Low-cost Composite Phase Change Material

Oak Ridge National Laboratory
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Project Summary

Timeline:
Start date: 10/1/2018
Planned end date: 9/30/2021

Key Milestones
1. Evaluation of as-received material - Acquire exfoliated graphite, conduct standard characterization, and infuse with salt hydrate and densify; 02/28/2019
2. 3 salt hydrate/CENG composites characterized -- Using commercially available graphite, three different salt hydrates composites are synthesized and evaluated; 03/31/2019

Key Partners:
- ORNL – Building Technologies Integration Center (BTRIC)
- ORNL – Center for Nanophase Materials Science (CNMS)
- Georgia Institute of Technology
- University of Tennessee, Knoxville

Budget:
Total Project $ to Date:
- DOE: $850k
- Cost Share: $0

Total Project $:
- DOE: $2550k
- Cost Share: $0

Project Outcome:
When successful, this project will advance the state of the art by realizing a 10x reduction in the cost of deploying phase change materials (PCMs) for building equipment or envelopes.
Multidisciplinary Project Team

Sample synthesis; PCM evaluation
Lead: Gluesenkamp¹
Team:
Jason Hirschey³, Samuel Graham⁴, Tim LaClair¹, Navin Kumar², Kaushik Biswas¹, David Keffer⁶

T2M; HVAC Integr.
Lead: Gluesenkamp¹
Team:
Tim LaClair¹, Navin Kumar², Bo Shen¹, Jin Dong¹, Orlando Rios¹, ORNL TTO

Materials characterization
Lead: Rios¹
Team:
Yuzhan Li², Michael Kesler², Thomas Proffen¹, Dami Akamo⁵, David Keffer⁶

Molecular modeling
Lead: Goswami¹
Team:
Orlando Rios¹

Principal Investigator: Gluesenkamp¹

Notes:
1. ORNL research staff
2. ORNL postdoctoral researcher
3. Georgia Tech PhD GO! student
4. Georgia Tech professor
5. UTK PhD Bredesen Center student
6. UTK professor
Challenge: Cost Effectiveness

- Traditional PCM solutions:
  - Passive
  - Integrated into wall/floor

- Problems:
  - Temperature mismatch: highly sensitive
  - High cost: payback exceeds product life
  - Poor fire safety: organic paraffin-based
  - Intrusiveness; inaccessibility: integrated into walls
  - Low utilization: only useful part of year, hurting economics
  - Low demand impact: PCM depleted by afternoon peak

Challenge: Cost

Energy Storage Material Cost ($/kWh)

Melting Temperature (°C)

- Salt Hydrates
- Other Organics
- Fatty Acids
- Waxes
Challenge: Technical Issues with Salt Hydrates

• Incongruent melting
  – Water/salt separation with repeated thermal cycling
    • Reduces thermal storage capacity over time

• Large supercooling
  – Unpredictable crystallization, delayed nucleation
    • Large temperature and volumetric fluctuations

• Low thermal conductivity
  – Slow thermal charging/discharging

• Corrosion
  – Liquid phase corrodes packaging
    • Shorten system lifespan
    • Alter chemical composition and thermophysical properties
Potential to transform energy storage:

- Billions of dollars have been invested into R&D of electric battery technologies, including
  - As of 2015, nearly $2B from renewable energy
  - As of 2015, nearly $2B from automotive industries
  - From 2017 to 2030, Bloomberg New Energy Finance (2017) predicts that global investments in electrical energy storage will double 6 times, with
    - $103B invested over this time period
    - $26B in the US
- By contrast, thermal energy storage has seen very little investment
- When this project is successful, a low cost PCM based on ORNL-developed IP can deliver energy storage services more cost effectively than electric batteries
HVAC integration

- HVAC-coupled PCM storage allows a range of possible phase change temperatures to be used.
  - Increases annual utilization factor to improve economics
- Configurations have been modeled and evaluated in ORNL’s Heat Pump Design Model (HPDM) software
Approach

- Develop a stable, low-cost salt hydrate, using a novel technique for incorporating compressed expanded natural graphite (CENG).
- Demonstrate prototype with >200 W thermal power, >800 Wh storage
When this project is successful, a low cost PCM based on ORNL-developed IP can deliver electric-equivalent storage more cost effectively than electric batteries.

**Impact**

- **Electric Battery**
- **Thermal Battery**

**Project outcomes:**
- **Demonstrate the stability**
  >100 cycles and cost of PCM < $2/ kWh
- **Demonstrate prototype with**
  >200 W thermal power, >800 Wh storage

**Current Organic PCM** (flammable)
**Current Inorganic PCM**
**ORNL PCM**
Progress

Sample synthesis

- Composite samples have been created
- Patent was filed on composition of matter and technique for creating it
- Sample handling procedure developed for XRD, SEM, and PDF evaluations

*Compressed graphite-salt “puck” before sealing with water vapor impermeable film.*

*Graphite-salt composite packed in bag*

*Humidity controlled glovebox for sample transfers*

*SEM image of composite sample*
Progress

Temperature-history calorimetry

• Accelerated thermal cycling with in-situ temperature, latent heat, heat capacity measurement for PCMs.
• Accuracy ± 3–6% of latent heat.
• Large sample throughput
  - Simultaneous evaluation of up to 150 samples
  - 24/7 operation
• Temperature range: -20°C to 60°C

\[ H_{fs} = \frac{m_w C_{pw} + m_{tw} C_{ptw}}{m_p} \frac{A_1}{A_1'} (T_0 - T_m) \]
Progress

XRD Characterization

- Rietveld method for quantitative phase analysis
- Thermal degradation with cycling
- New PCM degradation evaluation technique
- Outlines the degradation mechanism
  - By-product of degradation
  - Quantifies the rate of degradation

<table>
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<tr>
<th>Sample</th>
<th>Pure hydrate</th>
<th>Composite 1</th>
<th>Composite 2</th>
<th>Composite 3</th>
<th>Composite 4</th>
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<tr>
<td></td>
<td>Hydrate</td>
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MD Simulation

- Coarse-grain simulation of Na$_2$SO$_4$ + H$_2$O
- Understand the basic mechanism of phase-separation in the PCM
- Excellent phase separation under gravity and viscosity
  - Two phase separation: Hydrous and anhydrous
- 78K system vs. 28K System
  - Smaller system shows
  - Viscosity-dependent phase reversibility
- Ostwald ripening
  - Water motion is separate from all particles
Stakeholder Engagement: early stage project

- Multi-institution team

- Outreach to potential industry partners
  - Discussions held with 5 thermal storage companies
  - Coordination established with 2 graphite suppliers
  - Discussions ongoing with 3 HVAC OEMs
Stakeholder Engagement (continued)

• Inventions

• Reports and Publications
  – Three abstracts submitted to European Congress and Exhibition on Advanced materials and Processes (EUROMAT 2019).
Remaining Project Work

• Evaluate and publish different PCM characterization techniques, including:
  - Large scale parallel T-H calorimetry
  - XRD-based degradation

• Develop CENG-PCM and characterize on micro-level

• Perform technoeconomic analysis for applications

• Develop and characterize system prototype at the macro level
Thank You

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REFERENCE SLIDES
Project Budget: $850k/yr, FY19-21
Variances: None
Cost to Date: $297k
Additional Funding: None

## Budget History

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<th>FY 2018 (past)</th>
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<th>FY 2020 – FY 2021 (planned)</th>
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<td>DOE</td>
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Project Plan and Schedule

Project Schedule

Project Start: October 2018
Projected End: September 2021

Task

Past Work

Q2 Milestone 1: Characterization CENG-PCM
Q2 Milestone 2: Three different CENG-PCM characterized and cycle and Review Paper of Salt Hydrate

Current/Future Work

Q4 Milestone 3: Preliminary technoeconomic analysis
Q4 Milestone 4: Publish standard characterization
Q4 Milestone 4: One Composite Evaluation (Go/No-Go)
Q2 Milestone 5: Evaluation of milled + passivated material
Q3 Milestone 6: Refine technoeconomic analysis
Q4 Milestone 7: New material exploration
Q4 Milestone 8: 50 W HX prototype fabricated
Q4 Milestone 4: One Composite Evaluation (Go/No-Go)
Q1 Milestone 9: MD Simulations reported
Q3 Milestone 10: Cycling and latent heat evaluation
Q4 Milestone 11: Project Wrap Up
Q4 Milestone 12: Scaled Up Prototype Evaluation