Lab of Applied MultiPhase Thermal Engineering

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Inspiring Minds

Design of an Automated Thermal Cycler for Long-term Phase Change Material Phase Transition Stability Studies

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COMSOL CONFERENCE

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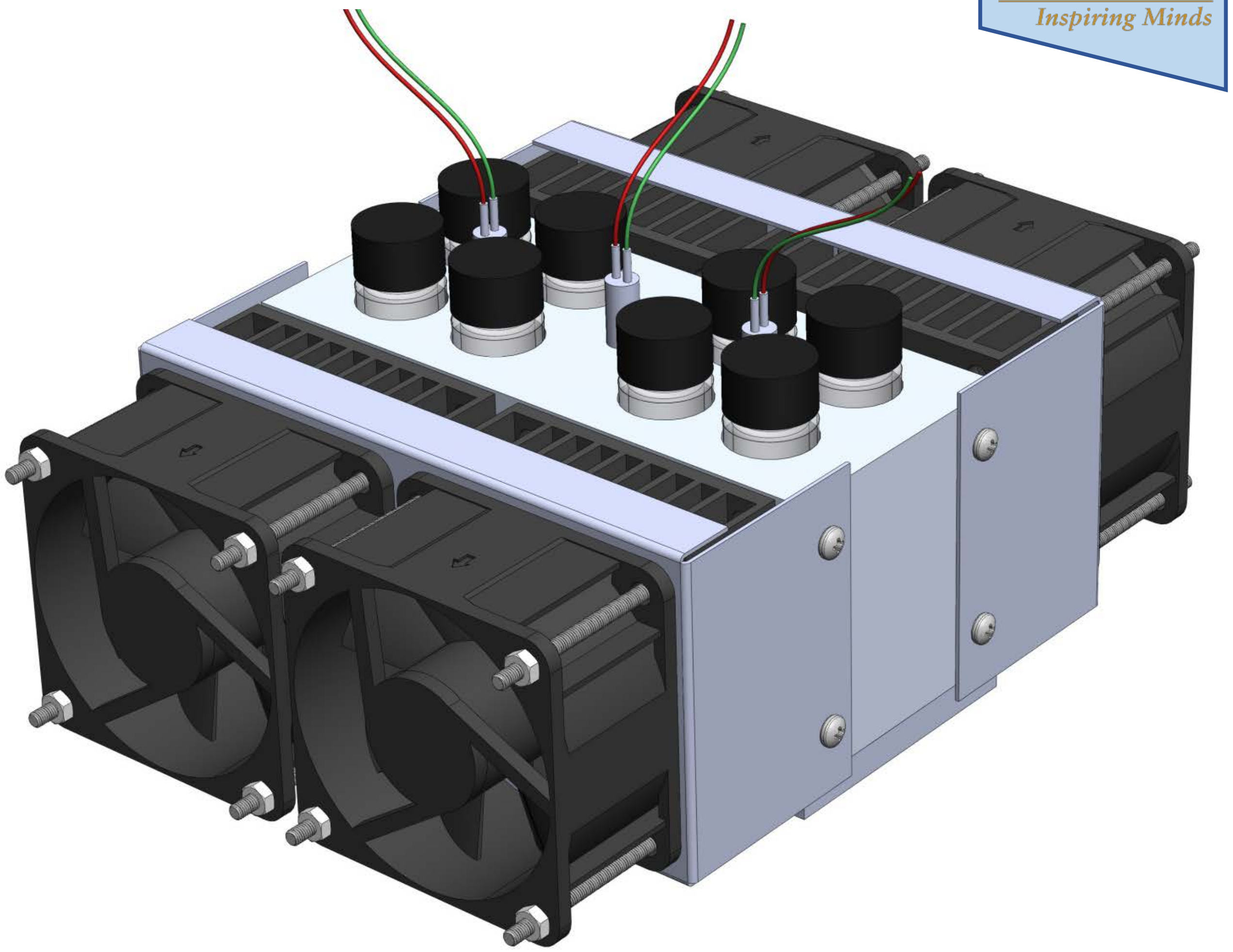
Thermal Cycler Overview

Melts and solidifies PCM samples:

- automated, no user interaction
- infinite number of cycles
- adjustable hot and cold temperatures

Main components:

- aluminum housing
- 8 dram vials of PCM
- thermistor probe
- 4 thermoelectric cooling assemblies
- 2 – 250 W cartridge heaters



Thermal cycler CAD model

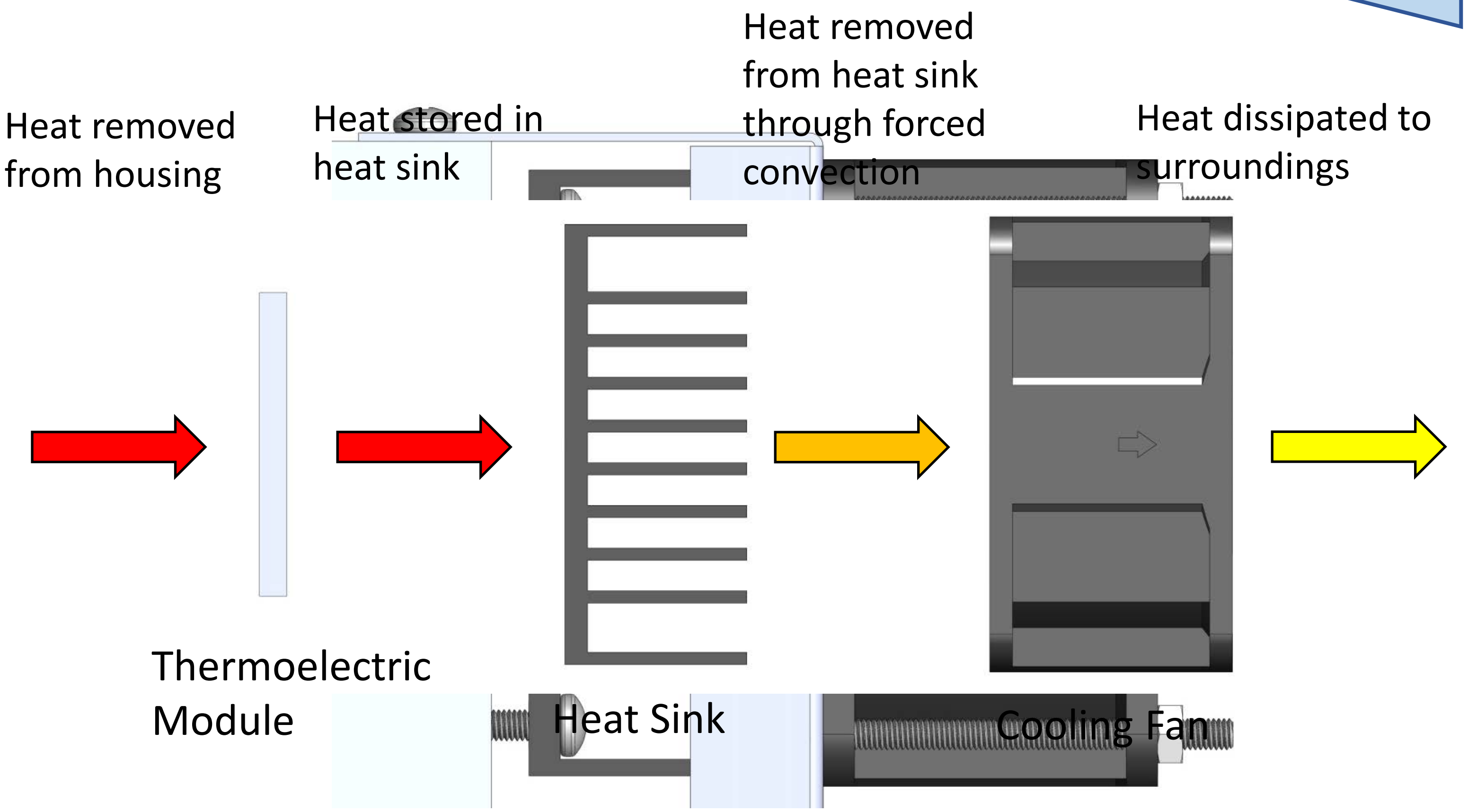
Thermal Cycler Cooling System

Removes heat through:

- solid state heat transfer
- forced convection

Main components:

- Thermoelectric module
  - 170 W
- Aluminum heat sink
- Cooling fan



Heat Transfer through thermoelectric cooling assembly

Top view of thermoelectric cooling assembly

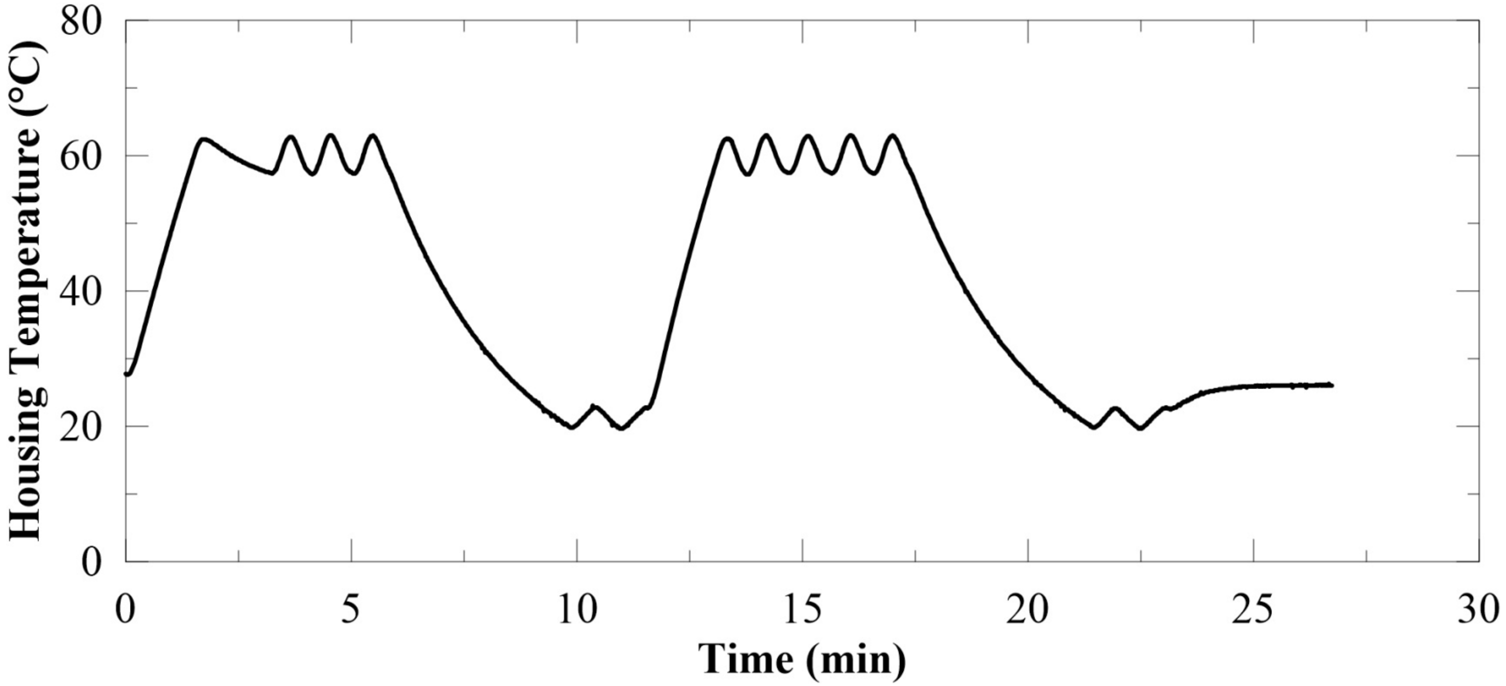
Thermal Cycler Control System

Physical components:

- Arduino Mega2560
- AC/DC solid state relays

Function:

- Reads housing temperature
- actuates relays to heat/cool system
- maintains housing temperature, T_d, with small fluctuation, $\pm \Delta T_f$



Sample operation of ON/OFF controller

COMSOL® Multiphysics

Use COMSOL Multiphysics to:

- simulate system response to ON/OFF controller
- Validate thermal management components
- estimate time required for full melt/solidification of PCM
    - T_m = 60 °C
    - ΔH_f = 200,000 J/kg
- desired cycle time (including melting and solidification)
    - 12 - 15 min

Simulated physics:

- “Heat Transfer in Solids”
    - phase change
    - ON/OFF temperature control
    - thermoelectric cooling (TEC)
    - conduction through TEC
    - forced & natural convection on heat sink

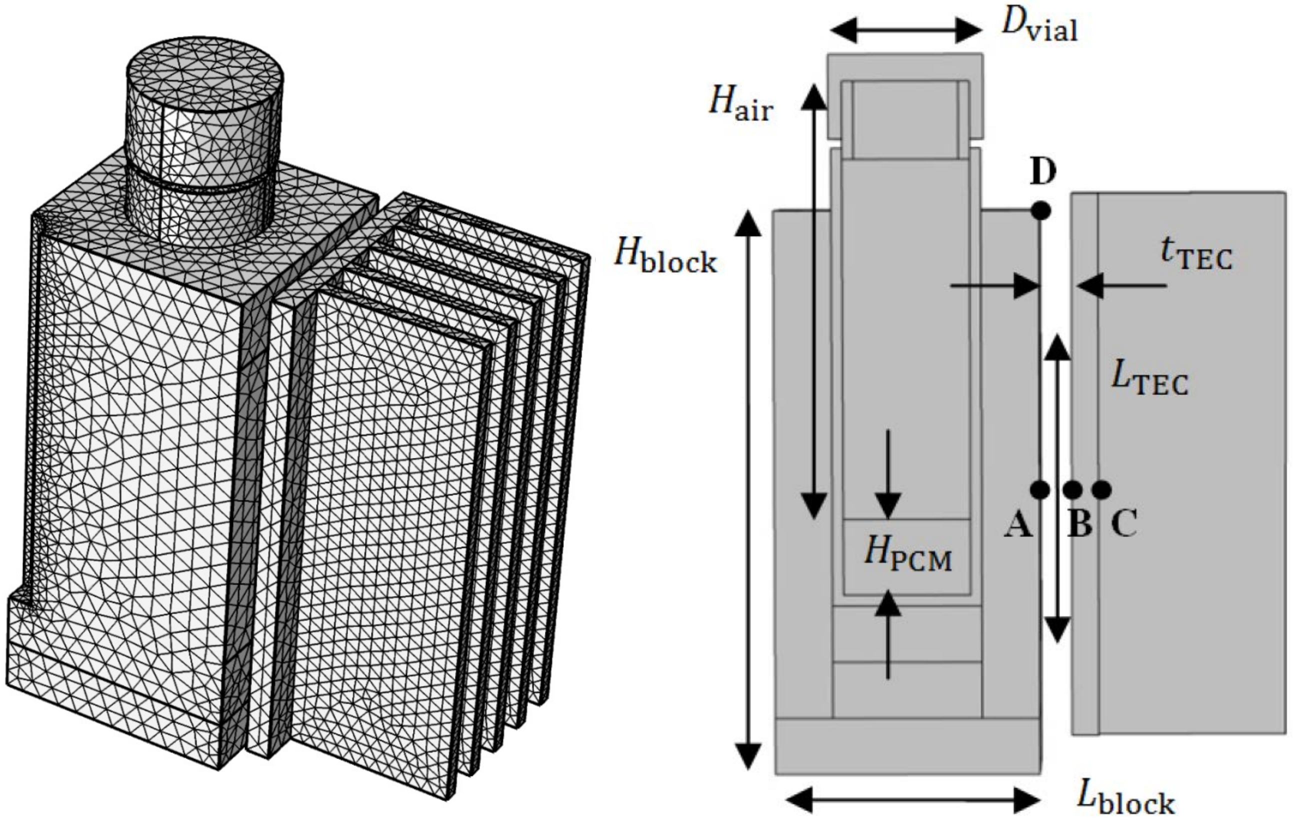
COMSOL® Geometry & Mesh

Geometry:

- 1/8 symmetric section of housing
- single dram vial
  - D_{vial} = 0.68 in
  - H_{PCM} = 0.335 in
- 1/2 symmetric section of heat sink

TEC not modeled:

- complex internal geometry
- conduction modeled instead as boundary condition



Eighth symmetric model and tetrahedral mesh

COMSOL® Phase Change

Specific heat capacity

- $C_\mathrm{p} = C_\mathrm{s} + \frac{C_\mathrm{l} - C_\mathrm{s}}{1 + \mathrm{e}^{-r(T - T_\mathrm{m})}} + \alpha \mathrm{e}^{-\beta (T - T_\mathrm{m})^2}$

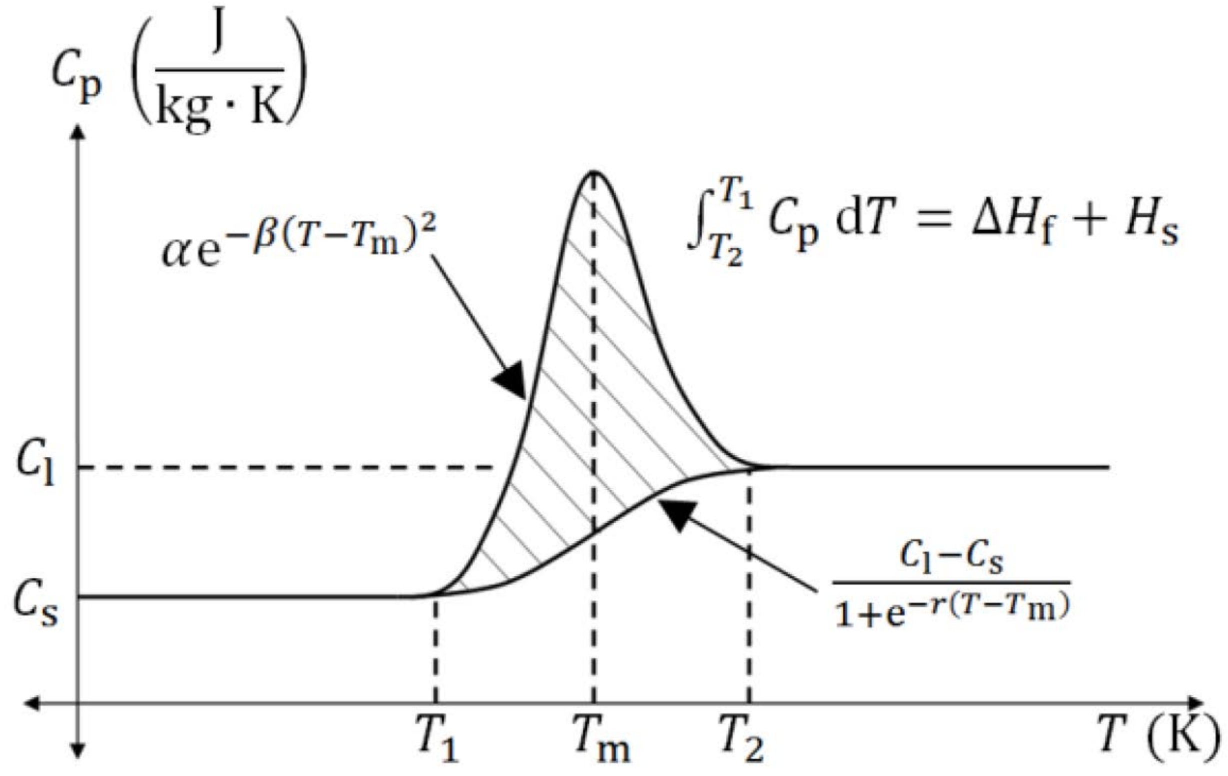
Thermal conductivity

- $k = k_\mathrm{s} - \frac{k_\mathrm{s} - k_\mathrm{l}}{1 + \mathrm{e}^{-r(T - T_\mathrm{m})}}$

α and β calculated numerically such that integral of Gaussian function is equal to latent heat of fusion.

For both equations:

- $r = \frac{10}{\Delta T}$



Specific heat capacity of material experiencing phase change over finite temperature range

COMSOL® ON/OFF Controller

Heating process controller ON/OFF status

- $X_{\text{heat}} = (T_{\text{Al}} < T_{\text{heat}} - T_{\text{f}}) + (T_{\text{Al}} > T_{\text{heat}} - T_{\text{f}}) \cdot (T_{\text{Al}} < T_{\text{heat}}) \cdot \left(\frac{\mathrm{d}T_{\text{Al}}}{\mathrm{d}t} > 0\right)$

Cooling process controller ON/OFF status

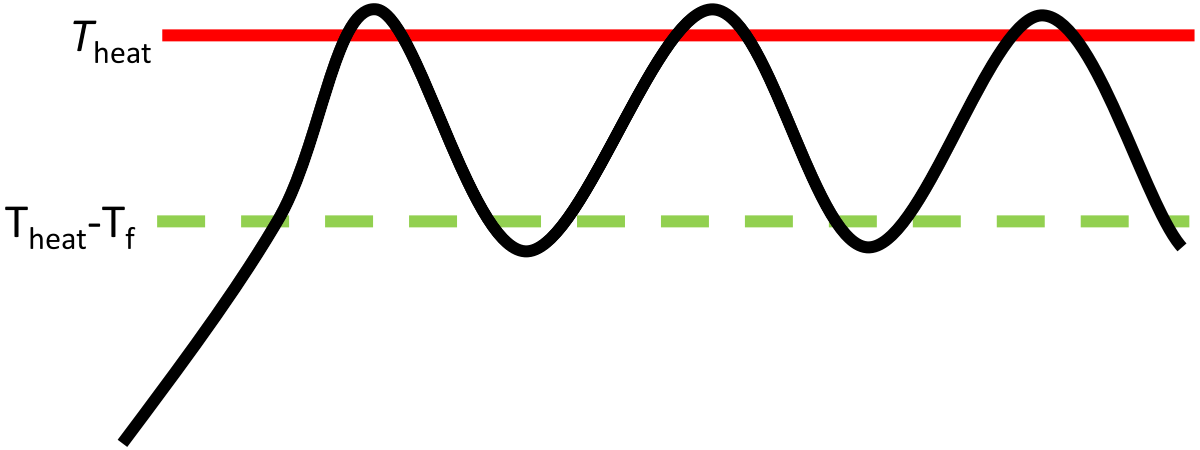
- $X_{\text{cool}} = (T_{\text{Al}} > T_{\text{cool}} + T_{\text{f}}) + (T_{\text{Al}} < T_{\text{cool}} + T_{\text{f}}) \cdot (T_{\text{Al}} > T_{\text{cool}}) \cdot \left(\frac{\mathrm{d}T_{\text{Al}}}{\mathrm{d}t} < 0\right)$

Heat added to system

- $Q_{\text{heat}} = X_{\text{heat}} \cdot Q_{\text{CH}}$

Heat removed from system

- $Q_{\text{cool}} = X_{\text{cool}} \cdot Q_{\text{TEC}}$



Temperature fluctuation about desired temperature

COMSOL® Thermoelectric Modules

Available information:

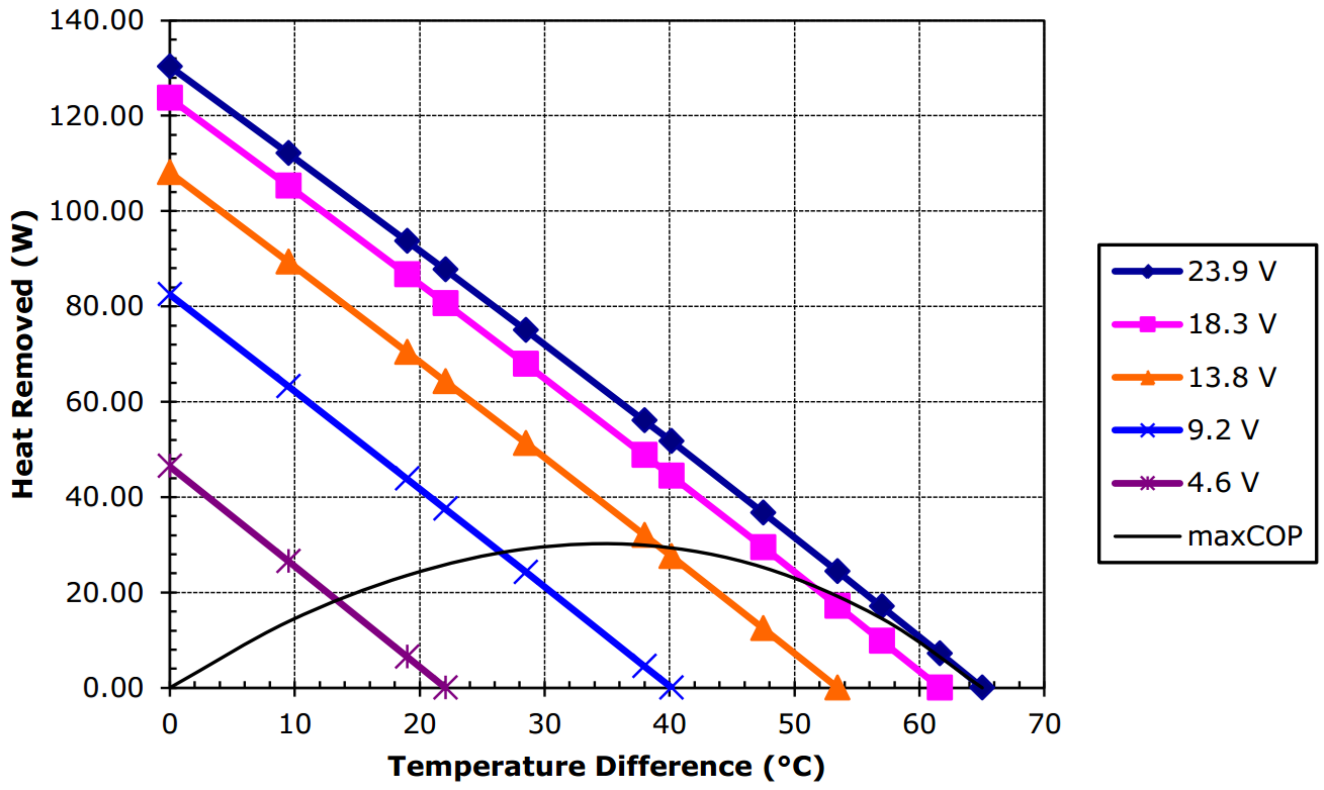
- $Q_{max}(V, T_H)$
- $\Delta T_{max}(V, T_H)$
- $Q(\Delta T)$

Resulting cooling rate:

- $Q_{\mathrm{TEC}} = \frac{1}{2} Q_{\max}\left(1 - \frac{\Delta T_{\mathrm{TEC}}}{\Delta T_{\max}}\right)$

Must identify at any V and T_H:

- $Q_{\max}$
- $\Delta T_{\max}$



Thermoelectric module performance curve at T_H = 30 °C
- Courtesy of TE Technology, Inc.®

COMSOL® Thermoelectric Modules

Q_{max}(V) 2nd order polynomial regressions:

- $Q_{max@30\,°C} = -0.2372V^2 + 11.118V - 0.1608$
- $Q_{max@50\,°C} = -0.2022V^2 + 10.650V + 1.7691$
- $Q_{max@70\,°C} = -0.1544V^2 + 9.1577V + 17.558$

ΔT_{max}(V) 2nd order polynomial regressions:

- $\Delta T_{max@30\,°C} = -0.1163V^2 + 5.5563V - 1.1939$
- $\Delta T_{max@50\,°C} = -0.1091V^2 + 5.6691V - 1.6536$
- $\Delta T_{max@70\,°C} = -0.1012V^2 + 5.6852V - 0.8129$

COMSOL® Thermoelectric Modules

Linear interpolation equations:

- $Q_{\mathrm{max}} = \alpha_{\mathrm{Q}} T_{\mathrm{H}} + \beta_{\mathrm{Q}}$
- $\Delta T_{\mathrm{max}} = \alpha_{\mathrm{T}} T_{\mathrm{H}} + \beta_{\mathrm{T}}$

Final cooling rate:

- $Q_{\mathrm{TEC}} = \frac{1}{2} Q_{\mathrm{max}} \left(1 - \frac{\Delta T_{\mathrm{TEC}}}{\Delta T_{\mathrm{max}}}\right)$

Interpolation parameters:

- $\alpha_{\mathrm{Q}} = \frac{Q_{\mathrm{max@70\,°C}} - Q_{\mathrm{max@30\,°C}}}{40\ \mathrm{°C}}$
- $\alpha_{\mathrm{T}} = \frac{\Delta T_{\mathrm{max@70\,°C}} - \Delta T_{\mathrm{max@30\,°C}}}{40\ \mathrm{°C}}$
- $\beta_{\mathrm{Q}} = Q_{\mathrm{max@70\,°C}} - \alpha_{\mathrm{Q}}(70\ \mathrm{°C} + 273.15\ \mathrm{°C})$
- $\beta_{\mathrm{T}} = \Delta T_{\mathrm{max@70\,°C}} - \alpha_{\mathrm{T}}(70\ \mathrm{°C} + 273.15\ \mathrm{°C})$

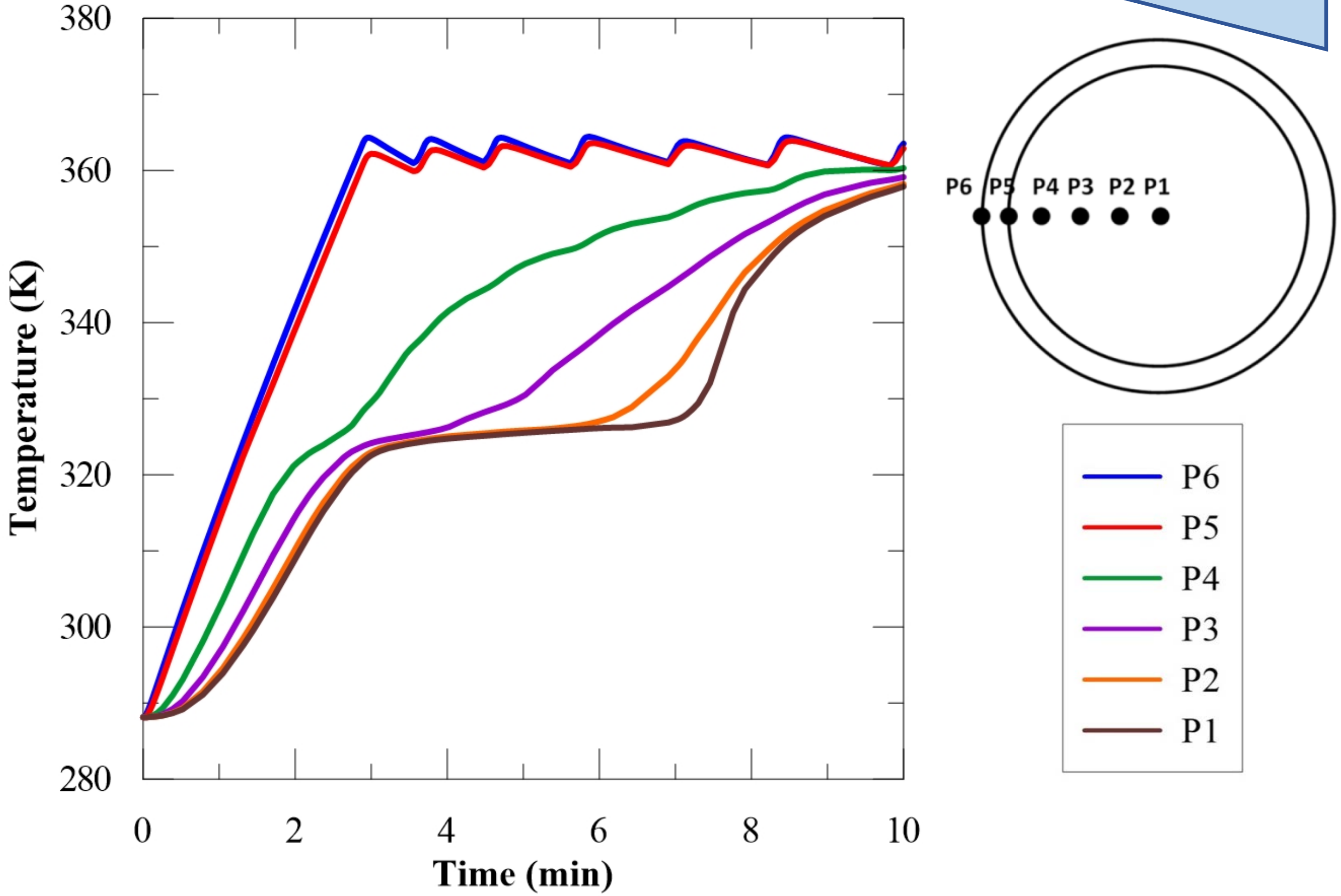
Results PCM Fusion

Numerical & experimental melt duration

PCM	Eicosane	Docosane	Myristic Acid
Experimental	~ 3 min	~ 4 min	~ 5 min
COMSOL	5.4 min	6.3 min	7.5 min
% Error	80 %	58 %	50 %
Sim. Time	54.7 min	74.3 min	52.6 min

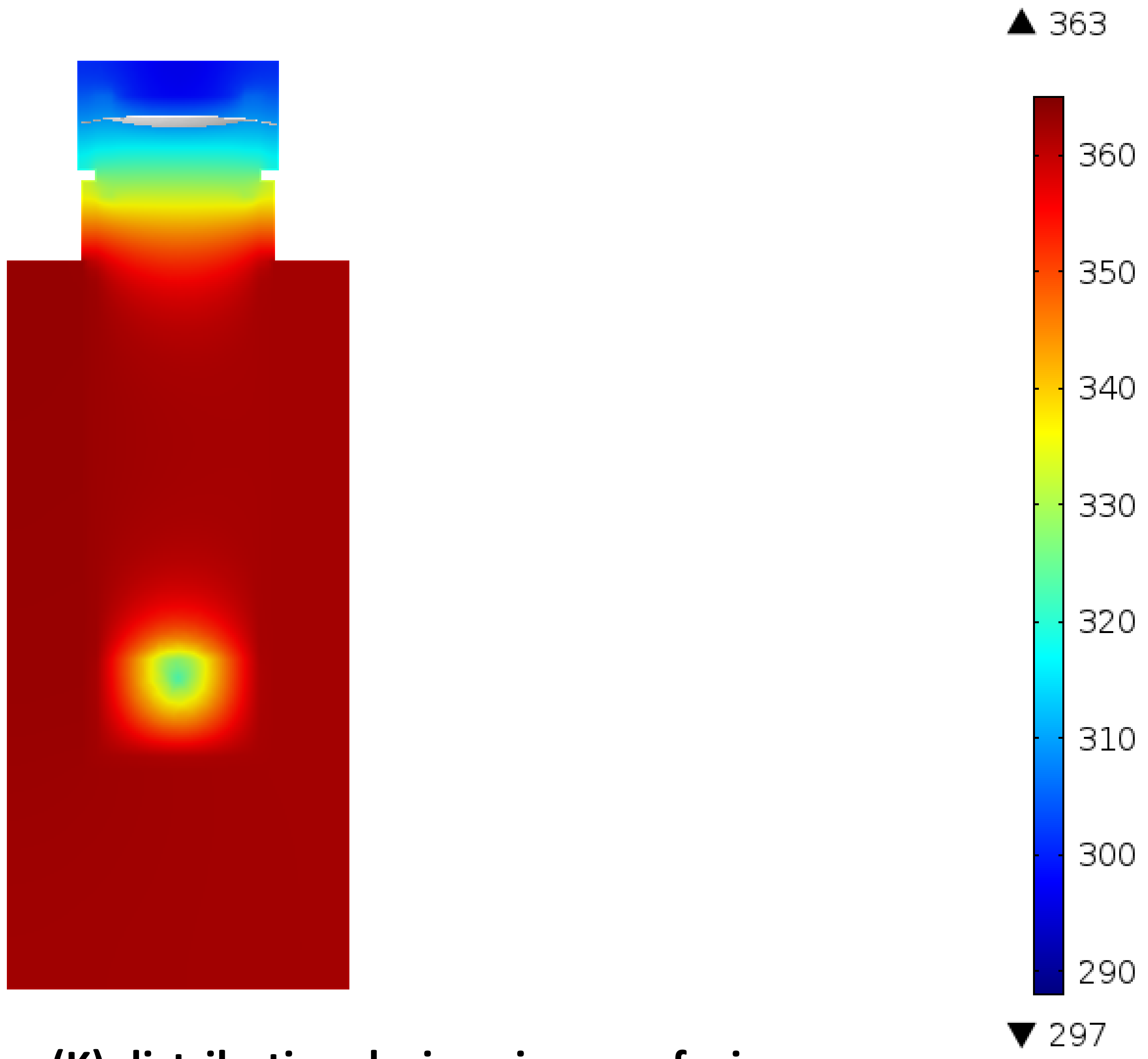
Primary errors:

- solid PCM body sinking within melted PCM (conservative approach)
- natural convection effects within liquid PCM



Myristic Acid melting (T_m = 54°C)

Results Fusion of Eicosane



Simulated temperature (K) distribution during eicosane fusion

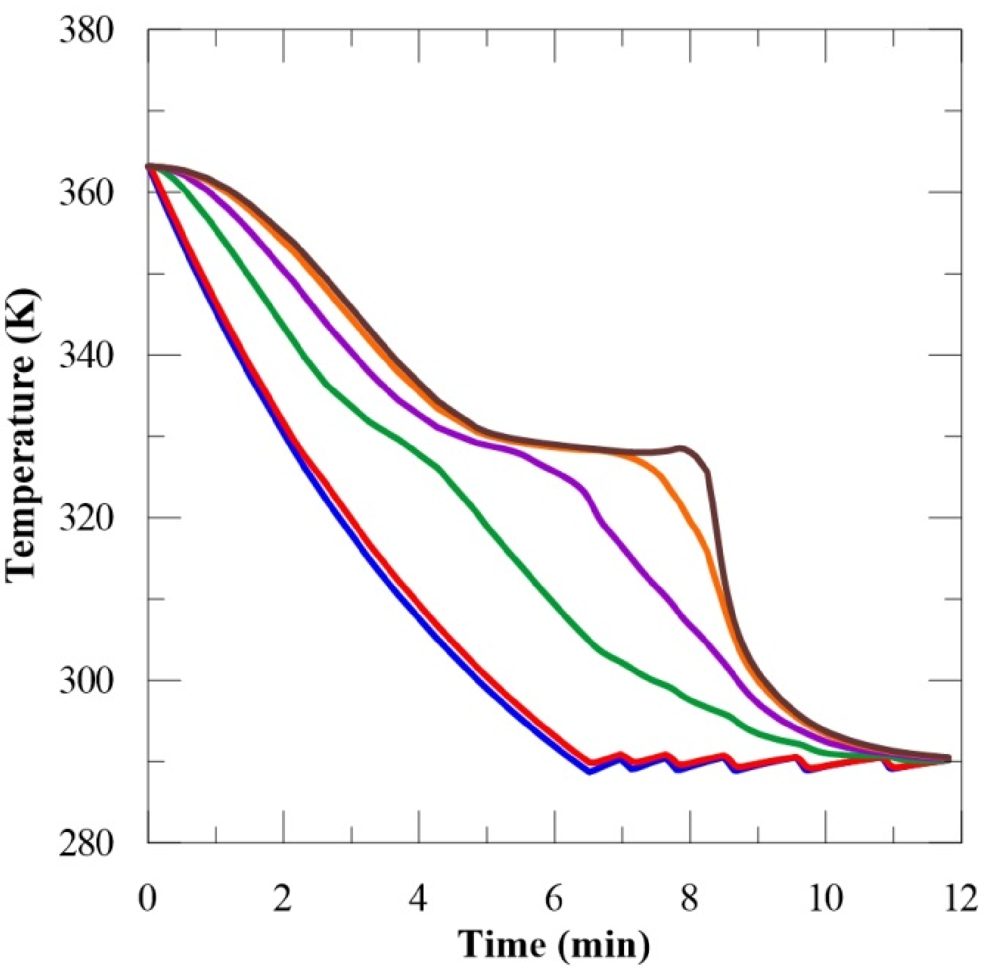
Results PCM Solidification

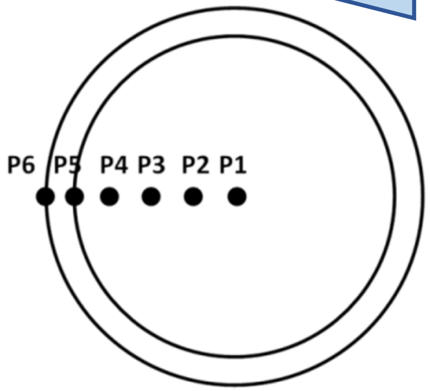
Numerical & experimental solidification duration

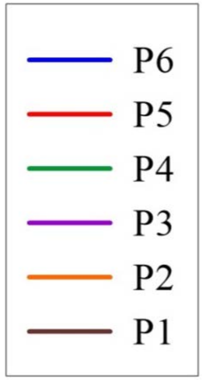
PCM	Eicosane	Docosane	Myristic Acid
Experimental	~ 10 min	~ 9 min	~ 8 min
COMSOL	10.9 min	9.6 min	8.3 min
Relative Error	9 %	6.6 %	3.8 %
Sim. Time	19.5 min	79.8 min	23.5 min

Primary error:

- natural convection effects within liquid PCM

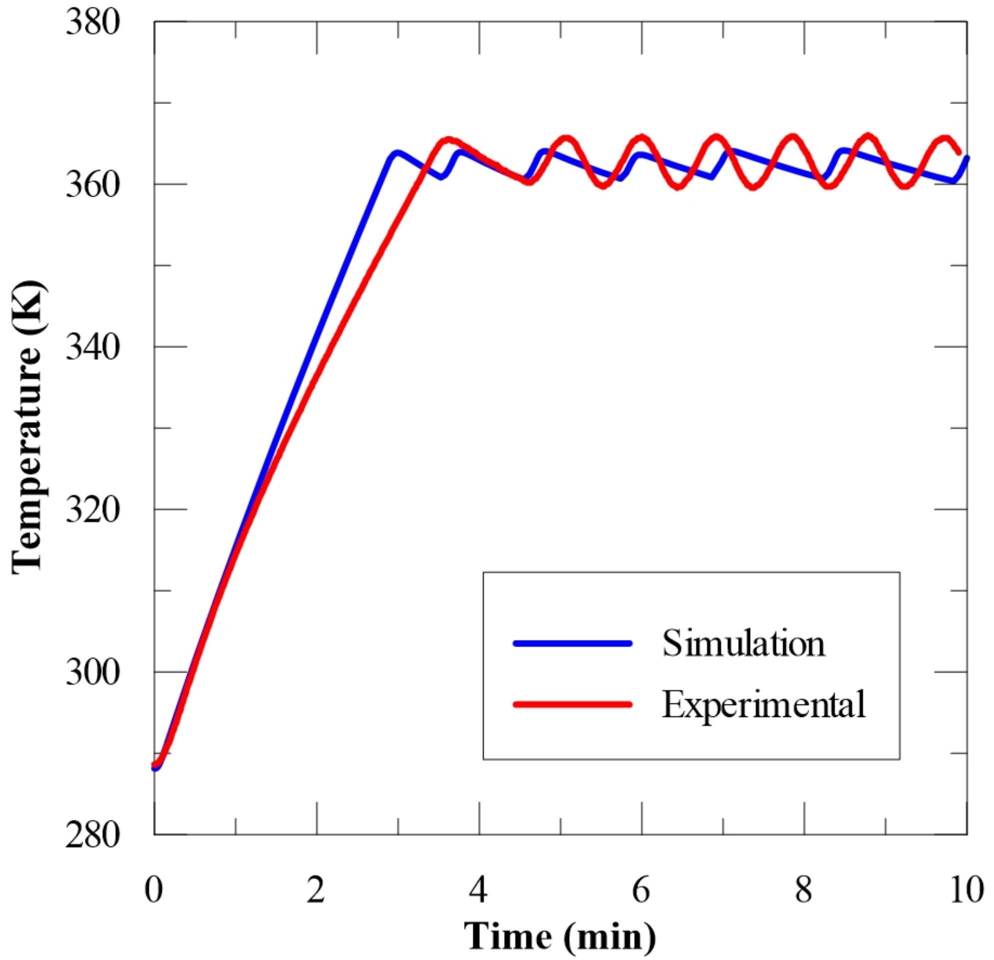




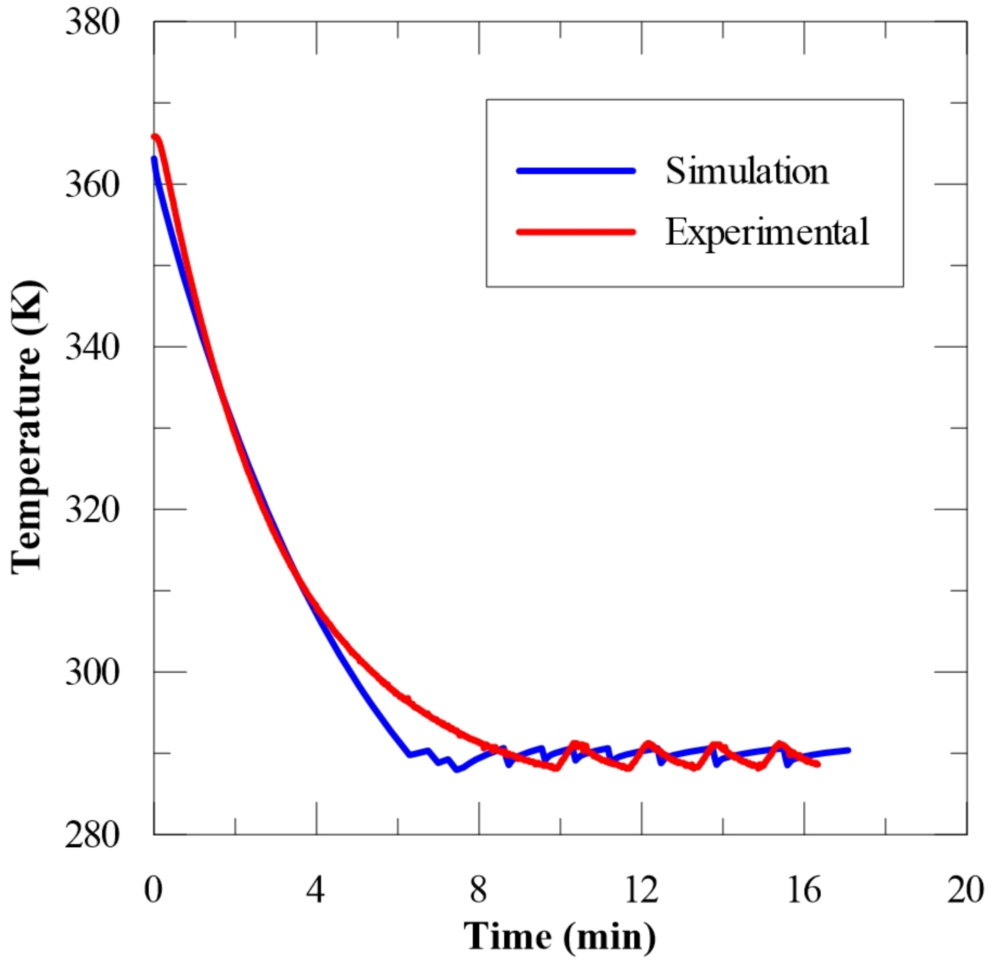


Myristic Acid solidification (T_m = 54 °C)

Results Housing Temperature



Numerical & experimental housing temperatures during heating process



Numerical & experimental housing temperatures during cooling process

Conclusions

Validation of thermal management components:

- full phase change within a desirable timeframe
- control system behavior
- prior to construction

Developed alternative ways to model:

- phase change
- ON/OFF temperature control
- thermoelectric cooling

Questions?

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COMSOL® Heat Sink & Fan

Convective heat loss from heat sink:

- $Q_{\text{conv}} = \frac{1}{2R_{\text{hs}}}(T_{\text{hs}} - T_{\infty})$

Thermal resistance during heating process:

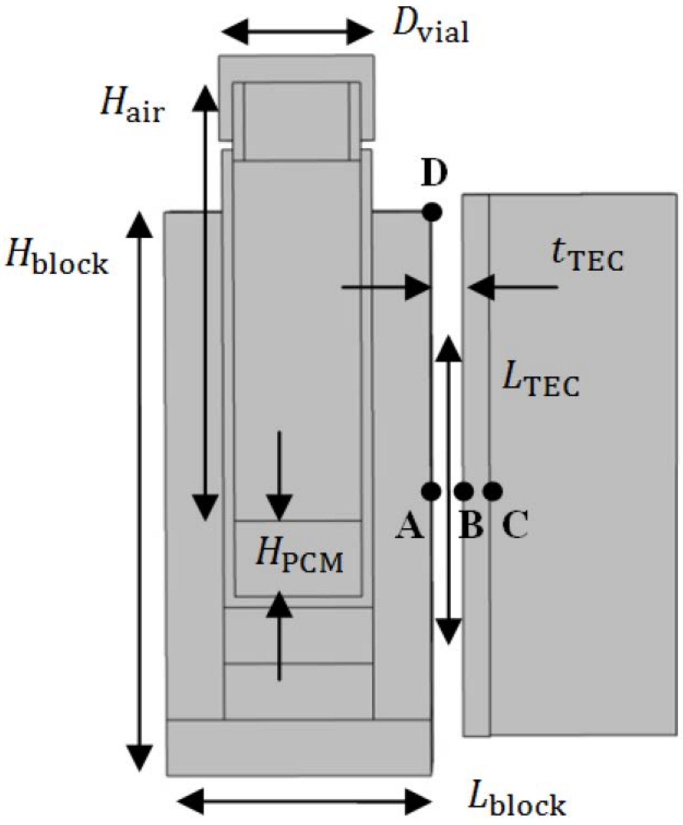
- $R_{\text{hs}} = R_{\text{n}}$

Thermal resistance during cooling process:

- $R_{\text{hs}} = R_{\text{n}} - (R_{\text{n}} - R_{\text{f}}) \cdot X_{\text{cool}}$

Conduction through thermoelectric module:

- $Q_{\text{cond}} = \frac{kA_{\text{TEC}}}{t_{\text{TEC}}} \Delta T_{\text{TEC}}$



COMSOL model cross-section