Simulation and Modeling of Reusable Phase-Change Packaging for Medical Applications

Akuratemp®

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Problem Statement

- Previous methods utilized by Akuratemp LLC calculated the latent heat needed by phase-change materials (PCM) in order to maintain specific internal temperatures of a shipped package while in transit.
- The goal was to reduce time and money needed to test these packages in a temperature chamber.
- An updated method was needed to calculate the holdover time instead of latent heat for the packages.

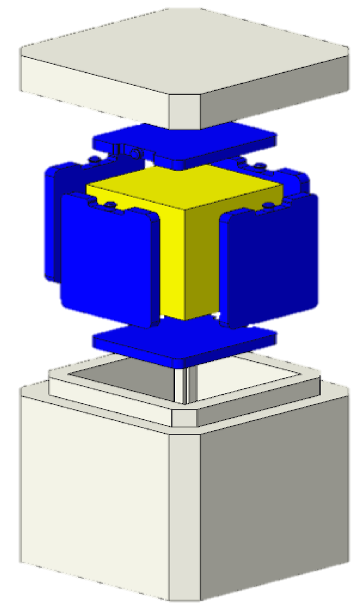


Figure 1. Final Shipping Container

Requirements

Table 1. Requirements Matrix

Number	Requirement Description	Value or Limit	Other Info
1	MATLAB-based code	High	Upgrade from Excel
2	Output is package holdover time	High	Provide an accurate result based on Akuratemp model
3	Develop a model in MATLAB	High	Start with 1D model, then 2D
4	Redefine thermal storage capacity of PCM used	High	Improved accuracy in calculations
5	Use thermal and heat transfer formulas for PCM	High	Phase change strictly between solid-liquid states
6	Include thermal properties of the insulation material	High	Polyurethane Foam (PUF)
7	Add additional parameters	Med	Switch container size and PCM

Concepts

- Concept 1 utilized Microsoft Excel and heat transfer equations to calculate holdover time.
  - Excel File calculated heat flow through each face of the insulating box made of Polyurethane Foam (PUF) but proved inaccurate.

Convection: $q = h_c A \Delta T$

Heat Transfer: $\dfrac{T_\infty - T_{in}}{\dfrac{1}{h_{out}A} + \dfrac{l}{kA} + \dfrac{1}{h_{in}A}}$

Fourier's Law: $q = -k\Delta T$

Table 2. Calculated vs Actual Holdover Time

Test Number	PCM Type	Latent Heat (J/kg)	PCM Quantity (kg)	Width (m)	Length (m)	Height (m)	Wall Thickness (m)	Holdover Time (h)	Actual Time (h)
1	HS26N	210000	4.5	0.38	0.38	0.38	0.05	22.52	30
2	HS26N	210000	9	0.46	0.46	0.46	0.05	31.28	37
3	HS26N	210000	9	0.51	0.51	0.51	0.08	33	24

- Concept 2 revolved around creating a MATLAB code that uses more complex, physics-based solutions along with the enthalpy method to simulate heat flow as a function of time.
- Concept 3 was added in a later stage in order to use the Stefan problem to calculate the transition of the PCM as it melts.
  - This was added to the code that focused on concept 2 in order to compare the two methods and verify results.

Final Design

Phase 1: Heat Conduction Partial Differential Equation (PDE)

- This phase incorporates the temperature difference between the PCM inside the package and the ambient, outside temperature.
- It is a representation of thermal conduction in a multi-component material system with varying thermo-physical properties.
- The equations simulate the temperature change as a function of time at points throughout the package.
- The PDE given below was solved numerically by using Finite Volume Method (FVM). The code is an extension of the FVTool, a toolbox for MATLAB
- This part of the code does not have any phase change considerations; it only shows the mechanisms of the heat transfer inside the package.

Heat Conduction in Multi-Component Material System

$$\rho Cp \frac{\partial T}{\partial t} + \nabla(-k\nabla T) = S_T$$

Transient Term: $\rho c_p \frac{\partial T}{\partial t}$

Heat Conduction Term: $\nabla(-k\nabla\emptyset)$

Heat Generation Term: S_T

Boundary Conditions: $a\nabla Te + bT = c$

Contours of temperature: $T_i = 20°C$

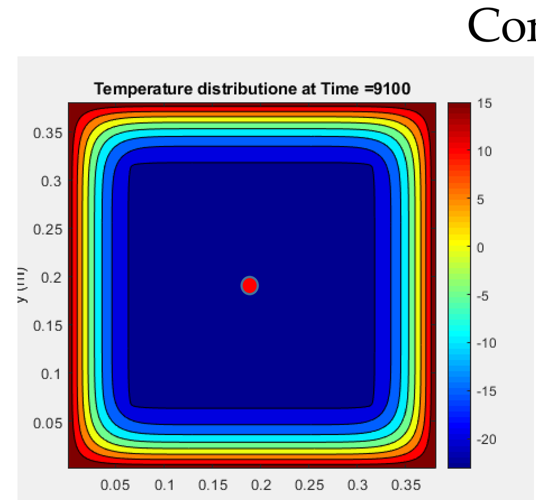


Figure 2. Thermocouple Location

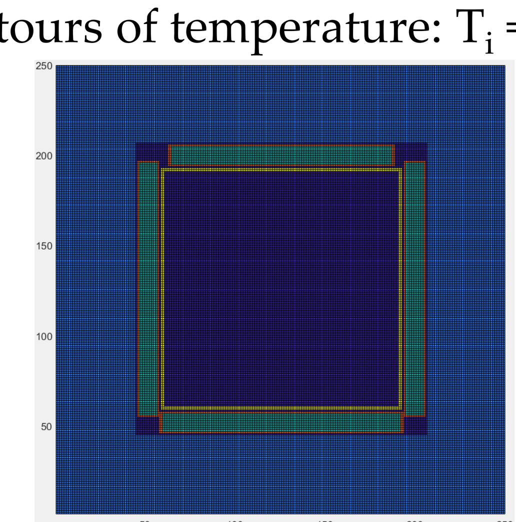


Figure 3. Mesh Grid of Package Geometry

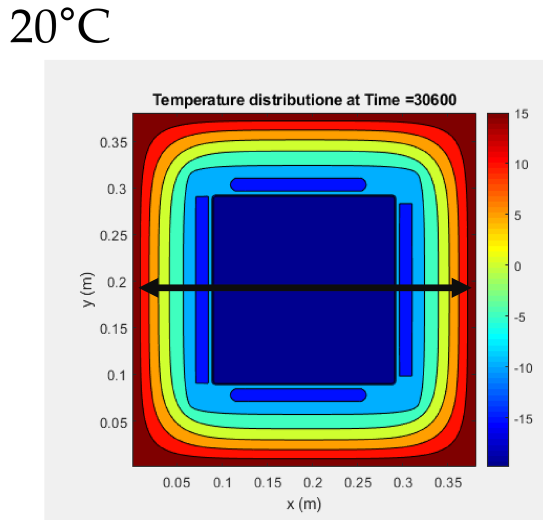


Figure 4. Profile Line

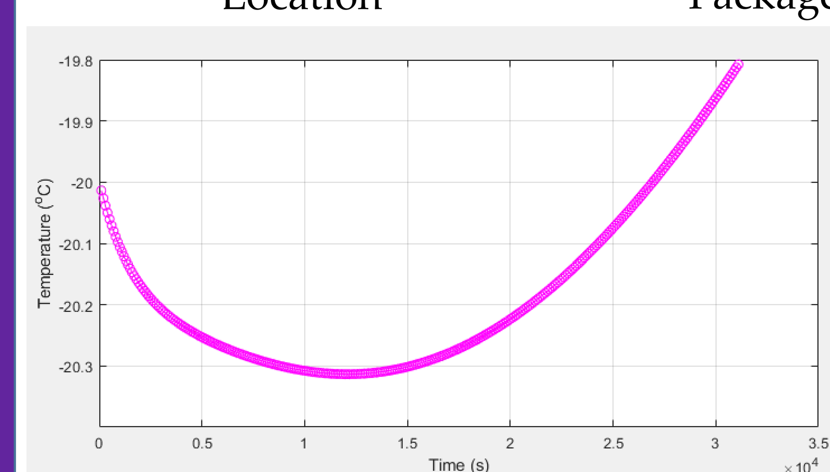


Figure 5. Temperature vs. Time at Thermocouple Location

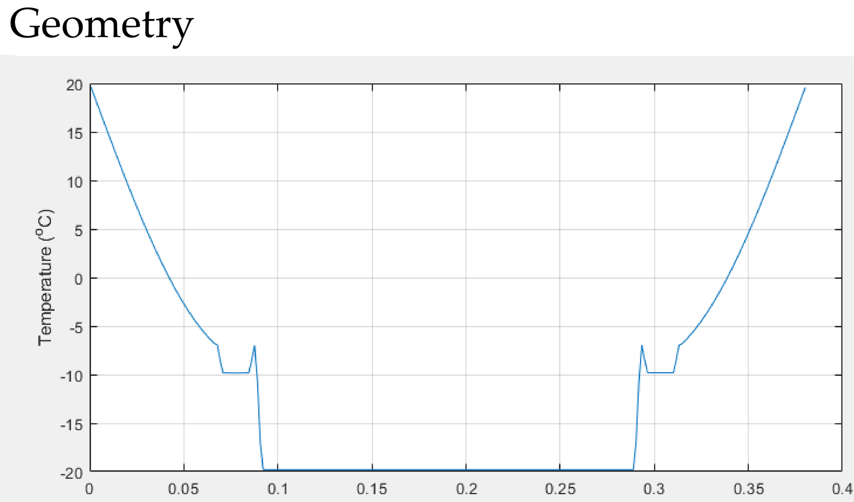


Figure 6. Temperature vs. Distance along Profile Line

Phase 2: Enthalpy Method and Stefan Problem

- In order to get accurate results, the heat transfer altered by phase change should be considered; the enthalpy method was added to accommodate for the transition of the PCM as it melts.
- This phase solves the problem using a 2D model; however, the convective motion due to the liquid part of the PCM is not considered due to complexity.
- This approach is validated against a 1D Stefan problem, and good agreement is achieved between analytical solution of the Stefan problem and the current phase field model for the materials properties obtained from Akuratemp LLC.

Results

Stefan Problem

Heat Equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \quad \text{in } \{T(x,t) : 0 < x < s(t), t > 0\}$$

Stefan Condition

$$\beta \frac{ds}{dt} = -\frac{\partial T}{\partial x}(s(t), t), \qquad t > 0$$

Enthalpy Method

Conduction

$$\rho C_p \frac{\partial T}{\partial t} = \nabla * (K\nabla T) + Q$$

Source Term

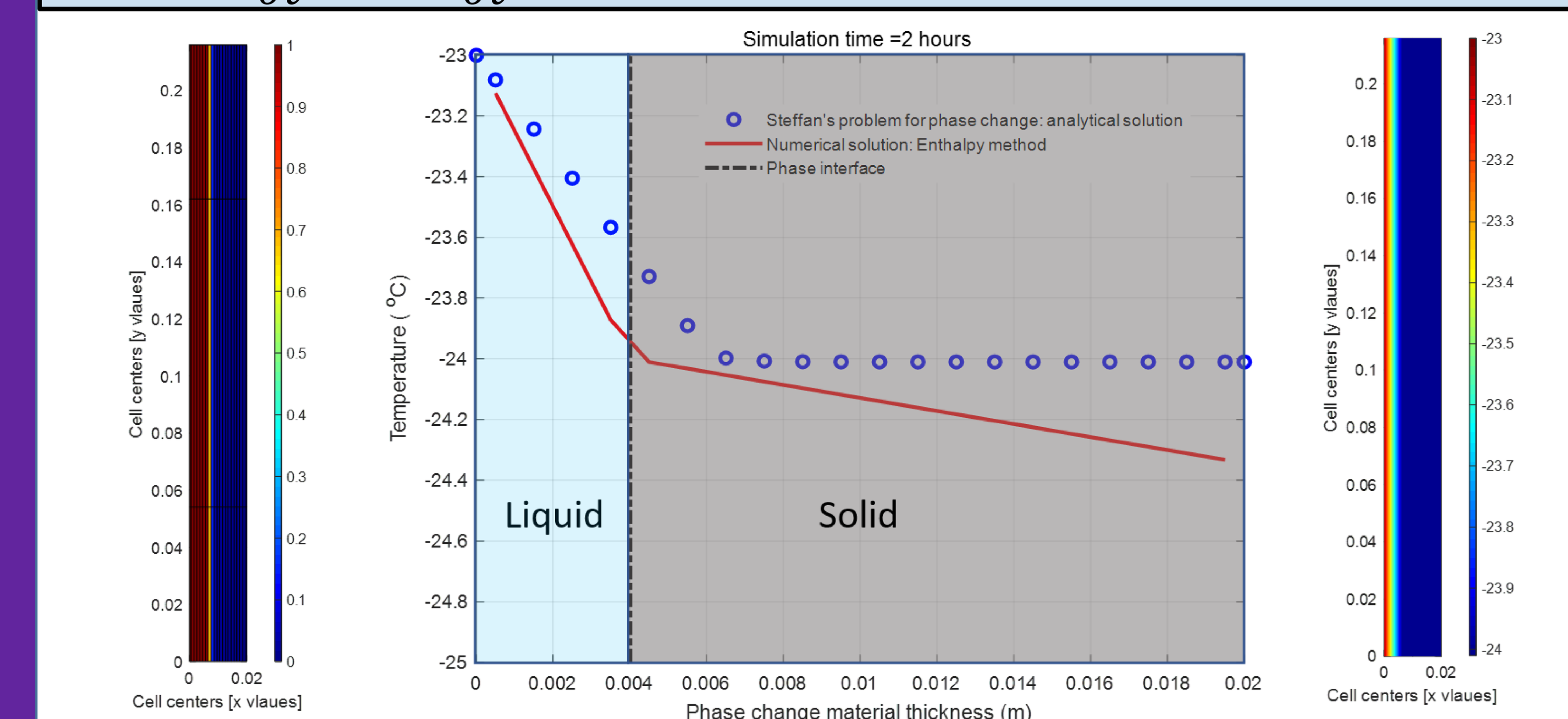
$$Q = -\frac{\partial(\Delta H)}{\partial t} = \frac{\partial(\rho L l_f)}{\partial t}$$

Enthalpy

$$\Delta H = c_p T + L l_f^{n-1}$$

Liquid Fraction

$$l_f = \begin{cases} 0 & \text{if } \Delta H < \Delta H_s = c_p T_m \\ \frac{\Delta H - \Delta H_s}{\Delta H_l - \Delta H_s} & \text{if } \Delta H_s < \Delta H \le \Delta H_l = \Delta H_s + L_m \\ 1 & \text{if } \Delta H \Delta > \Delta H_l \end{cases}$$



Summary

- Three concepts were tested and compared:
  - Simple heat transfer equations in Excel were fast, but not efficient enough to accurately predict holdover time.
    - Physics-based heat transfer models, like the enthalpy method, are required to get an accurate result.
  - Transient thermal diffusion equations and the enthalpy method is used to simulate the internal temperature of the package while the PCM melts via 2D model.
  - Enthalpy method was used along with a one-dimensional Stefan problem to verify results.

Team & Acknowledgements

- Arturo Adame-Nava, B.S.E.; Luis Martinez Gonzalez, B.S.E.; Luke Meares, B.S.E.; Ulises Ortiz Vargas, B.S.E.
- Mentor: Dr. Hayri Sezer

- Capstone Sponsor: Harshul Gupta

Sources:

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