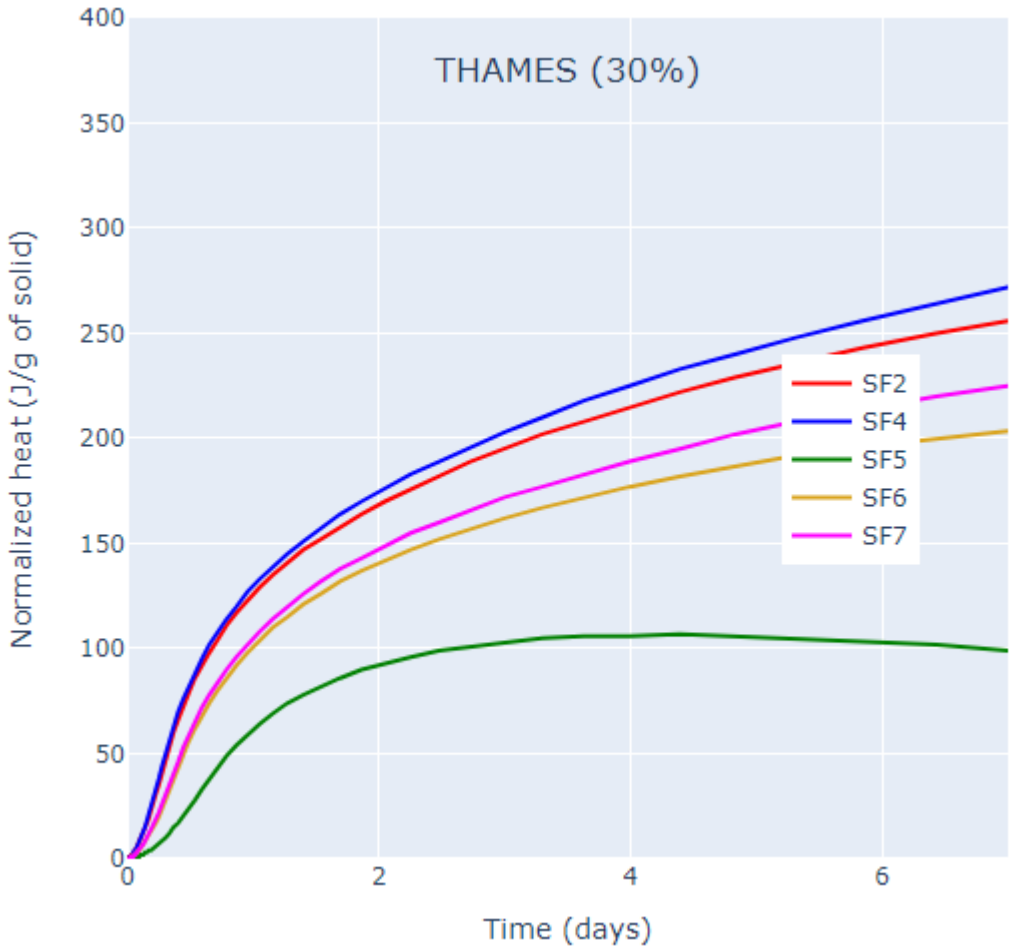
Experimental and THAMES with 20% SF



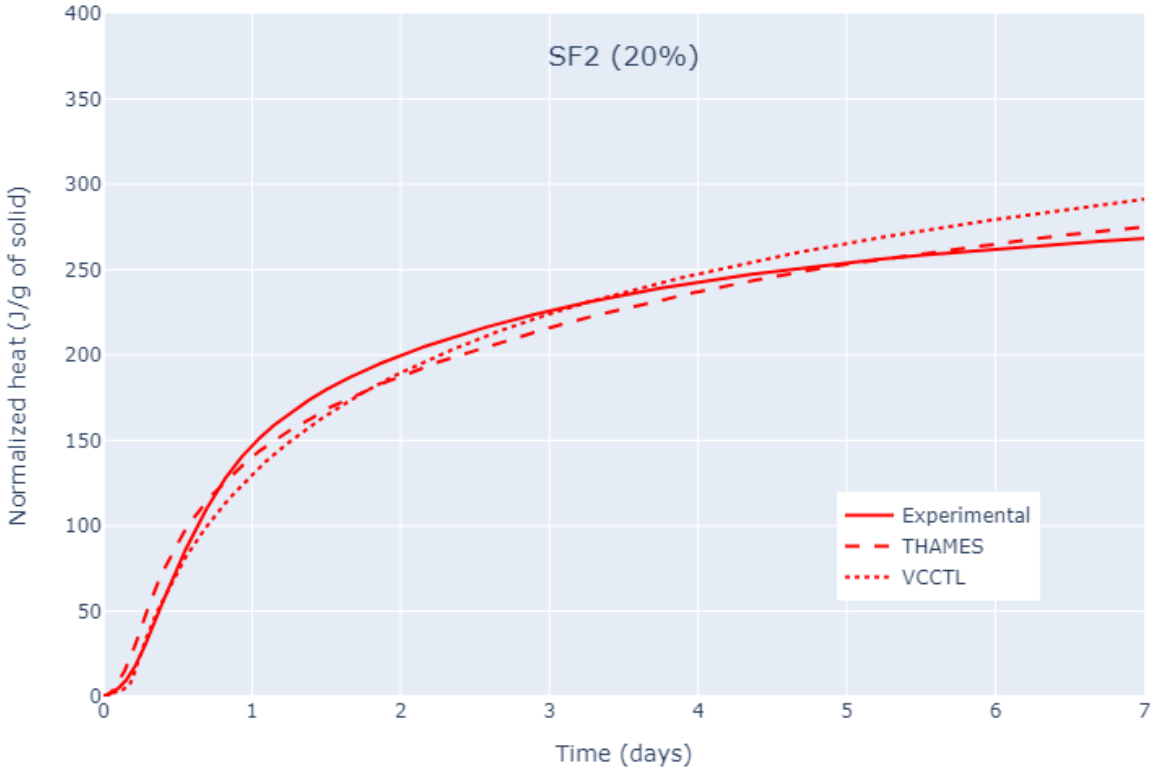


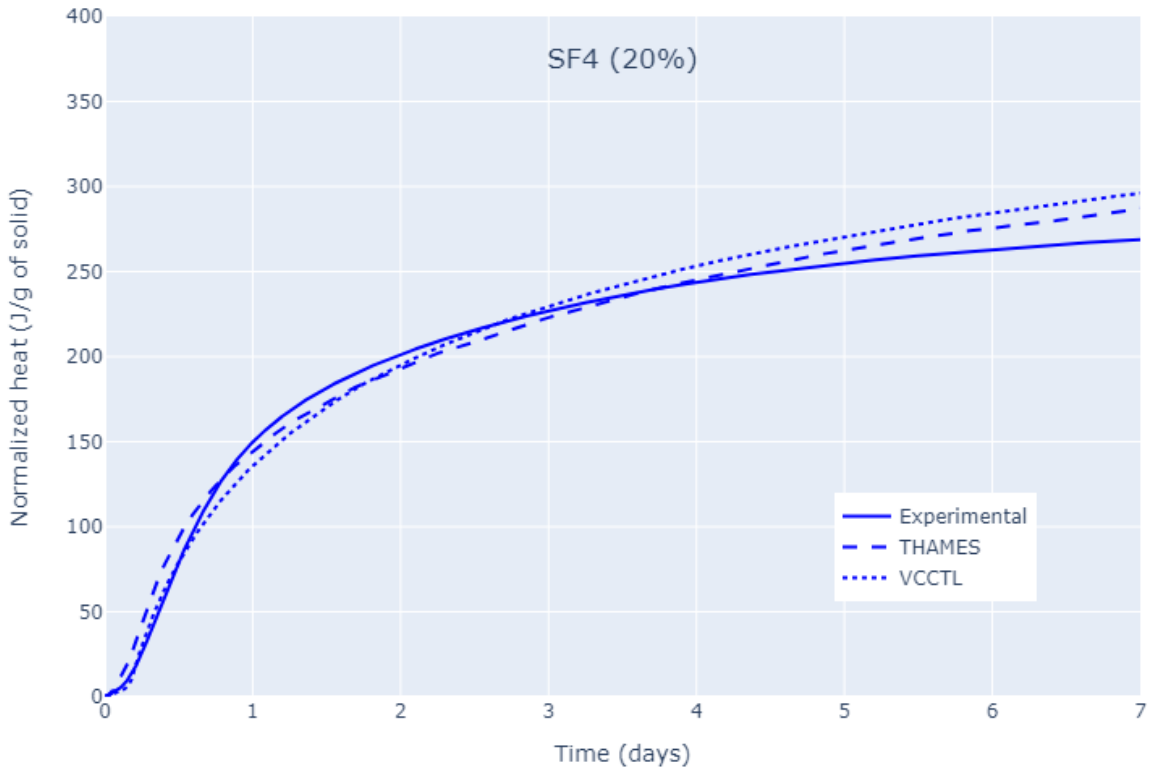
Experimental and THAMES with 30% SF



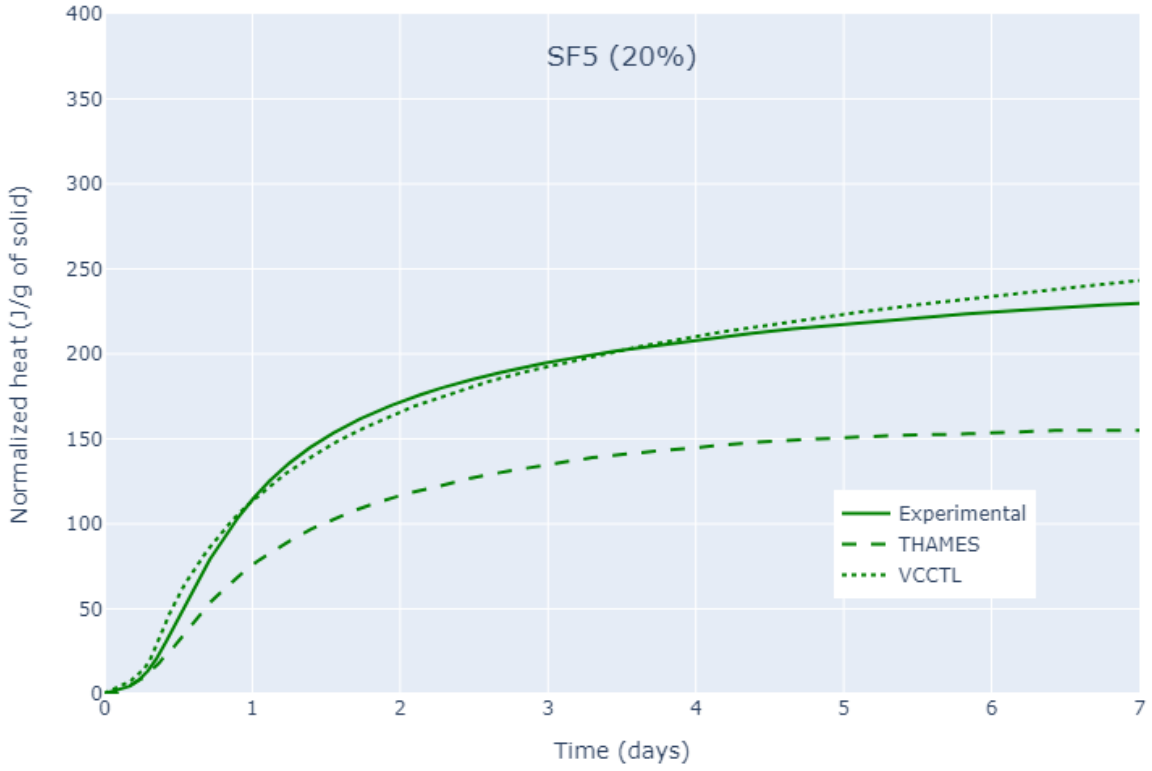


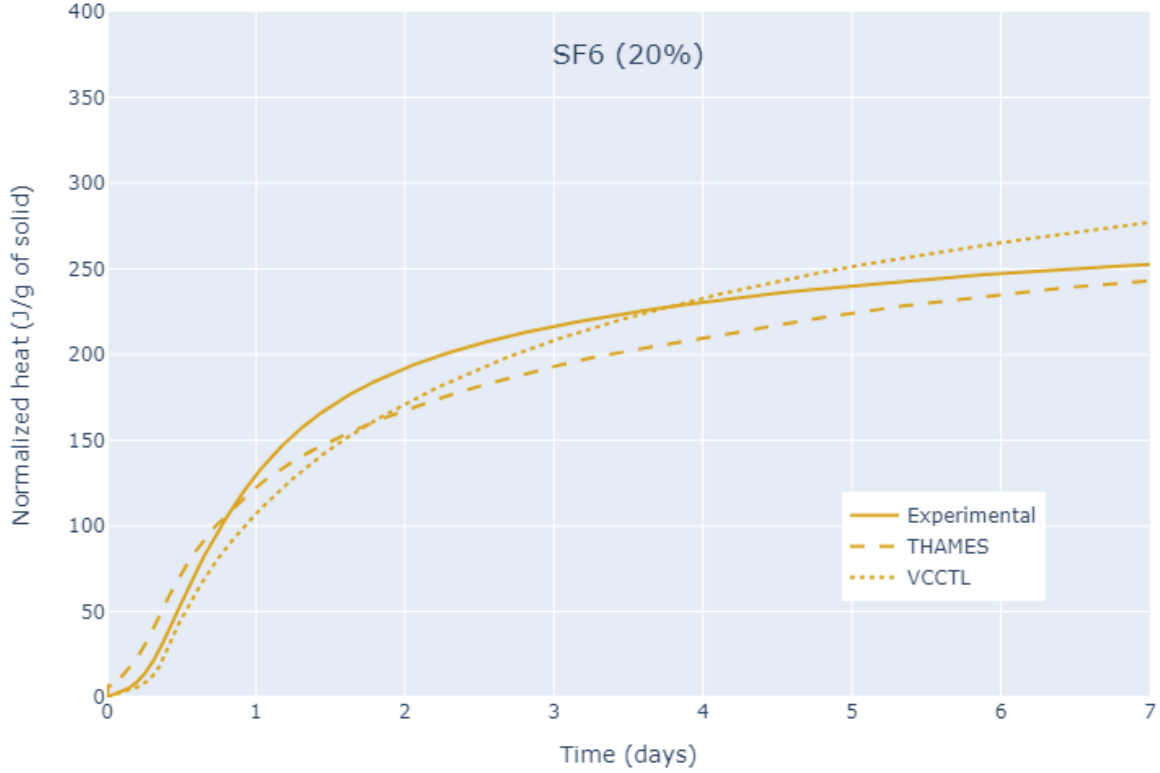
Experimental – VCCTL – THAMES
SF2 and SF4 with 20% SF



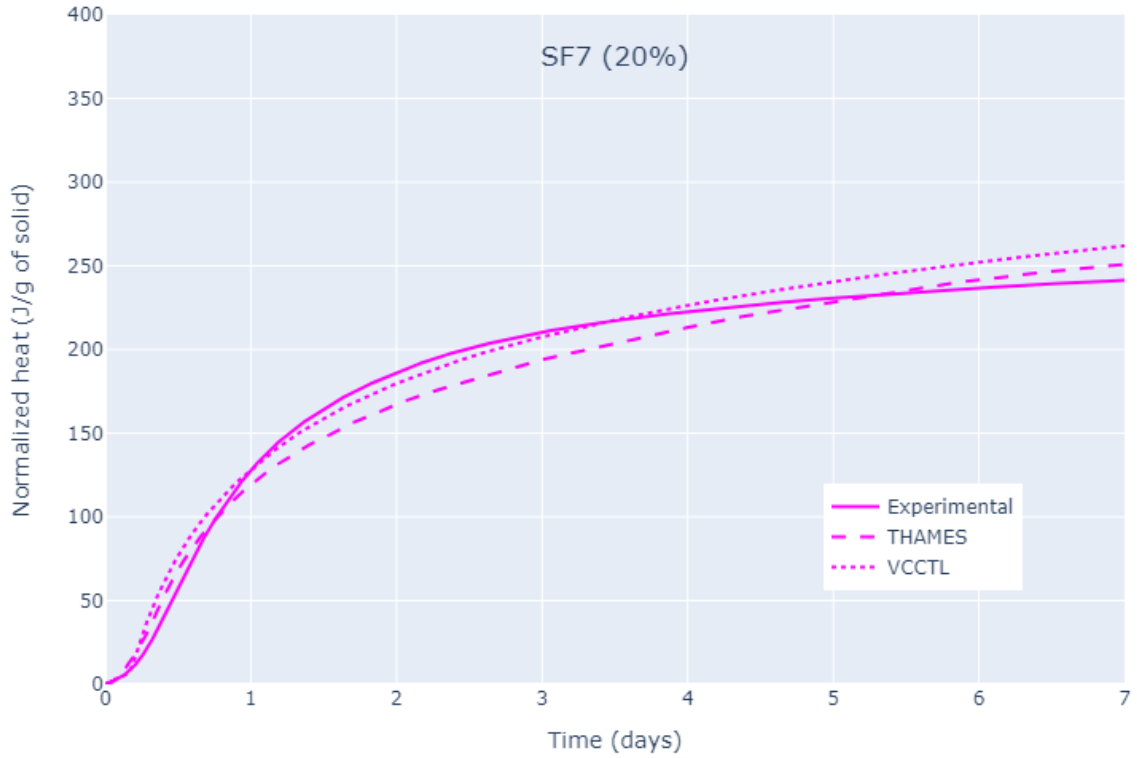


Experimental – VCCTL – THAMES
SF5 and SF6 with 20% SF

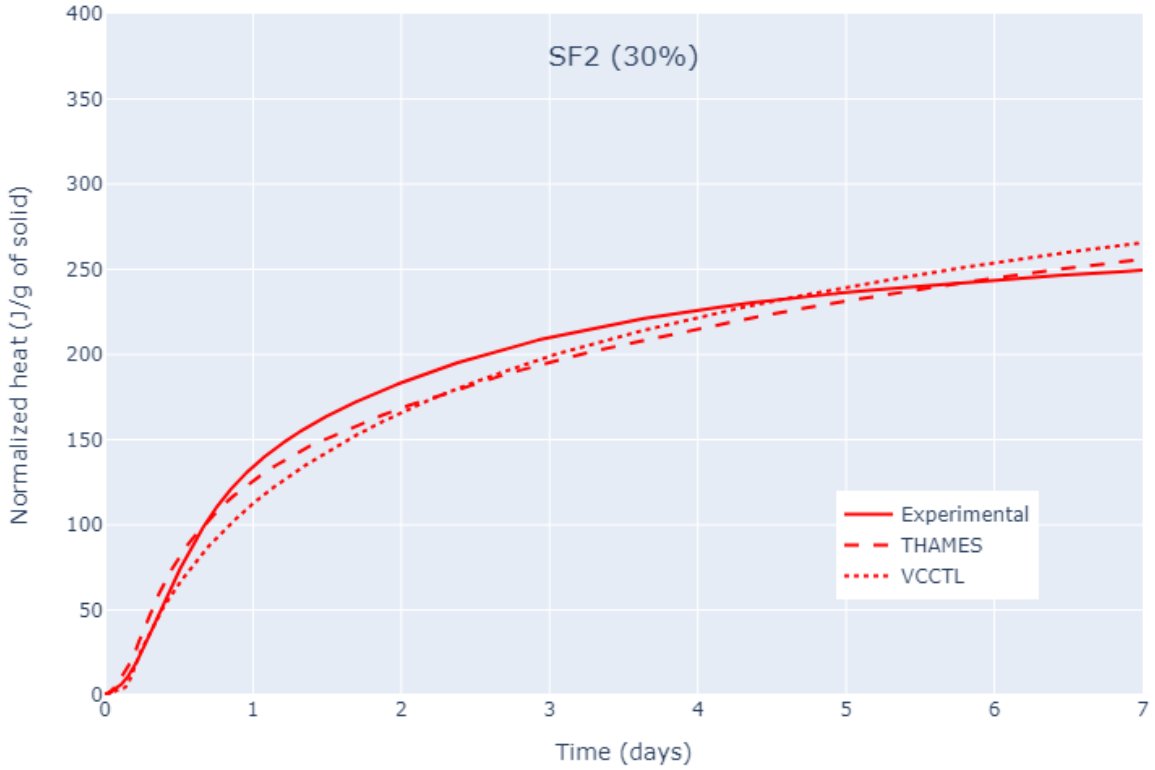


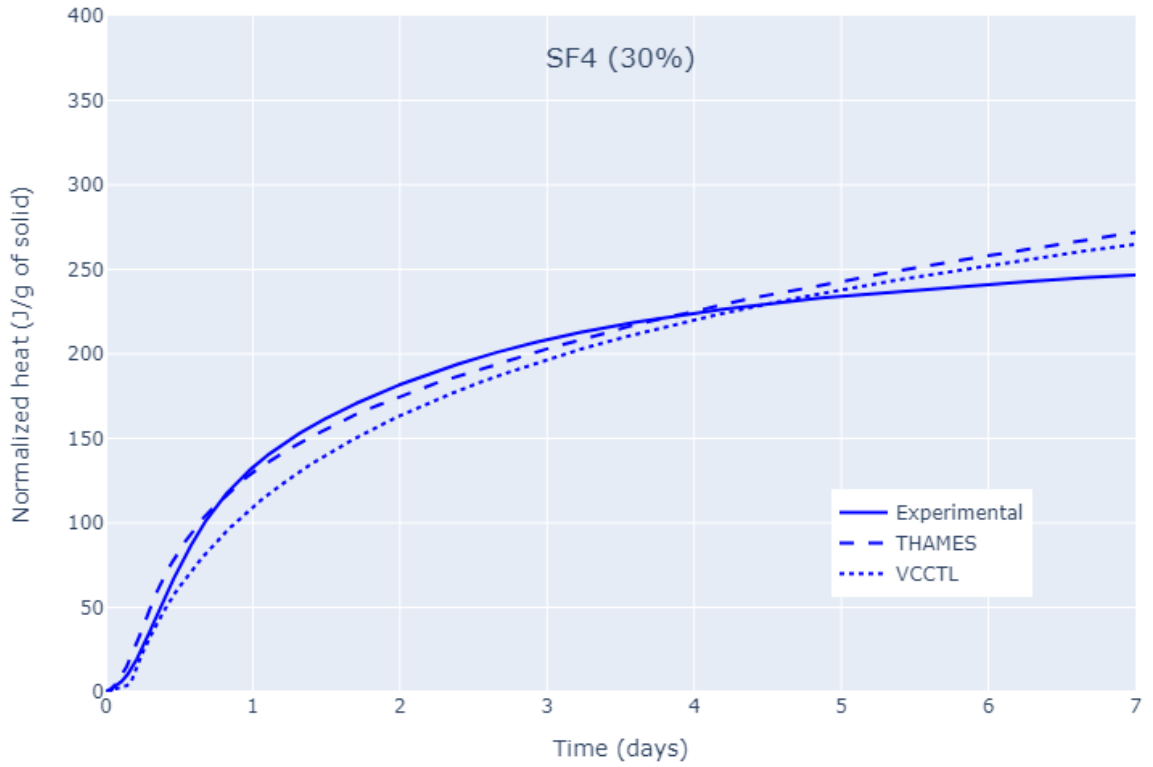


Experimental – VCCTL – THAMES
SF7 with 20% SF

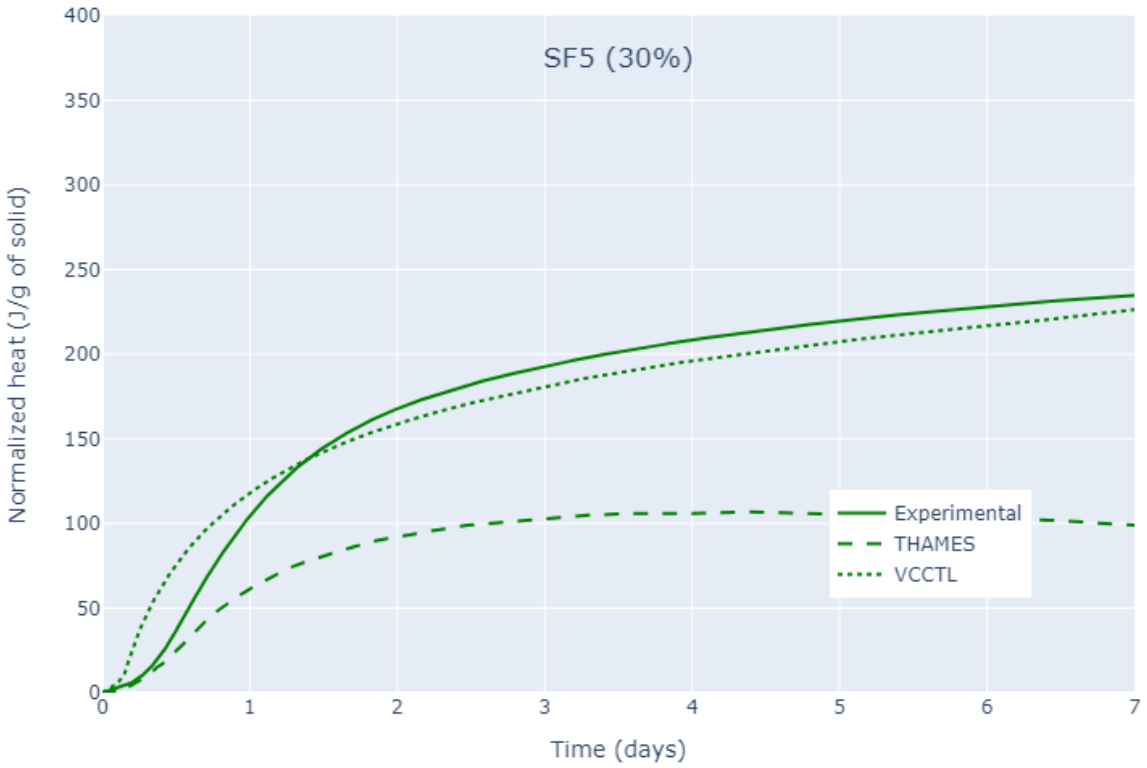


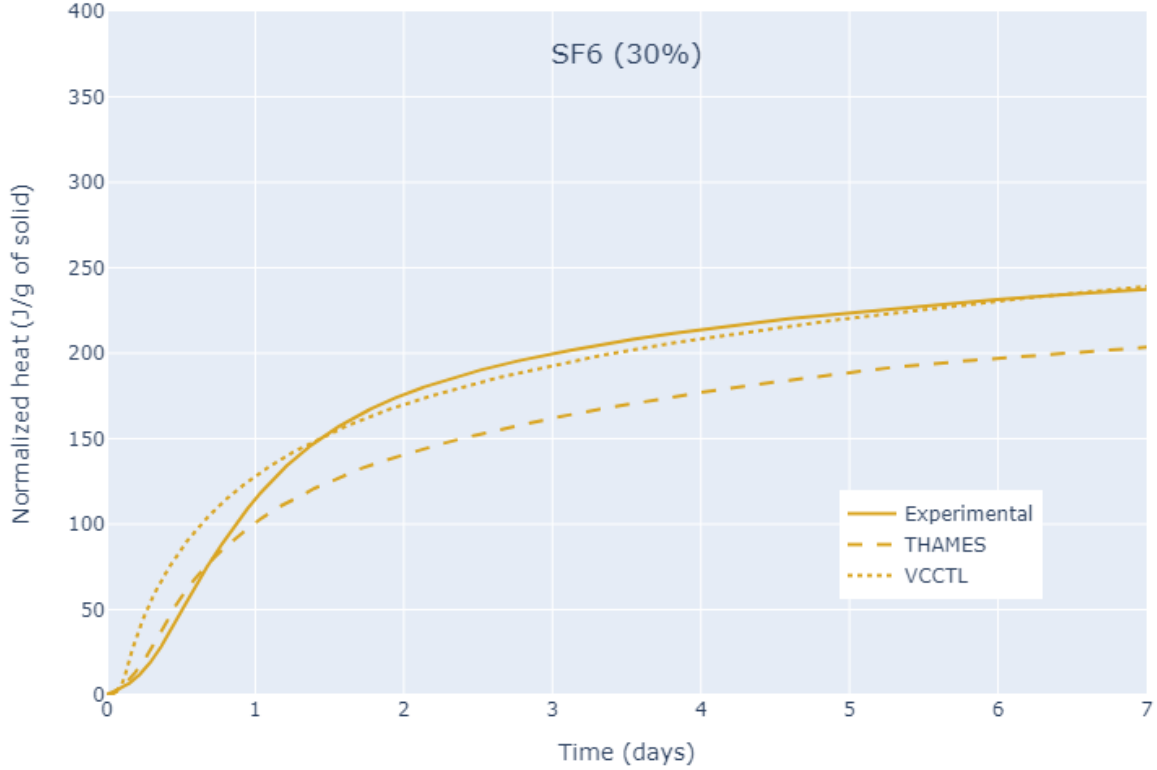
Experimental – VCCTL – THAMES
SF2 and SF4 with 30% SF



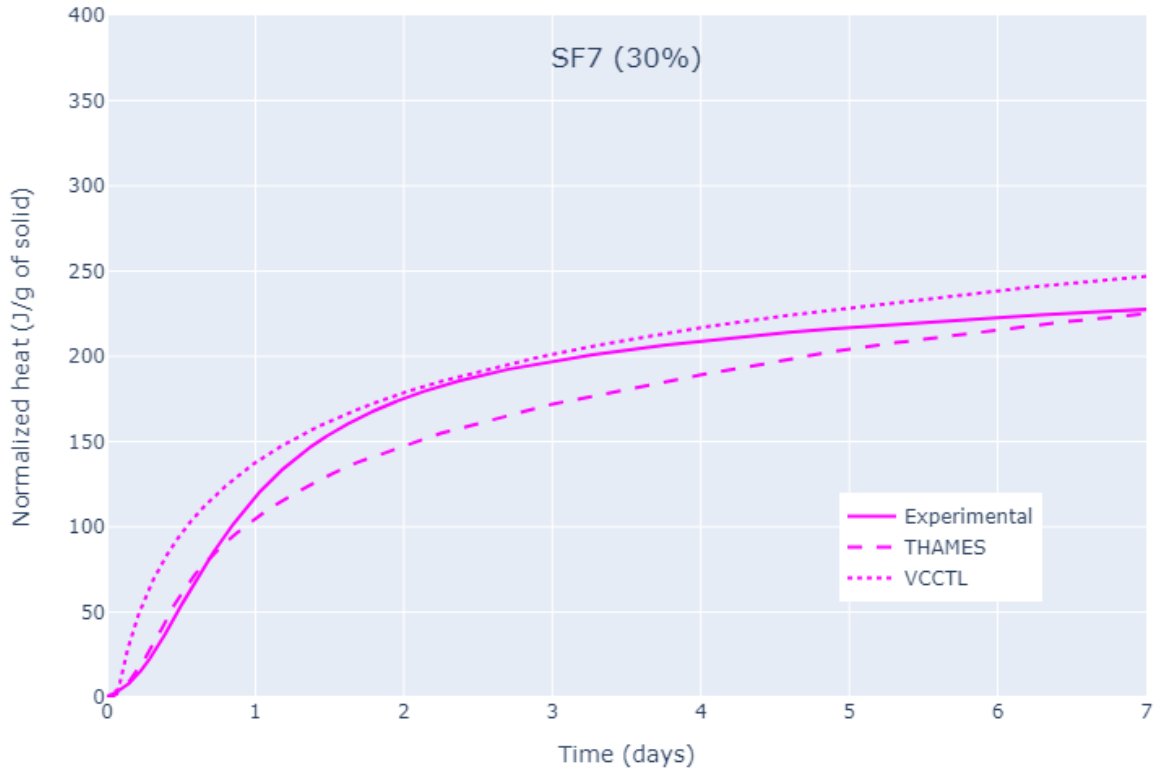


Experimental – VCCTL – THAMES
SF5 and SF 6 with 30% SF

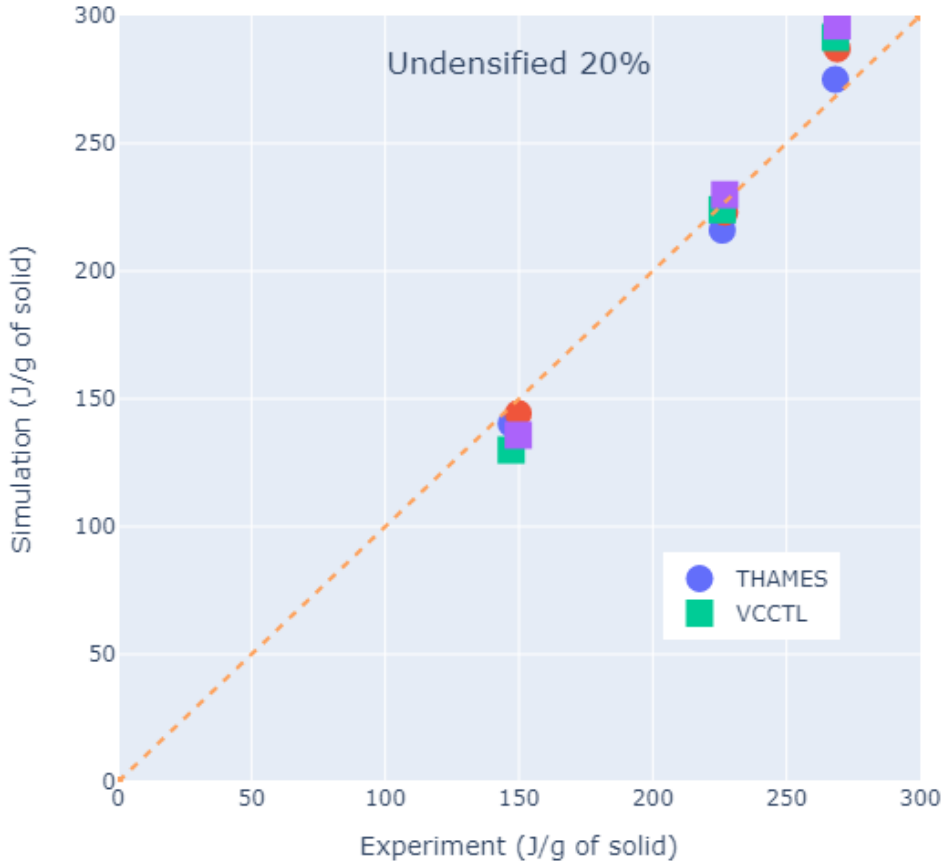


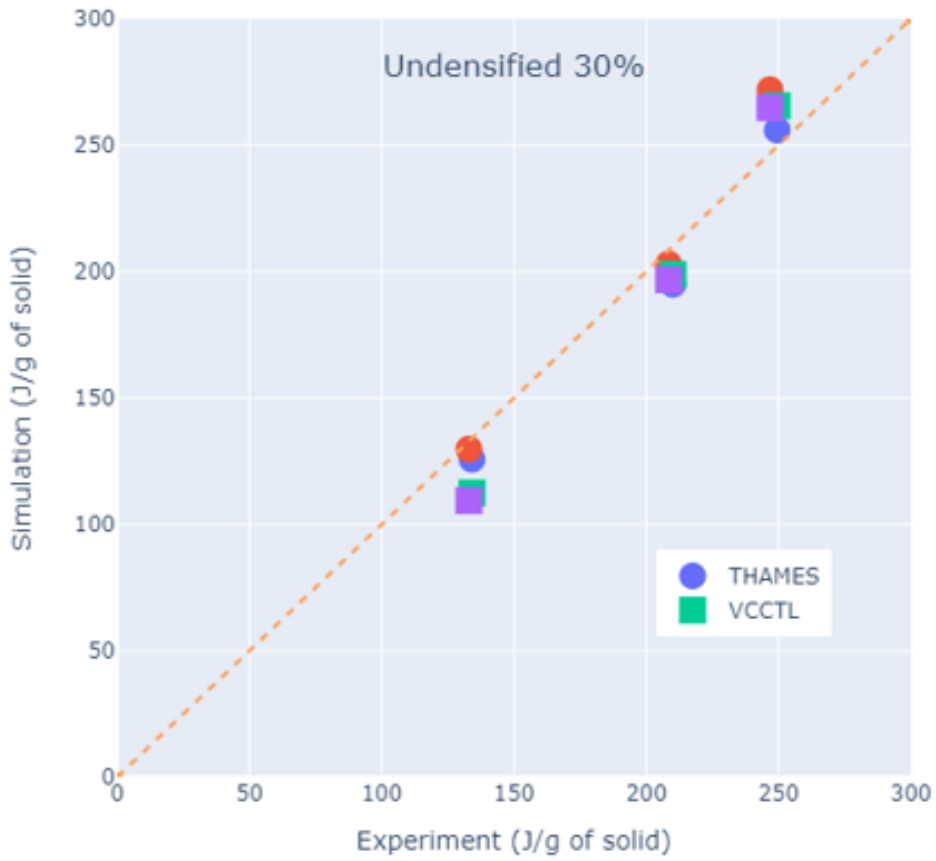


Experimental – VCCTL – THAMES
SF7 with 30% Silica Fume



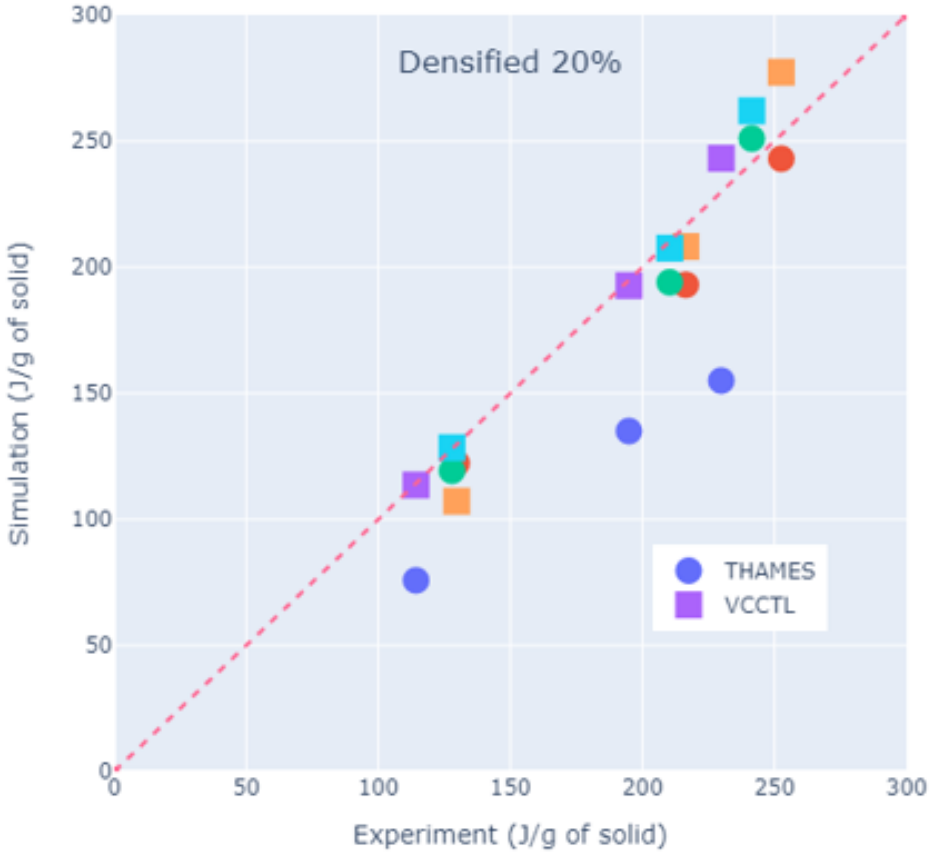
Undensified - SF2 and SF4 – 20 and 30% SF Replacements

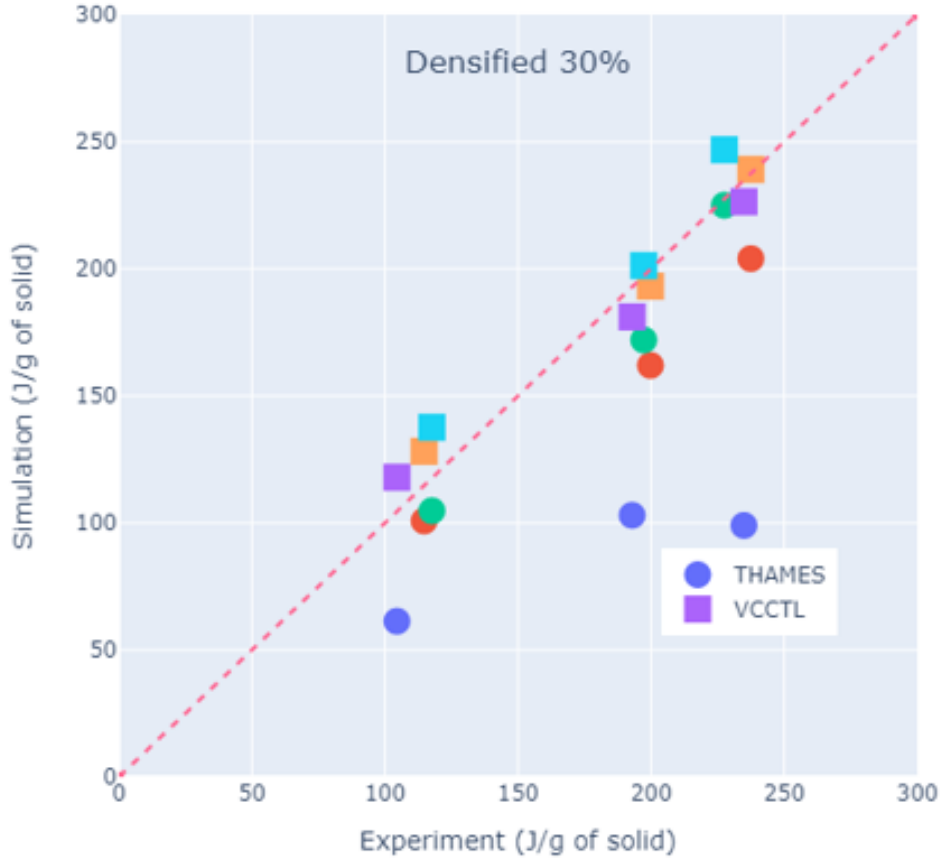




Hydration periods 1, 3, and 7 days, respectively.

Densified - SF5, SF6, and SF7 – 20 and 30% SF Replacements





Hydration periods 1, 3, and 7 days, respectively.

Conclusions

- Silica fume can be used as a replacement to cement.
- Experimental, and simulation - VCCTL and THAMES – analysis showed a reasonable agreement for the SF samples with similar physical properties.
- In general, VCCTL and THAMES simulation analysis resulted in a similar trends for all SF samples.
- SF5 sample showed a significant difference in its SiO_2 wt% and LOI wt% values different than the other SF samples, which may be reflected in the worst agreement for SF5's experimental and THAMES simulation among all samples studied.

Conclusions Cont'd…

- $Ca(OH)_2$ reaction to form C–S–H gel and for C–S–H gel to nucleate heterogeneously on SF particles have been formulated and regressed to the experimental reaction data for mixtures of Class H oil well cement with any of the five different SFs.
- THAMES and VCCTL models correctly differentiates among different SFs based on SiO_2 (wt%) content, LOI (wt%), and BET specific surface area characteristics.
- SFs on hydration can be realistically simulated at replacement levels up to at least 30% by mass, which is an important step forward in simulating cements' hydration behavior with significant pozzolanic proportions, such as in ultra-high-performance concrete binders.

Future Work:

Structure change, kinetic modeling of THAMES, and properties of individual phases for different cementitious material additives will be investigated.

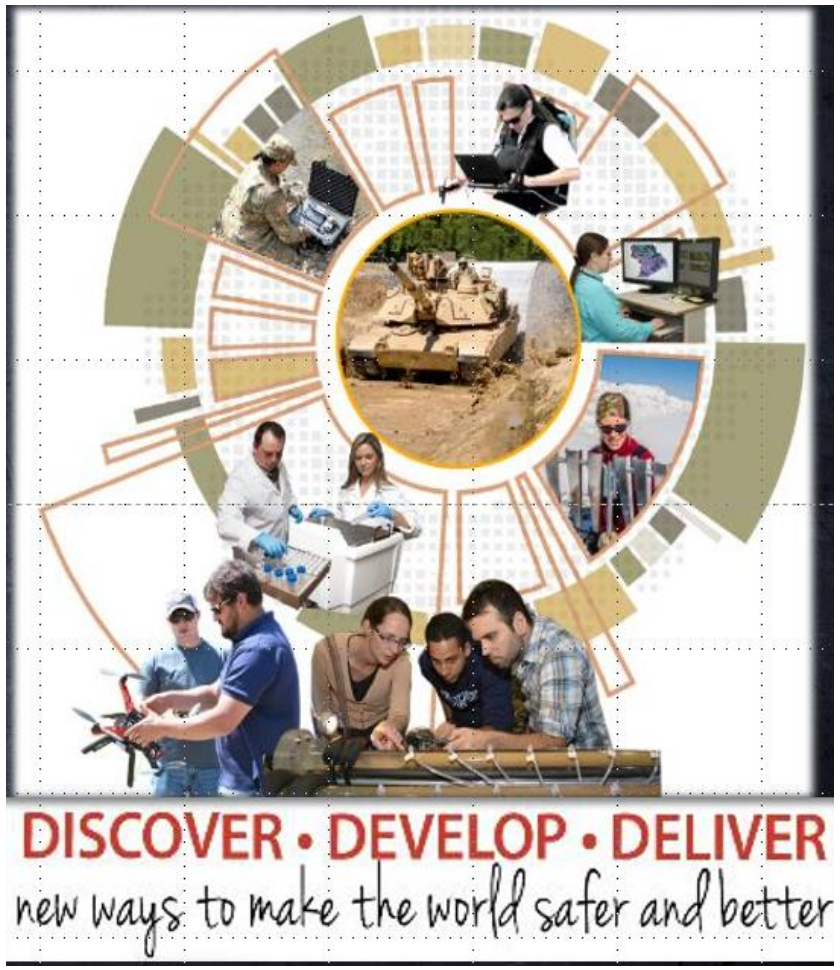
- Continue testing on different compositions of materials in cement at various simulation conditions.
- Validate microstructure and more sensitive properties (e.g., permeability).
- Compute Powers gel-space ratio to show how C-S-H binds the material together with optimum amount of additive.
- Compute the linear elastic moduli and the transport factor of the microstructures.

ACKNOWLEDGEMENTS

TEXAS A&M UNIVERSITY
Department of Materials Science and Engineering

TEXAS A&M UNIVERSITY
Zachry Department of Civil & Environmental Engineering

TAMU
Yoonjung Han
Jonathan Lapeyre
Umme Zakira
Jeffrey W. Bullard



ERDC
Mine Ucak-Astarlioglu
Serdar Astarlioglu
Jedadiah Burroughs

Research performed at Texas A&M University was supported by a grant from the U.S. Army Corps of Engineers, Engineer Research and Development Center, Contract W912HZ19C0042.

Contact: Mine.g.ucak-Astarlioglu@usace.army.mil

Permission to publish was granted by Director, Geotechnical & Structures Laboratory.