Using Thermal Simulation to predict thermal performance of Temperature Controlled Packaging

Thermal Management Expo 2022

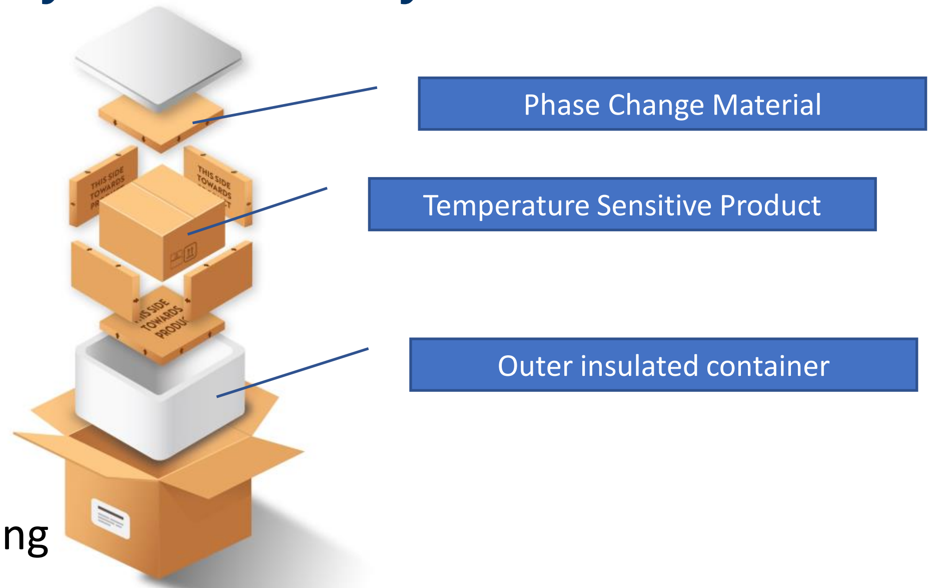
Iftekhar Ahmed

Director, Thermal Engineering

CAVU Group

Protecting Temperature Sensitive Pharmaceuticals

- Temperature controlled transportation of pharmaceutical, biological and active ingredient products
- Cold chain products have different temperature criteria
  - Refrigerated - 2ºC to 8ºC
  - CRT – Controlled Room Temperature -15ºC to 25ºC (typical)
  - Frozen – Below -20 ºC (typical)
- Maintaining temperature control during transportation events, ensures product stability and efficacy



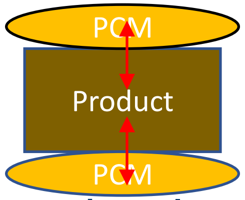
Temperature Controlled Packaging

Thermal Physics of Temperature Controlled Packaging

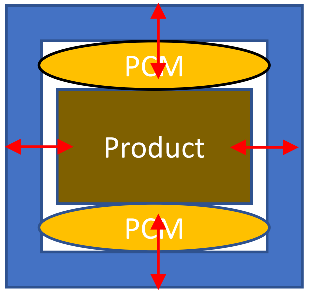
- Heat transfer in TCP (Temperature Controlled Packaging) takes place due to Conduction, Convection and Radiation.
- The effect of radiation is minimal and is usually not considered in thermal modeling.
- Convection becomes significant based on the amount of air present in the packaging.
- Conduction is the dominant mode of heat transfer.
- Phase change from solid/liquid and liquid/solid occurs due to the presence of Phase Change Materials.

Thermal Physics of Temperature Controlled Packaging

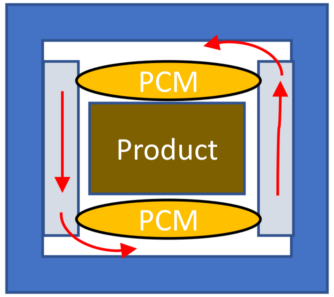
- How do the modes of heat transfer apply in TCP design?
  - Product in contact with PCM gels (conduction)



  - Heat transfer through an insulated wall (conduction)



  - Ribs in containers promoting airflow (convection)



The Need for Thermal Simulation of TAP

- Thermal design of TCP (Temperature Controlled Packaging) can be a complex exercise; following factors drive the design process
  - Product temperature requirements i.e Refrigerated, CRT or Frozen
  - Total duration the packaging is expected preserve product temperatures
  - Ambient conditions in the transportation lane
  - Use of passive, active or hybrid systems for maintaining temperatures
  - Product characteristics i.e. density, thermal conductivity and specific heat
- Thermal physics in a TCP involves multiple physical phenomenon
  - Conduction
  - Phase Change
  - Convection
  - Radiation
  - Transient Thermal Response

The Need for Thermal Simulation of TCP

Without Simulation: Customer Requests → Concept Design → Build Prototype, followed by testing (iterative) → Production

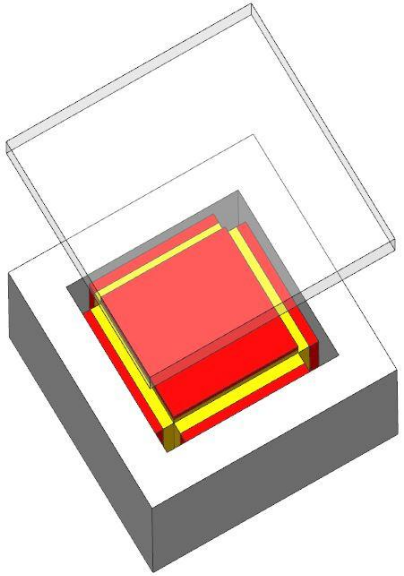
A single <u>build/test iteration</u> typically takes <u>weeks or months</u>

With Simulation: Customer Requests → Concept Design → Thermal Simulation → Final Testing → Production

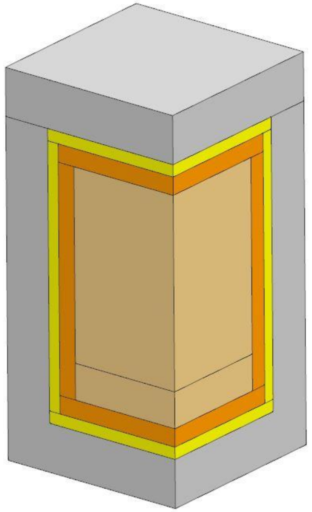
A single <u>simulation iteration</u> typically takes <u>hours</u>

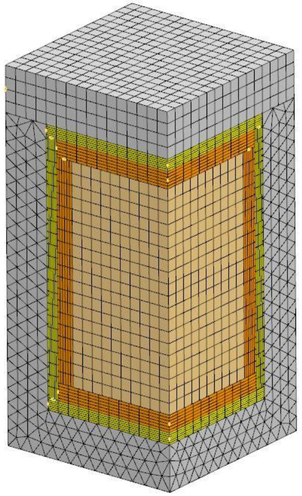
Developing a Thermal Simulation Model

Create 3D Solid Model



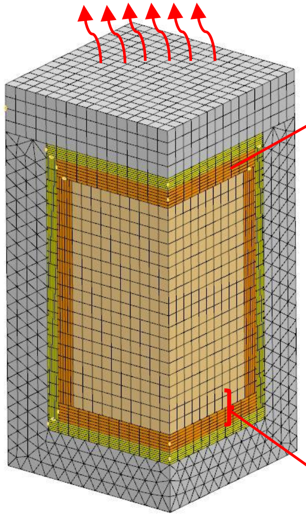
Apply geometric and
physics symmetry





Create a Finite
Element Model

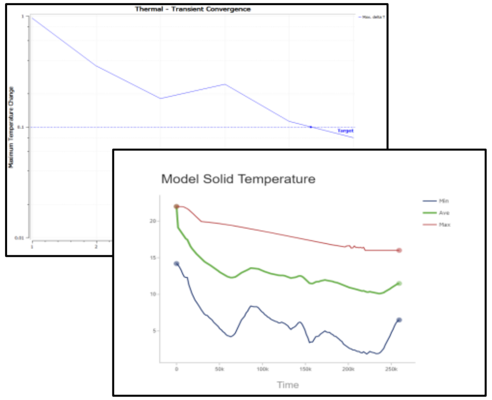
Convection to Ambient



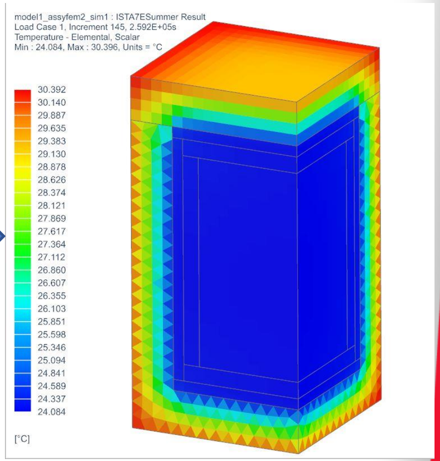
Ti =22^{o}C

Thermal
Contact

Apply Boundary
Conditions



Solve for Transient
Thermal Response



Results:
Temperatures
Heat Fluxes
Phase Quality

Numerical Approach to Thermal Analysis

- The Numerical approach is a variation on the Finite Element Method, which is used to solve the three-dimensional heat conduction equation, shown below

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right) + q_v$$

where:

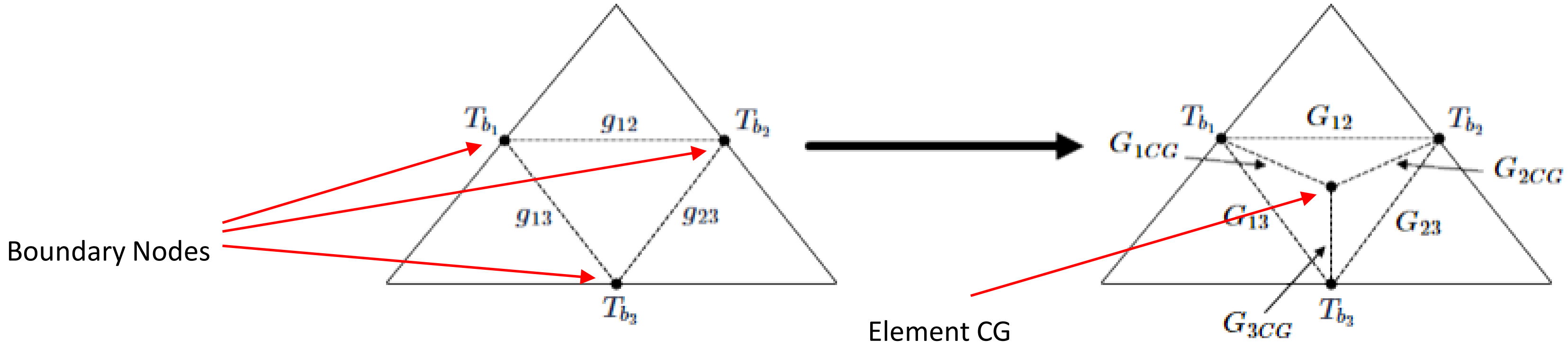
- ρ is the material density.
- c is the specific heat capacity.
- k is the thermal conductivity, where subscripts x, y and z are the anisotropic specifications in space directions.
- q_v is the heat generation per unit volume.

- The 3D heat conduction formulation is solved by integrating it over the domain or control volume under consideration

$$\underbrace{\int_A q_n da}_{\text{Heat flow across CV boundaries}} + \underbrace{\int_V q' dV}_{\text{Heat generation in CV}} = \underbrace{\int_V \rho c \frac{\delta T}{\delta t} dV}_{\text{Change of energy in CV}}$$

Numerical Approach to Thermal Analysis

- This approach considers a finite element as a control volume and develops a conductance network based on boundary mid points and element Center of Gravity



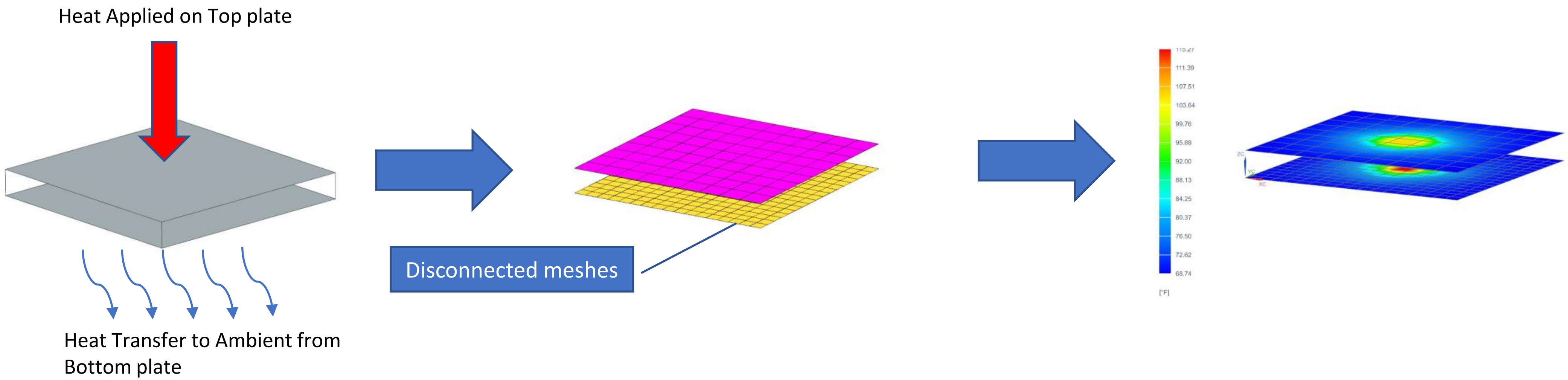
- The integral formulation of the 3D conduction equation can be expressed in terms of the Finite Control Volume approach as follows:

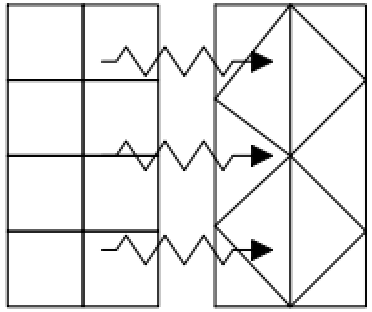
$$\underbrace{\mathbf{Q}_i}_{\substack{\text{Heat generation}\\ \text{in CV}}} + \underbrace{\sum_j [\mathbf{G}_{ij} \ \mathbf{x} \ (\mathbf{T}_i - \mathbf{T}_j)]}_{\substack{\text{Heat flow across}\\ \text{CV boundaries}}} = \underbrace{\mathbf{C}_i \frac{\mathbf{dT}_i}{\mathbf{dt}}}_{\substack{\text{Change of}\\ \text{energy in CV}}}$$

- FCV approach is more robust, less dependent on element shapes, provides flexibility and ease of use in creating thermal connection. Heat transfer is not dependent on nodal continuity. Conservation of Energy is applied on each elemental control volume, unlike FEM.

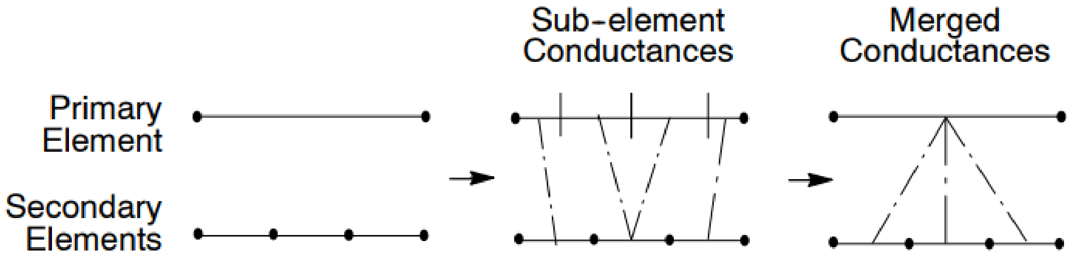
Numerical Approach to Thermal Analysis

- Thermal solver allows the user to define heat flow between disconnected meshes, this approach is known as a Thermal Coupling. Thermal couplings can be established between any two sets of elements





A Thermal Coupling is a conductance between unconnected elements with dissimilar meshes. It is an additional heat path through which heat may flow. Normally, thermal couplings connect adjacent parallel surfaces or edges. Conductance value is based on element area and a user specified parameter

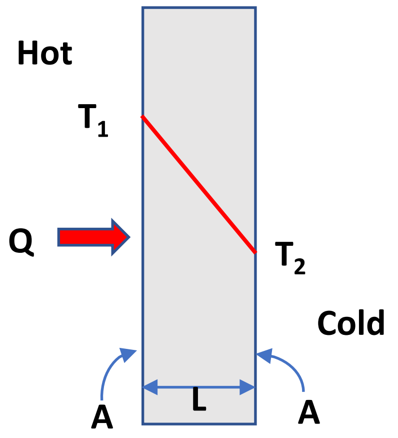


Impact of Mesh Density on Model Accuracy

- Heat Conduction physics is a **linear function** as expressed by Fourier's law

$$\frac{Q}{t} = \frac{kA\,\Delta T}{L}$$

- Q/t = Heat energy per unit time
- K = thermal conductivity
- A = Area of crossection
- L = Thickness
- Δ T = Temperature Difference (T_1- T_2)

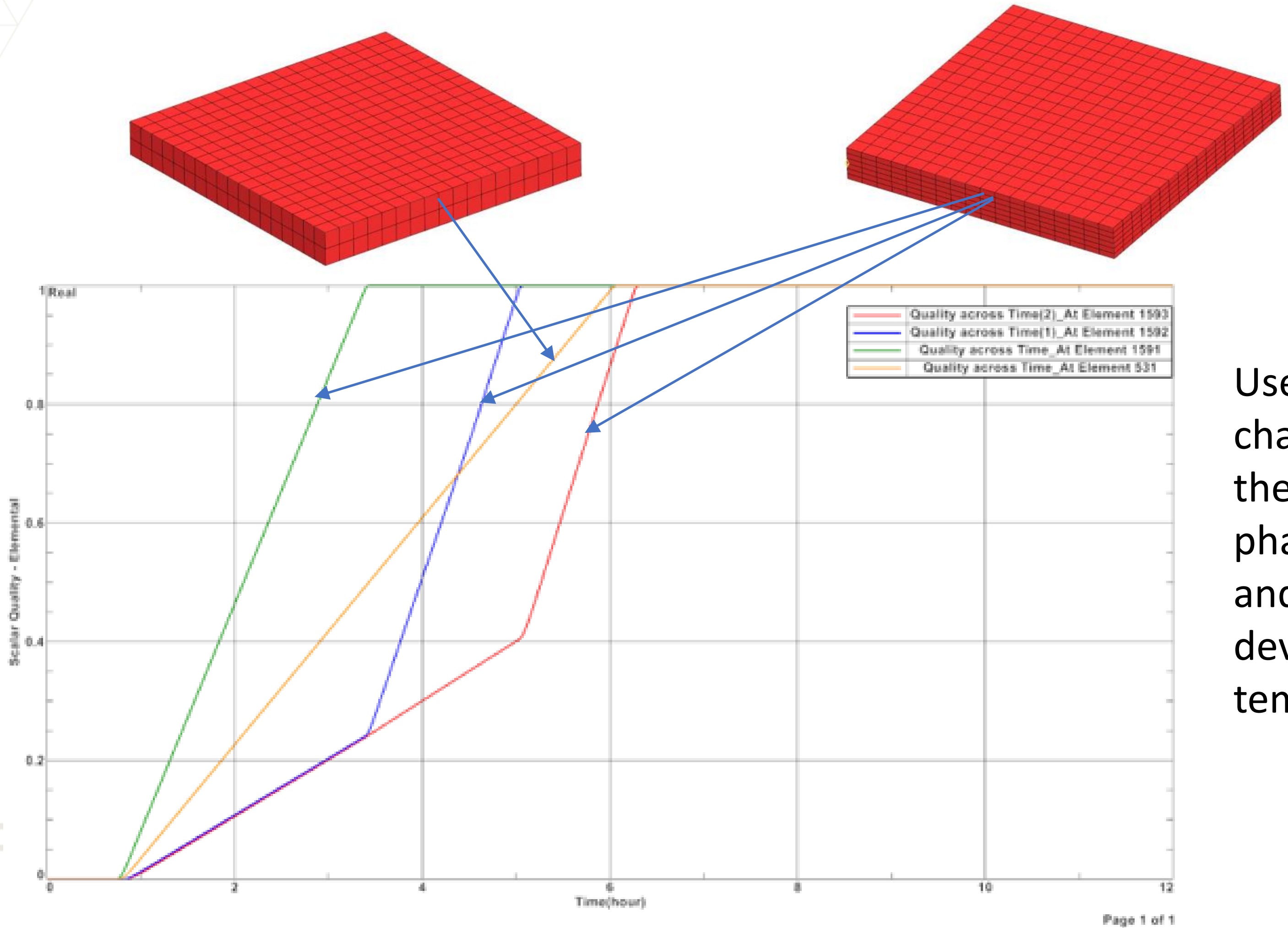


- Two temperature calculation points or nodes, say between two surfaces is enough to get accurate results.

- Non-linear heat transfer will require higher mesh density for higher accuracy
  - Convection
  - Radiation
  - Phase Change

Phase Change Accuracy

- Phase Change physics is dependent on mesh density; a coarse mesh will not model the phase change front accurately
- Phase Quality represents state of PCM between solid and liquid, 0 = fully solid, 1= fully liquid



Use of coarse mesh does not capture the change in phase quality as accurately along the thickness of the PCM. Correctly capturing phase change behavior, including phase change and warm up/cool down times is KEY to developing a thermal model that correctly predicts temperature distribution in a shipping system.

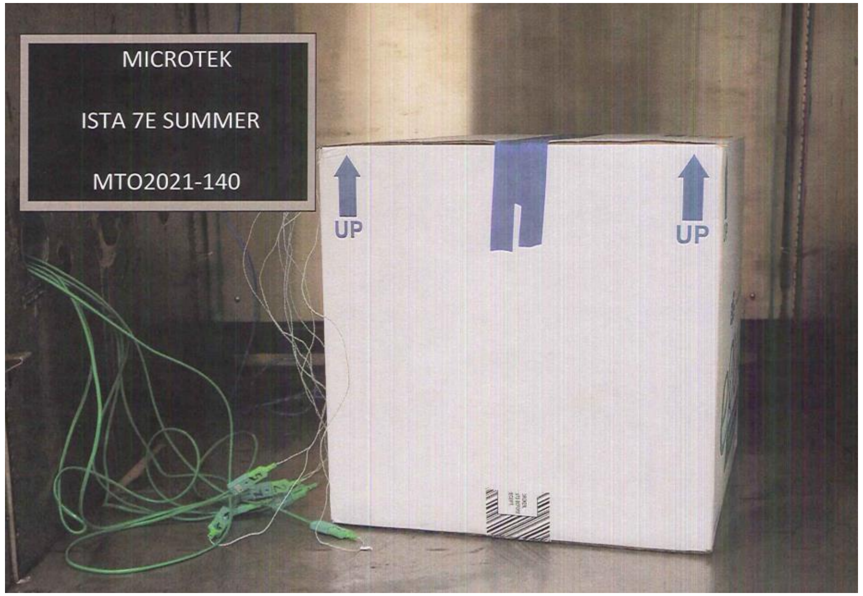
Case Study- Description

- A temperature controlled packaging system was used to develop a thermal simulation model
- Packaging system was tested in a thermal chamber and product temperatures were obtained over a period of time
- The packaging system utilized PCMs for temperature control of the product, product temperatures are to be maintained between 15ºC to 25ºC.
- Product consisted of 10 ml vials with water fill
- Packaging system was tested using a standard ISTA 7E Summer profile for 72 hours
- Packaging system specifications:
  - Product description
    - 60 vial cartons (1.5”x1.5”x2”) - Vials are glass with a liquid fill volume of 10- mL and a twist-on cap - Each weighs 28.9 g
  - Phase Change Materials
    - 6 x PCM panels, positioned on each side of the product, conditioned at 22ºC
  - EPS insulated container
    - OD = 16.2”x16.2”x16.2”, wall thickness = 2.5”
  - Thermal Test Profile
    - ISTA 7E Summer Profile
    - Duration 72 hours

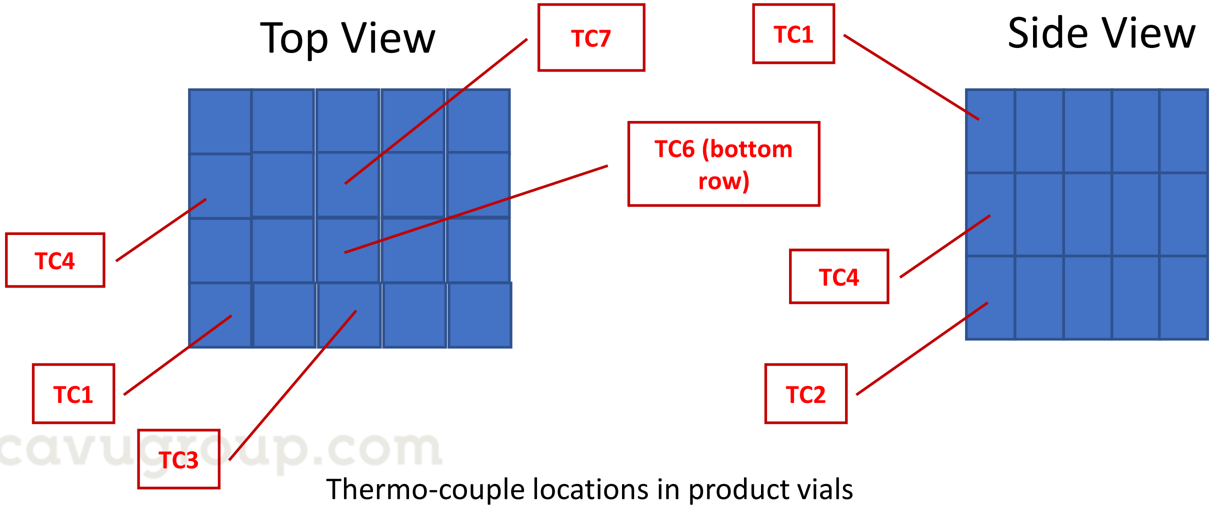
Case Study- Test Setup

Product vial placement in shipper

PCM placement in shipper



Shipper located in thermal chamber



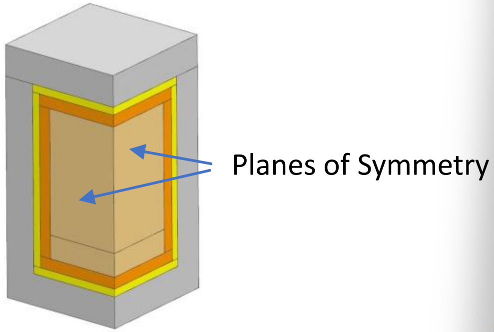
Thermo-couple locations in product vials

Thermo-couple Locations

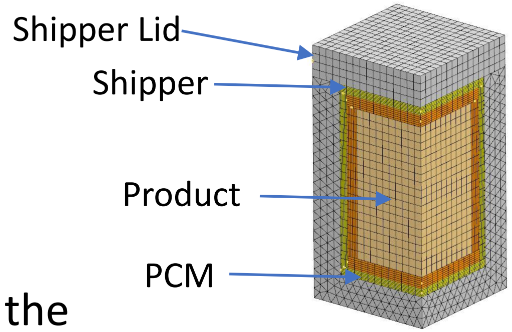
- TC1 – Top Left Corner
- TC2 – Bottom Left Corner
- TC3 – Top Side Center
- TC4 – Left Side Center
- TC6 – Bottom Center
- TC7 – Top Center

Case Study- Simulation Model

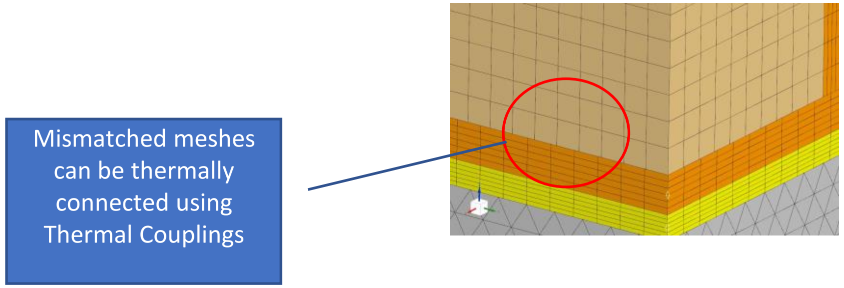
- The insulated shipper assembly was modeled as a 3D CAD assembly model
- In order to reduce computation time, a quarter symmetry model was created along planes of symmetry for geometry and thermal physics
- The CAD assembly is then used to develop a Finite Element assembly model. Assembly FEM consists of independent FEMs which are assembled based on the parent assembly geometry
- Component FEMs in the assembly are defined with thermal material properties, including:
    - Density
    - Specific Heat
    - Thermal Conductivity
    - Latent Heat
    - Phase Temperature
- From the assembly FEM of the model, a simulation model is created, wherein the the thermal boundary conditions are defined, including
    - Thermal couplings – to define conduction between different components e.g. Product to PCM, PCM to PCM, PCM to Shipper etc.
    - Initial Temperatures on Product, PCM and Shipper
    - External Convection to Ambient
    - Ambient Profile – ISTA 7E Summer



Quarter Symmetry Model

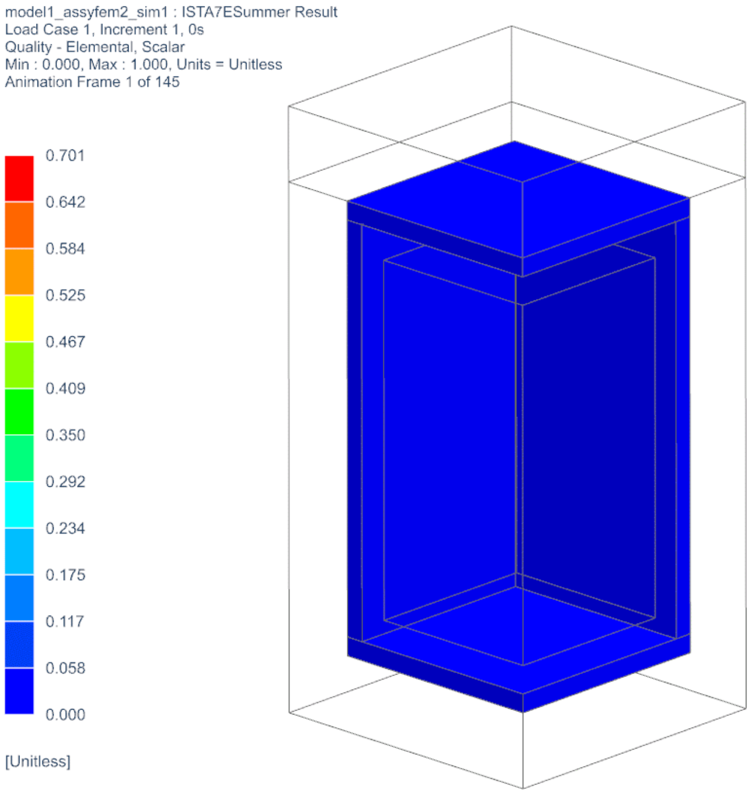


Assembly FEM

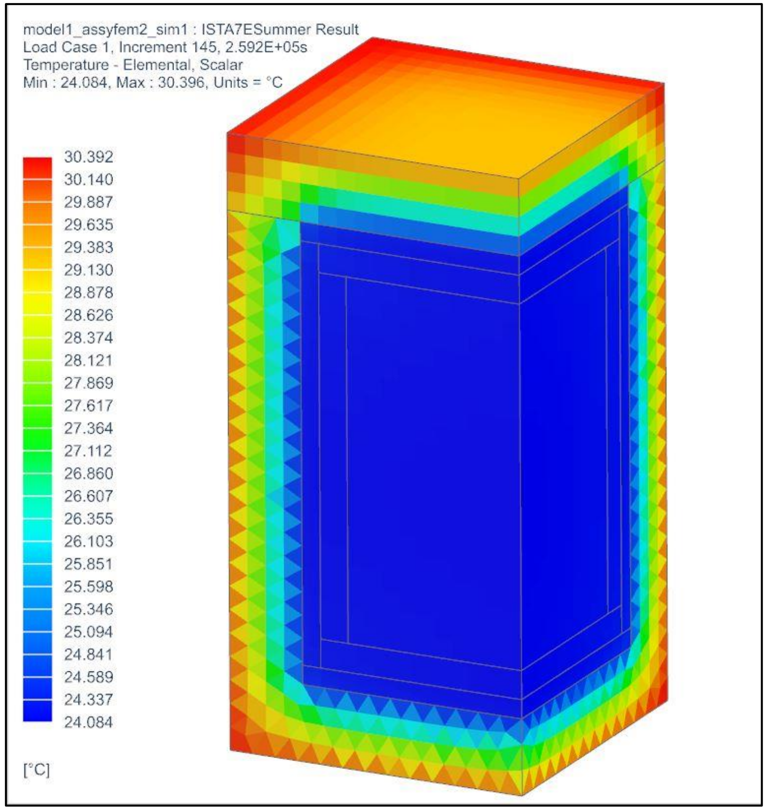


Case Study- Simulation Model

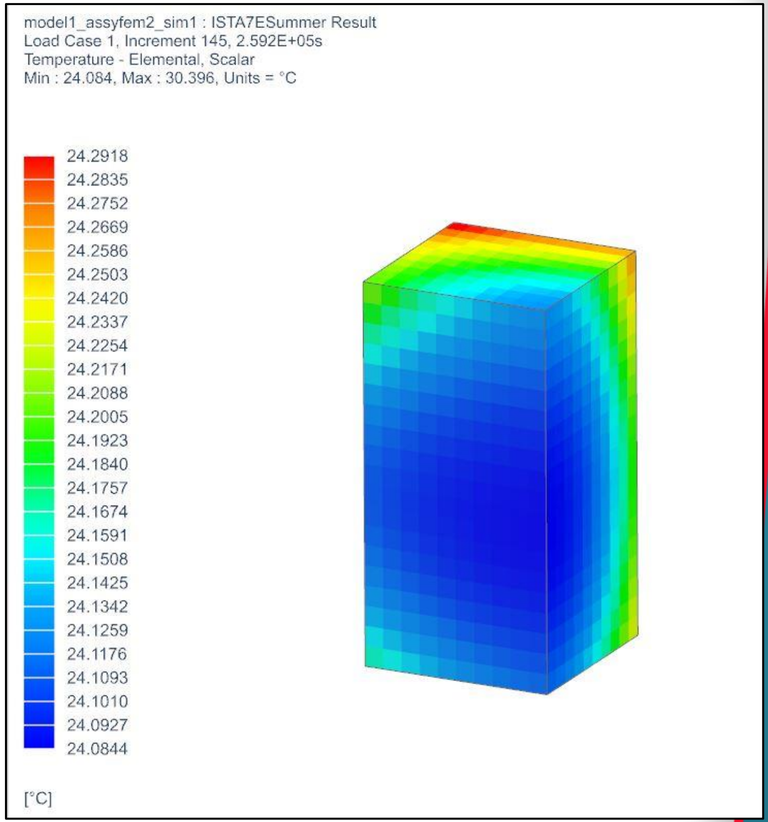
- The simulation model is solved as a Transient analysis, i.e. the FEM is solved for temperatures over the entire assembly as a function of time
- Results are recovered as elemental temperatures over the entire FEM assembly
- Secondary results such as phase quality and heat fluxes are also recovered



PCM Quality Plot

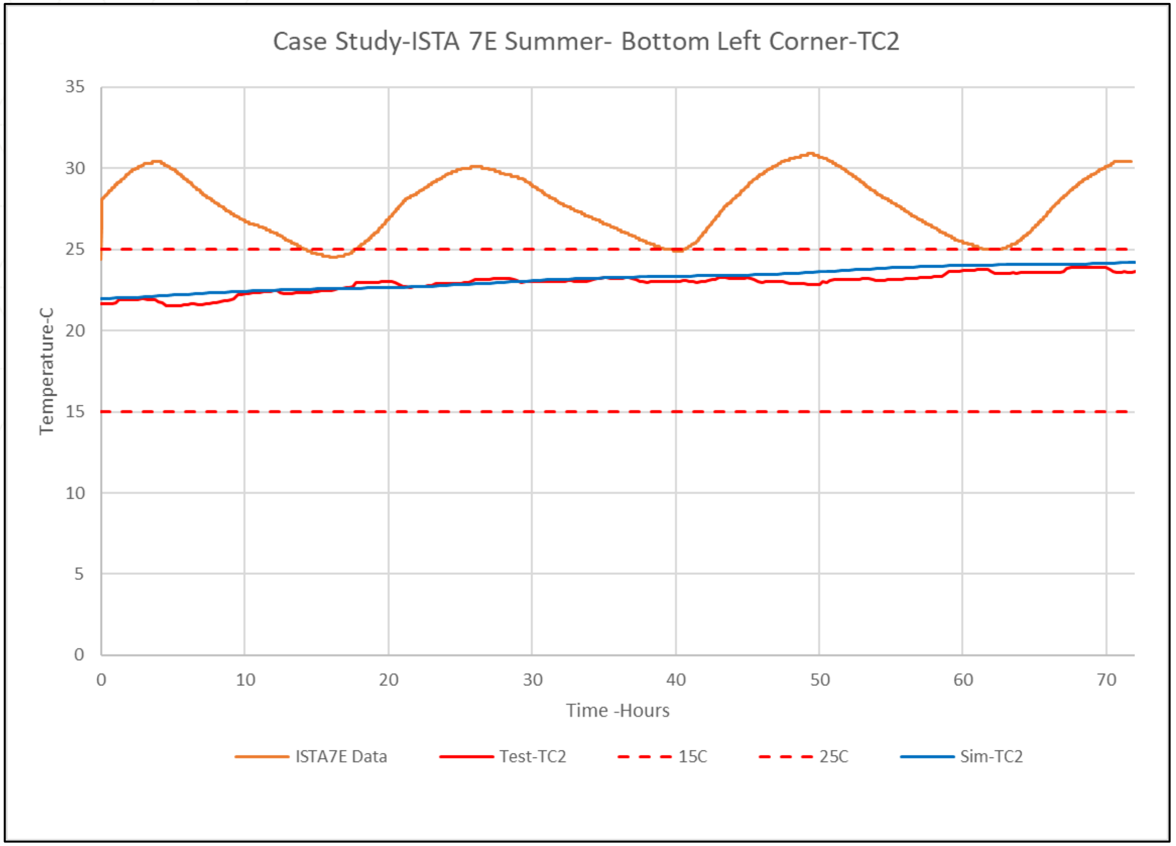


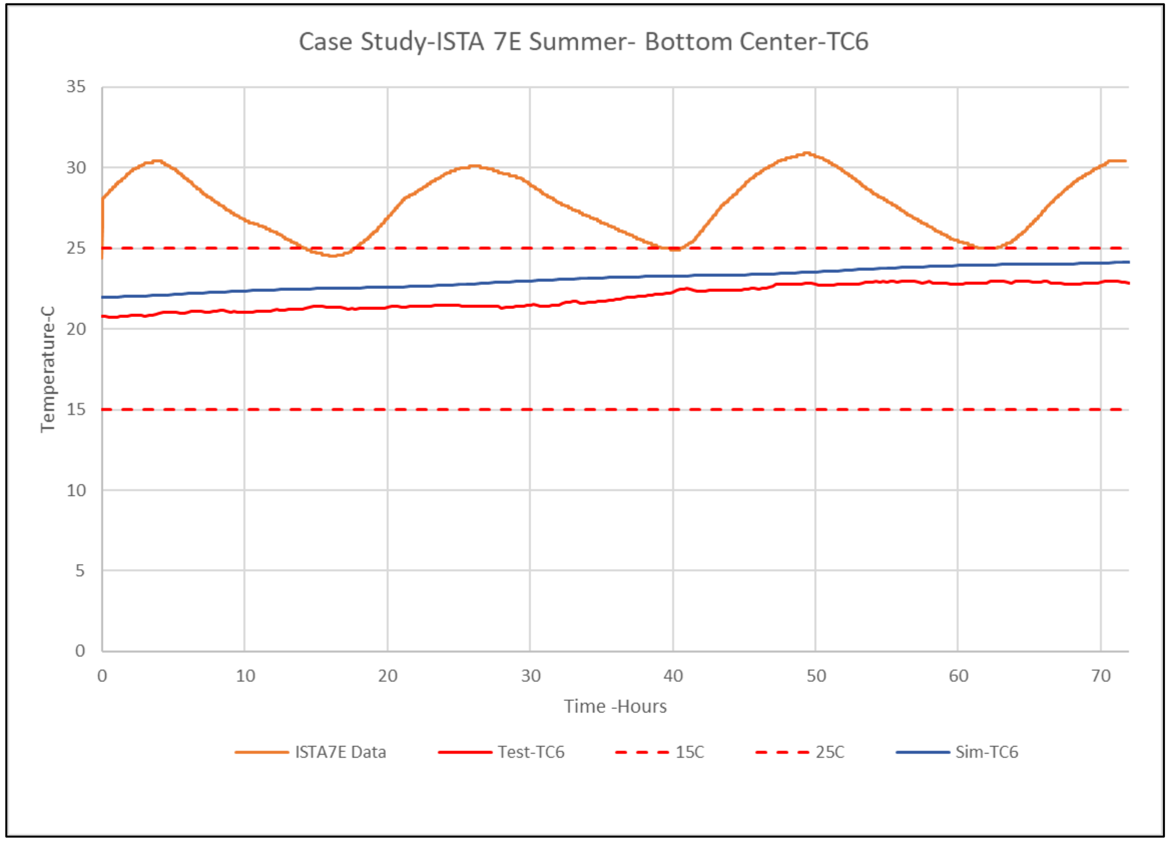
Temperatures on shipper assembly



Temperatures on product

Case Study- Results Comparison





TC 2 location shows good correlation between test and simulation, similar results for TC1 and TC3

TC6 location shows test data generally colder than the simulation results, similar results for TC7

Case Study- Conclusions

- There is generally good correlation between test and simulation results
- For TC4, TC6 and TC7 the difference between test data and simulation is higher, with TC6 (Bottom Center) being the largest difference
- These 3 TCs are running colder than prediction by simulation. Likely reason is the non-uniform distribution of PCM is pouches, where are represented as uniform cuboids in simulation model.
- Model can be made more accurate by determining PCM distribution and surface contact during packout
- This shipper has very small/few air gaps to cause any significant amount of convection, hence a conduction model is sufficient to get good results
- For shippers with significant air gaps, particular vertical columns of air, convection will have to be modeled explicitly in CFD to get accurate results.