COLD CHAIN TECHNOLOGIES

Use of Advanced Modeling to Effectively Predict Convection and Phase Change while Optimizing Thermal Packaging Designs and Increasing Speed to Market

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Section I. Background on Thermal/Fluid Modeling

1.1 General Overview of the Shipper Modeling Process

Mathematic modeling is the process where a real life system is represented by a set of mathematical relationships (the model) after certain approximations and assumptions have been made. In general, this modeling process can be divided into the following steps **(1):**

- Determine Objective
- Establish System Background Including Data & Laws
- Develop Approximations & Assumptions
- Perform (execute) Modeling
- Validate the Model
- Compound the Model

This paper provides a discussion of typical thermal modeling methods as well as how such modeling has been used to accelerate the development of Cold Chain Technologies (CCT) products, thereby bringing them to market more quickly.

Simulation of thermal packaging is a complex problem. Specifically, the problem is a coupled thermal/fluid problem, involving both thermal and fluid effects. To completely model the physics of the shipper, three equations must be solved, specifically: conservation of mass, conservation of momentum and conservation of energy. Two key areas to be simulated correctly are a) free convection and b) phase change. A brief background of each is provided below, followed by the equations and corresponding approximations and assumptions.

<u>Free Convection in Enclosures (Shipper)</u>

Fluid motion due entirely to the action of a body force (such as gravity) is typically called “free convection,” in contrast to forced convection, which is brought about by an external means, such as a fan. The movement of a fluid (gas or liquid) in free convection results from the buoyancy force on the fluid when its density is decreased via heating (or increased via cooling). The presence of a buoyancy force is required for natural convection to occur. Typically, this buoyancy arises from density differences which are the results of a temperature gradient within the fluid.

Specific to the simulation of thermal packaging, free convection (of air) will occur in the void volumes (enclosures) that are present in the shipper. This convective flow will occur due to the difference in the (initial) temperature of shipper components, namely the frozen refrigerants (-20ºC), the liquid refrigerants and/or product load (+5ºC) and the shipper itself (+22ºC).

In the analysis of free convection, it is assumed that the fluid is incompressible, the fluid properties (specific heat, thermal conductivity and viscosity) are constant and that viscous dissipation is negligible **(2)**. The governing equations must be solved simultaneously for five unknowns (v_x, v_y, v_z, p and T). This requires that the hydrostatic pressure and well as boundary/initial conditions are specified. Because of the complexity of the governing equations, there are no exact solutions for natural convection in enclosures; in practice, solutions to such problems are normally obtained via numerical methods.

Phase Change of Refrigerants (Passive Refrigeration)

Phase change materials (PCMs), relative to cold chain packaging, can be defined as a passive thermal energy storage mechanism used to protect pharmaceutical products in several temperature ranges. Specifically, thermal energy can be stored as sensible (specific) heat or latent heat (e.g. heat of fusion). To keep a product hot (or cold) relative to the surrounding environment, PCMs change phase at a constant temperature, called the phase change temperature, whereby they absorb or release heat. To increase the duration of refrigeration at a given temperature, PCMs are selected such that their phase change temperature is near (or within) the desired refrigeration temperature range of the product being shipped. As the PCM changes its phase (for example, from ice to water at 0ºC) it effectively extends refrigeration duration by cooling the product via its latent heat. If PCMs are not used, only the sensible (specific) heat of the packaging material will resist temperature increase, and the time that the package will be within temperature criteria will be significantly reduced.

PCM geometry and placement in the package will have an impact on the duration that the product will remain within temperature specification. As discussed below, CCT is developing advanced modeling techniques to optimize both the geometry and placement of PCMs within a given package to maximize refrigerative duration, and minimize cost, weight and volume. As phase change is a non-linear thermal behavior, its simulation is challenging. The following sections discuss the specific methods used to characterize the physics of phase change.

Simulation of Thermal Packaging: Conservation of mass, momentum and energy

To completely simulate the flow of a fluid in a shipper, all three equations (mass, momentum and energy) are needed. To simulate the temperature distribution in a solid, however, only the energy equation is required.

Conservation of Mass [Fluid only]

The continuity equation, which is simply a statement of the conservation of mass, can be written for a path following the fluid motion using the operator $\frac{D}{Dt}$ as shown below in equation 1.

$$\frac{D\rho}{Dt} = -\rho(\boldsymbol{\nabla} \cdot \boldsymbol{v}) \qquad [1]$$

This form of the continuity equation describes the rate of change of density (ρ) as seen by an observer "floating along" with the fluid. In dealing with thermal shippers, variations in density are insignificant, and can be ignored. For this special case (incompressible fluid with ρ = constant) the continuity equation becomes:

$$(\boldsymbol{\nabla} \cdot \boldsymbol{v}) = 0 \qquad [2]$$

Conservation of Momentum [Fluid only]

The equation of motion, which is the conservation of momentum, is a restatement of Newton's second law (e.g. sum of the forces = mass x acceleration, or F = ma). In vector notation, the equation of motion, can be written as shown below in equation 3 **(3)**:

$$\frac{\partial}{\partial t}\rho\boldsymbol{v} = -(\boldsymbol{\nabla} \cdot \rho\boldsymbol{v}\boldsymbol{v}) - \boldsymbol{\nabla}p - (\boldsymbol{\nabla} \cdot \boldsymbol{\tau}) + \rho\boldsymbol{g} \qquad [3]$$

In equation 3, the left hand side term represents the rate of increase of momentum per unit volume. The right hand side terms represent, per unit volume, the following:

- The rate of momentum ($\rho\boldsymbol{v}\boldsymbol{v}$) gain by convection (1st term)
- The pressure (p) force (2nd term)
- The rate of momentum gain by viscous (μ) transfer (3rd term)
- The gravitational ($\boldsymbol{g}$) force (4th term)

Rewriting equation 3 in terms of the substantial derivative ($\frac{D}{Dt}$) equation 3 becomes:

$$\rho\frac{D\boldsymbol{v}}{Dt} = -\boldsymbol{\nabla}p - (\boldsymbol{\nabla} \cdot \boldsymbol{\tau}) + \rho\boldsymbol{g} \qquad [4]$$

Equation 4, which is similar in form to equation 1, represents conservation of momentum for a reference that flows along with the fluid. To use equation 4 to determine velocity distributions, however, the stresses must be expressed in terms of velocity gradients. For a Newtonian fluid equation 4 can be re-written as shown below:

$$\rho\frac{D\boldsymbol{v}}{Dt} = -\boldsymbol{\nabla}p + \mu\boldsymbol{\nabla}^2\boldsymbol{v} + \rho\boldsymbol{g} \qquad [5]$$

Equation 5, the celebrated Navier-Stokes equation, is the generic form of the equation used to simulate fluid flow in thermal shippers. There are two "limiting" types of heat transfer in fluids, namely forced convection and free convection. Forced convection results when the flow patterns are determined by some external force (e.g. fan), while free convection results when the flow patterns are determined by the buoyancy effect on a heated fluid (e.g. density differences). In forced convection, the velocity profiles are found, and are used to find the temperature profile. *In free convection, however, the velocity profiles and the temperature profiles are intimately connected, and must be determined at the same time.* For these cases, the modified Navier-Stokes equations are:

Forced Convection: $\rho \frac{D\boldsymbol{v}}{Dt} = \mu \boldsymbol{\nabla}^2 \boldsymbol{v} - \boldsymbol{\nabla} p + \rho \boldsymbol{g}$ [6]

Free Convection: $\rho \frac{D\boldsymbol{v}}{Dt} = \mu \boldsymbol{\nabla}^2 \boldsymbol{v} - \rho \beta \boldsymbol{g} (\mathrm{T} - \mathrm{T_o})$ [7]

The approximations used to develop equation 7 are the Boussinesq approximations **(2)**. The first of these approximations is that, like forced convection, equation 2 is valid. The second approximation is that the density difference which causes the flow can be approximated as a pure temperature effect (i.e., effect of pressure on density is neglected). Specifically, the density difference is estimated for thermal buoyancy using $[\rho - \rho_o = \rho\beta(\mathrm{T} - \mathrm{T_o})]$ where the subscript (o) indicates properties outside the fluid boundary layer, and β is the thermal expansion coefficient of the fluid. The validity of this approximation is for $\beta(\mathrm{T} - \mathrm{T_o}) << 1$.

To simulate fluid flow effects inside a shipper (e.g. free convection in an enclosure), equation 7 is used. To simulate fluid flow effects outside of the shipper, either free convection or forced convection (equation 6) may be required, depending on the shipper's surrounding environment.

Conservation of Energy [Fluid & Solid]

To develop the temperature profile in the fluid, the energy equation must be added to the continuity and momentum equations (above), and all three equations must be solved simultaneously. In addition, the energy equation is also needed to simulate the temperature field in solid components of the shipper (foam, bricks, gel packs) which involve the physics of conduction and phase change. The general form of the energy equation is listed in equation 8.

$$\rho \frac{DU}{Dt} = -(\boldsymbol{\nabla} \cdot \boldsymbol{q}) - (\boldsymbol{\tau} : \boldsymbol{\nabla} \boldsymbol{v}) - p(\boldsymbol{\nabla} \cdot \boldsymbol{v}) \qquad [8]$$

In equation 8, the left hand term represents the rate of gain of internal energy (U) per unit volume. The right hand side terms represent, per unit volume, the following:

- The rate of internal energy input by conduction (1st term)
- The irreversible rate of internal energy increase by viscous dissipation (2nd term)
- The reversible rate of internal energy increase by compression (3rd term)

For a fluid with constant viscosity (μ) and thermal conductivity (k), equation 8 becomes:

$$\rho c_p \frac{DT}{Dt} = = \; k\boldsymbol{\nabla}^2\mathrm{T} + \mu \boldsymbol{F} \qquad [9]$$

Where c_p is the specific heat of the fluid and F is a dissipation function (for free convection, the dissipation function can be neglected). For solids, the dissipation function is zero, and the substantial derivative becomes a partial derivative, so the energy equation can then be written:

$$\rho c_p \frac{\partial T}{\partial t} = = \; k\boldsymbol{\nabla}^2\mathrm{T} \qquad [10]$$

To account for phase change, the transient term of energy equation must be modified as follows:

$$\rho \frac{\partial T(h)}{\partial t} = \; k\boldsymbol{\nabla}^2\mathrm{T} \qquad [11]$$

where h(T) = $\int_{T1}^{T2} CpdT$

Here, h(T) = is the enthalpy function of the material, and includes the latent heat (e.g. heat of fusion) of the substance at the phase change temperature.

In summary the equations needed to determine the temperature profile in a fluid are:

<u>Conservation Equations (FLUID):</u>

Conservation of Mass: $(\boldsymbol{\nabla} \cdot \boldsymbol{v}) = 0$

Conservation of Momentum (Forced Convection): $\rho \frac{D\boldsymbol{v}}{Dt} = \mu\boldsymbol{\nabla}^2\boldsymbol{v} - \boldsymbol{\nabla}p + \rho\boldsymbol{g}$

Conservation of Momentum (Free Convection): $\rho \frac{D\boldsymbol{v}}{Dt} = \mu\boldsymbol{\nabla}^2\boldsymbol{v} - \rho\beta\boldsymbol{g}(\mathrm{T}-\mathrm{T_o})$

Conservation of Energy: $\rho c_p \frac{DT}{Dt} = k\boldsymbol{\nabla}^2\mathrm{T} + \mu\boldsymbol{F}$

<u>Conservation of Energy (SOLID):</u> $\rho \frac{\partial T(h)}{\partial t} = k\boldsymbol{\nabla}^2\mathrm{T}$ where h(T) = $\int_{T1}^{T2} CpdT$

1.2 Typical Methods used for Coupled Thermal/Fluid Problems

For most real engineering problems involving complicated geometries, nonlinear material properties, and mixed heat transfer mechanisms, the analytical solution of the constitutive equations for mass, momentum and energy conservation is not tractable. To achieve a numerical solution, these equations are typically discretized in space and time, and the resulting discretized equations are solved using iterative solution techniques. The most common discretization methods can be classified into one of the following three categories: finite difference methods, finite element methods, and finite volume (or control volume) methods.

Finite Difference Methods

Finite difference methods are conceptually one of the simplest methods for the numerical solution of ordinary or partial differential equations. They rely on being able to discretize the domain of interest into regularly spaced computational points: the points are often aligned with the axes of the coordinate system in which the computational domain is defined. Derivatives of dependent variables are approximated by "finite differences" along the axis directions. The advantage of finite difference methods is that they are easy to construct and program. The disadvantage of these methods is that they are not well suited to problems with real geometries, because boundary conditions cannot be accurately defined unless the boundaries also align with coordinate system axes.

Finite Element Methods

Finite element methods are more appropriate for complex geometries: they permit discretization of the computational domain into polyhedral elements (typical elements in 3D include tetrahedra, hexahedra, wedges, and pyramids). These elements can be constructed as an irregular mesh, allowing the elements to conform to the natural boundaries of the problem. To solve a set of equations on a finite element mesh, a set of basis functions is constructed on each element, and the coefficients of the basis functions are determined such that they satisfy the original constitutive equations in their *weak form*. The coefficients define values of the dependent variables at the finite element *nodes* (computational points, including their vertices). *The main drawback of finite element methods for fluid flow and heat transfer problems is that they do* ***not*** *naturally satisfy conservation principles*: conservation of mass, momentum and energy must be ensured through utilization of a very fine mesh, which quickly drives up computational time.

Finite Volume (Control Volume) Methods

Finite volume, or control volume methods allow the domain to be discretized into regular or irregular polyhedra, but automatically impose conservation principles as part of the solution formulation. For real engineering applications, finite volume methods typically use the same kind of discretization as a finite element mesh, but solve the constitutive equations on those elements differently.

Example of Control Volume Formulation

As an example, consider the term for convective transport of a quantity ϕ, shown below in equation 12.

$$\frac{\partial(\rho U_j \phi)}{\partial x_j} \qquad [12]$$

When this term is integrated over a control volume, Gauss' theorem can be applied to express it instead as an integral over the control volume boundary, as shown below:

$$\int \frac{\partial(\rho U_j \phi)}{\partial x_j} dV = \oint_A \rho U_j n_j \phi dA \qquad [13]$$

In its discretized form, the right hand side of equation 13 can be approximated as follows:

$$\oint_A \rho U_j \; n_j \phi \; dA \approx \sum_{ip} \dot{m}_{ip} \phi_{ip} \qquad [14]$$

where

$$\dot{m}_{ip} = \rho U_j n_j \Delta A$$

is the discrete mass flow through a finite sub-surface of the finite volume, *ip* denotes the integration point of this sub-surface, ΔA is the sub-surface area, ϕ_{ip} is the discrete value of ϕ at this sub-surface and the sum is over all surfaces of the finite volume.

Control volumes may be constructed from the actual elements, or may be centered around nodes of elements. A node-centered finite volume is depicted in 2D in **Figures 1a** and **1b**, below.

Each finite volume sub-surface is an element bi-sector plane, where a complete finite volume results from the subsectors of two surrounding quadrilateral elements and three triangular elements. These sub-surfaces are called integration point surfaces, and the integrand to be evaluated is computed at their mid-points. This method of finite volume definition extends directly to 3D.

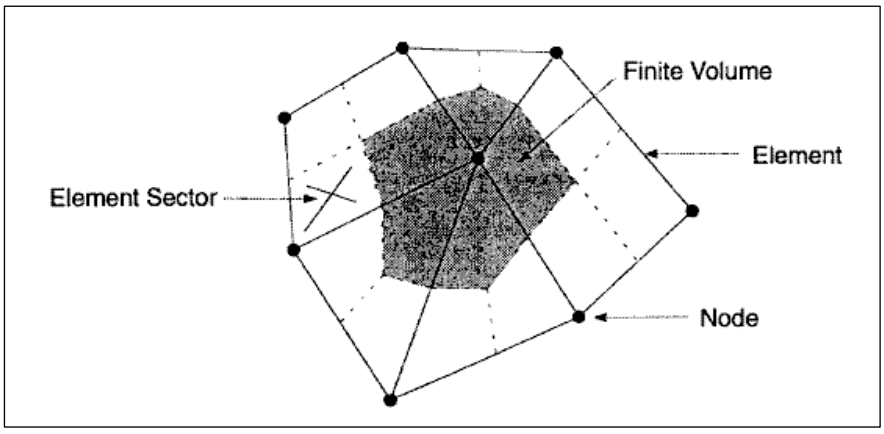

Figure 1a: Node Centered Finite Volume in 2D

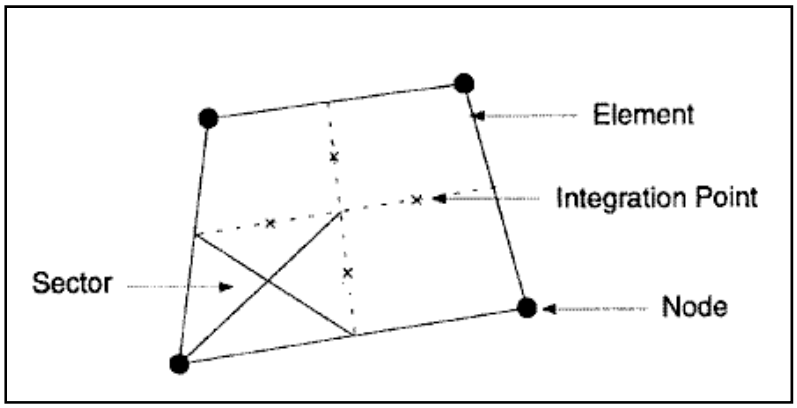

Figure 1b: Element from Figure 1a, Showing Integration Points

The discretization scheme thus entails representing discrete approximations to the volume integrals over the element sectors and discrete approximations to the surface integrals on the element integration point surfaces. The overall equation assembly proceeds by visiting each element in turn, making the discrete approximations to the terms in the integrals, so that when all elements have been visited, every node has a completed finite volume equation for each conservation law. In co-located finite volume methods, all the dependent variables, including pressure and the velocity components, are stored at the element nodes.

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This finite volume integration procedure can, for example, be performed for the conservation of mass and conservation of momentum equations, to yield:

Conservation of mass (equation 15):

$$V\frac{(\rho-\rho^{o})}{\Delta t}+\sum_{ip}\dot{m}_{ip}=0 \qquad [15]$$

Conservation of momentum (equation 16):

$$V\left(\frac{\rho U_j - \rho^o U_j^o}{\Delta t}\right) + \sum_{ip} \dot{m}_{ip} U_{j,ip} = -\sum_{ip} \left(P \Delta n_j\right)_{ip} + \sum_{ip} \left(\mu_{eff} \left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \Delta n_j \right)_{ip} + S_{U_j} V \quad [16]$$

where the superscript ^{0} denotes values of dependent variables at old time steps.

These concepts are readily extended to energy and other conservation equations, and are equally applicable for element-centered (rather than node-centered) control volumes. The unique conservation properties of the control volume methods make them the preferred choice for heat transfer and fluid flow problems, over finite difference and finite element methods.

1.3 Use of Thermal/Fluid Modeling for Cold Chain Shippers: Advanced Methods

CCT/MAYA's thermal/fluid modeling technology is extremely well suited for numerical simulation of the thermal performance of cold chain shippers. The system incorporates sufficient breadth of capability to model the full range of heat transfer physics in cold chain shippers, including conduction, convection, phase change, and radiation. The solution strategy and architecture is highly optimized for treatment of coupled thermal flow effects, especially conjugate heat transfer and natural convection. And finally, an advanced solver technology enables the simulation to be carried out for extended periods, predicting transient response over the full span of a complete shipping cycle (up to 120 hours or more). The FEMAP/TMG Thermal/Flow software technology enables effective thermal modeling of cold chain shippers by providing accurate and efficient treatment of the following physics:

Conductive Heat Transfer

FEMAP Thermal/Flow provides comprehensive handling of conductive effects in complex geometries. The system is based on a conservative element-based control volume formulation to compute accurate conductive and capacitive terms for arbitrary, unstructured meshes. The proprietary scheme is based on an element temperature function constrained at calculation points on the boundaries and at the geometric centroid. The numerical formulation is second-order accurate, and is insensitive to element skewness and distortion; this permits accurate computation of transient response even with coarse meshes.

A wide range of element types can be used to model the conductive domain, including shells, solids, and beams, as well as axisymmetric elements. Orthotropic and temperature dependent thermal conductivity is supported for all element types.

Thermal Contact Resistance, Air Gaps and Bonded Joints

This technology includes extensive capabilities for the treatment of thermal contact effects. The Thermal Couplings feature in FEMAP Thermal/Flow provides a highly effective mechanism for modeling conductive or radiative heat transfer between contacting surfaces. The algorithm supports fully disjointed meshes, thereby facilitating construction of complex assembly models. Thermal Couplings are ideally suited for modeling heat transfer across small air gaps, or between bonded surfaces.

Natural (Free) Convection

Convective heat transfer can and does occur in air gaps in cold chain shippers, and can be used to improve packaging designs (e.g. reduced weight), or if the shipper is not sealed, can cause a major source of heat leakage. CFD modeling is required for accurate characterization of this phenomenon. The FEMAP/TMG solution technology provides effective treatment of buoyancy-driven airflow, and accurate computation of the resulting convective heat transfer.

Natural convection simulations are very often compute-intensive. A fully coupled implicit solution of the conjugate heat transfer problem is beneficial for the accurate simulation of natural convection: it permits relatively large time-steps while maintaining numerical stability. This coupled solver technology efficiently solves the solid-domain conduction and fluid domain Navier-Stokes equations in a segregated manner, exploiting the different properties of the linearized equations in each domain. For full implicit coupling, iterations are performed on the segregated solutions to converge the globally nonlinear problem. This solver technology is necessary for natural convection simulations to be both accurate and stable. Other key tools for simulation of natural convection include Boussinesq buoyancy models and a natural convection thermal wall function. The validity of the wall function has been demonstrated over a wide range of Rayleigh numbers, and is an effective tool in moderately turbulent natural convective flows.

Refrigerant Phase Change

A key aspect governing the thermal response of cold chain shippers is the latent heat effects associated with the phase change of the refrigerant materials. As discussed above, effective treatment of these effects is critical in order to achieve accurate simulation results.

The FEMAP Thermal/Flow software incorporates a rigorous and conservative enthalpy-based formulation for computing the energy balance and temperature response in elemental control volumes transitioning from one phase to another. Unlike methods based on temperature-varying specific heat, this approach yields accurate results even for very large time steps or temperature changes. The system includes facilities to define distinct thermal properties (i.e. conductivity, specific heat) for each of the material's phases.

Modeling Efficiency

A major challenge in the simulation of cold chain shipper thermal performance is the need to solve the numerical model for transient response over large periods of time, usually several days. Such extended time cycles significantly augment the computational expense of the simulation. Therefore, to maximize fidelity within reasonable limits on solve time, it is essential that the computational meshes be as concise and efficient as possible. The FEMAP software incorporates a very broad array of tools for the construction of finite volume meshes for thermal/fluid problems. The toolset includes:

- Global and local controls with default sizing
- Define element size or spacing with bias
- Free surface meshing, quads or triangles only
- Mapped meshing with quads or bricks
- Direct generation of line, shell and solid elements
- Extrude and revolve geometric curves or line elements into shell elements; shell elements can be extruded or revolved to form solid elements
- Connected shell elements can be extruded normal to themselves to turn thin-shell models into solid ones
- Mesh refinement and smoothing
- Subdivision and semi-automatic meshing of solids
- Automatic solid meshing with tetrahedral elements

FEMAP Thermal/Flow also supports and exploits planar symmetry; since many CCT shippers are designed to be symmetric about orthogonal planes, this offers a four-fold reduction in model size. The software also supports disjointed meshes at the fluid/solid boundaries; this permits the construction of more tailored meshes, with element densities appropriate for the local physics of the relevant domain.

Solution Efficiency

A key technology underpinning high fidelity simulation of cold chain shippers is the numerical solver. The complex physics, long operating cycles, and high accuracy requirements demand a highly efficient solver.

FEMAP Thermal/Flow offers state-of-the-art solution technology for coupled thermal/flow problems. The thermal solver is based on an advanced iterative conjugate gradient scheme that delivers high performance and robustness. The CFD solver incorporates adaptive correction multigrid solver technology, enabling it to handle very large problems with ease.

As mentioned above, the FEMAP/TMG implicit solution technology permits relatively large time steps for the long transient simulations required for analysis of cold chain environments. Variable time step sizes, as well as the ability to take different time steps in fluid and solid regions gives the analyst a large degree of flexibility in the analysis. A critical feature for long transient simulations is the freeze flow capability: this suspends recalculation of the continuity and momentum equations when the flow field has stabilized, and only restarts calculation after a prescribed change in temperature. Freeze flow criteria thus become an enabling technology for the simulation of very long transient phenomena.

Summary: Advantages of the Approach

Overall, the above simulation approach for cold chain shippers brings a number of important benefits, which when combined, result in more accurate solutions and faster solve times. As discussed above, these include, but are not limited to:

- Thermal solver uses a finite difference control volume approach (vs. finite element approach) which allows the use of disconnected meshes to model thermal physics such as thermal couplings and non-geometric elements
- Local conservation of energy allows non-linear behavior (e.g. phase change) to be more accurately modeled
- Fewer elements are required with this approach
- Thermal couplings can be used to connect disconnected thermal meshes; specific advantage on thermal contact resistance between solids
- Individual and/or coupled solvers for thermal & flow solutions (independent fluid and thermal meshes are automatically connected at solve time)
- Option of using an implicit solver (unconditionally stable, large time steps possible)
- Fast/efficient transient solver w/automatic time step

The benefit to industry includes a quick turnaround for design concepts, reduced development time and increased speed to market.

1.4 References

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2. Case Study: Thermal/Fluid Modeling of a 2" wall PUR Shipper

2.1 Objective & Background

The objective of this modeling effort was to demonstrate that simulation could be utilized to design a 2" wall PUR shipper that would hold a product temperature of 2 to 8ºC for a 96 hour summer cycle. To this end, a 2" PUR shipper was fabricated and used as the basis of a thermal packaging design. The design consisted of the following components:

- Qty 1, Molded PUR base [OD = 20.5" (L) x 19.88" (W) x 21.63" (H)]
- Qty 1, Molded PUR lid [OD = 20.5" (L) x 19.88" (W) x 2" (H)]
- Qty 1, Molded PUR inner box [dimensions 14.5" (L) x 13.88" (W) x 19.5" (H)]
- Qty 1, Corrugated Product box [ID = 11.13" (L) x 10.5" (W) x 16.5" (H)]
- Qty 12, 338F Refrigerant Brick [Dimensions 11.5"L x 8.88"W x 0.75"H]
- Qty 8, 339F Refrigerant Brick [Dimensions 11.5"L x 5.445"W x 0.75" H]

In this shipper design, temperature is passively controlled by pre-conditioned frozen (-20ºC) and liquid (+5ºC) refrigerants in combination with an insulated polyurethane (PUR) foam container (with inner product box). An exploded view of the PUR shipper is shown in **Figure 2.**

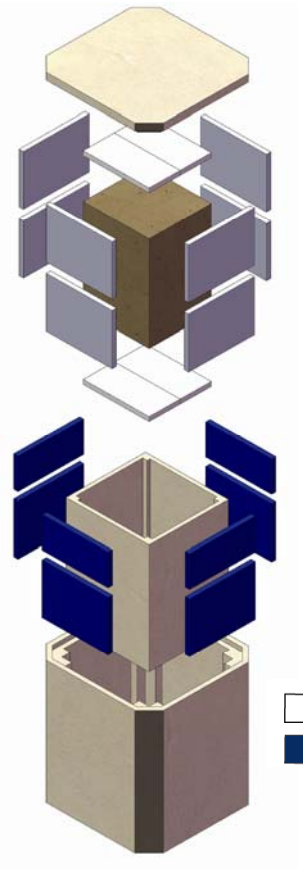

Figure 2: Exploded View of PUR Shipper (-20ºC Refrigerants in Blue, +5ºC Refrigerants in White).

For the PUR components, all pre-conditioning is done at room temperature (+22ºC) for a minimum of 24 hours. As shown in the figure, a total of twelve 338F bricks were used, eight refrigerated (+5ºC) surrounding the sides of product box and four frozen (-20ºC) surrounding the bottom of the PUR inner box. A total of eight 339F bricks were used, four refrigerated (+5ºC) on the top/bottom of the product box, and four frozen (-20ºC) surrounding the top of the PUR inner box. Without product, this design weighs ~55 lbs, including 28 lbs of refrigerated bricks (+5ºC) and 17 lbs of frozen (-20º) bricks.

2.2 Approximations & Set-up of Model

As described in section 1.1, all mathematical models are idealizations to some degree, which place certain limitations on the validity of the solution; for the model to be complete, all approximations and assumptions must be stated along with the results.

The geometry of the shipper was constructed using the actual components, which were generated via solid modeling software (SolidWorks). To limit the simulation model size, a ¼ size model was utilized, and all thermally insignificant features (e.g. radii, fillets, etc) were removed. The solid model was then saved as a parasolid file, with everything at a 1:1 scale (default in meters). The quarter model used to make the simulation is shown below in **Figure 3**.

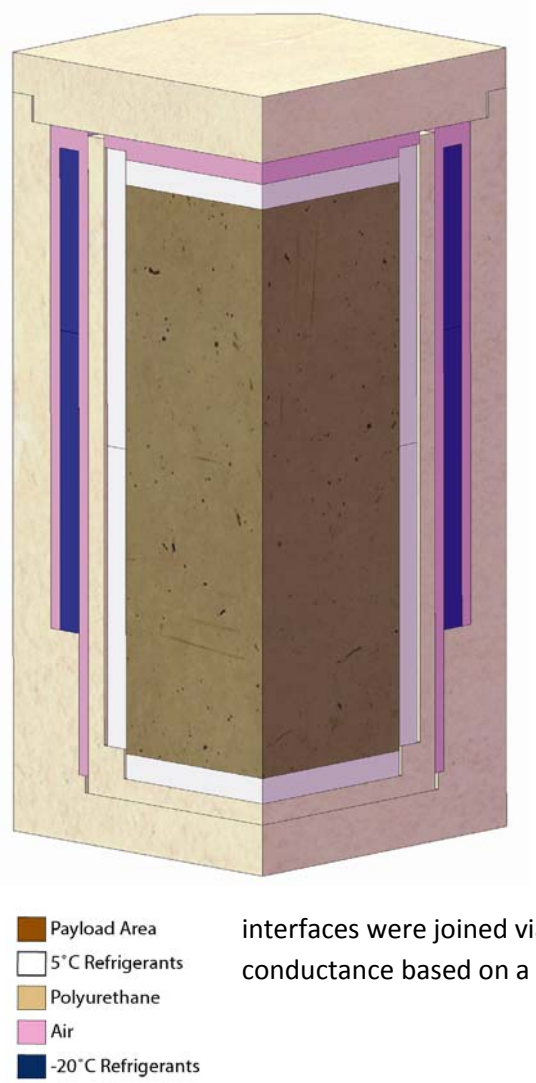

Figure 3: Solid Model (Quarter Size) Used to Develop Simulation (Pink = Air gaps, Blue = -20ºC Frozen Refrigerants, White = +5ºC Refrigerants)

As is typical in such simulations, the geometry was divided into discrete volumes (or elements) and inspected and corrected to eliminate any interferences and/or discontinuities between parts. For all solid materials (shipper, refrigerants and outside of product box) 3D isotropic elements, of either tetrahedral or hexahedral type, were used and thermal properties (density, specific heat and thermal conductivity) were assigned to these elements. These properties were assumed to be constant with both direction and temperature. Furthermore, materials expected to change phase (e.g. frozen refrigerants) were assigned a phase change temperature, latent heat and a specific heat for their liquid phase. Likewise, for fluid materials (air in the shipper, air in the product box) 3D fluid elements, of either tetrahedral or hexahedral type, were used and the required fluid properties (thermal conductivity, specific heat, density, viscosity and gas constant) were assigned. Each component, be it solid or liquid, was meshed at a size appropriate for the physics involved. All solid to solid element interfaces were joined via “thermal couplings,” and each coupling was assigned a conductance based on a combination of test data and experience.

As we are most interested in temperature of the payload over time, the type of analysis run was selected as a 3D transient thermal/fluid model [T = T(x,y,z,t)], with a predetermined ambient temperature profile (summer in this case). In this model, the surface temperature of the shipper was determined using a forced convection boundary condition; specifically, an ambient temperature and ambient heat transfer coefficient were assigned to the shipper surroundings. The appropriate initial conditions were assigned to all solids, as described above. Any solid material that impedes fluid flow was defined as a blockage. Furthermore, symmetry plane was defined on the surface of all fluid elements in the plane of symmetry. Fluid ambient conditions, which include ambient pressure and gravity vector, were defined, and the transient thermal and flow solvers were activated. The thermal solver was set to output (write) results every hour, while the fluid solver was set to output (write) results every 2 hours. The solver parameters, such as integration time step, were adjusted to obtain a reasonable balance between solution accuracy and overall solve time. The results, discussed below, were used to validate and further compound the model.

2.3 Post Processing & Simulation Results

During the simulation, at each time step the minimum and maximum temperatures were monitored, along with the mass, momentum and energy balances. Once the simulation was finished, the results were loaded into the post-processor and reviewed. Specifically, the transient profiles of both the (frozen) refrigerants and the product load were reviewed. Once the phase change and product load transient temperature profiles were determined to look reasonable, all solids (including thermal couplings) were reviewed at the initial, middle and final time steps of the simulation. Finally, flow vectors (or temperature contours) of the fluid were reviewed and inspected for a) symmetry and b) expected flow direction.

Figure 4 is graph of actual and simulated results of the shipper's product load temperature versus time for the imposed 96 hour (summer) ambient temperature profile. As shown in the figure, the simulation compares very well with the actual data (within 1ºC at all times). Furthermore, the locations of the highest and lowest product load temperatures correspond with the simulation. The simulation results near the bottom of the product load (shows the highest overall temperature) track nearly the same as the thermocouple (TC) at that location. Likewise, the simulation results near the center of the product load (shows lowest overall temperature) track very closely to the TC in that location.

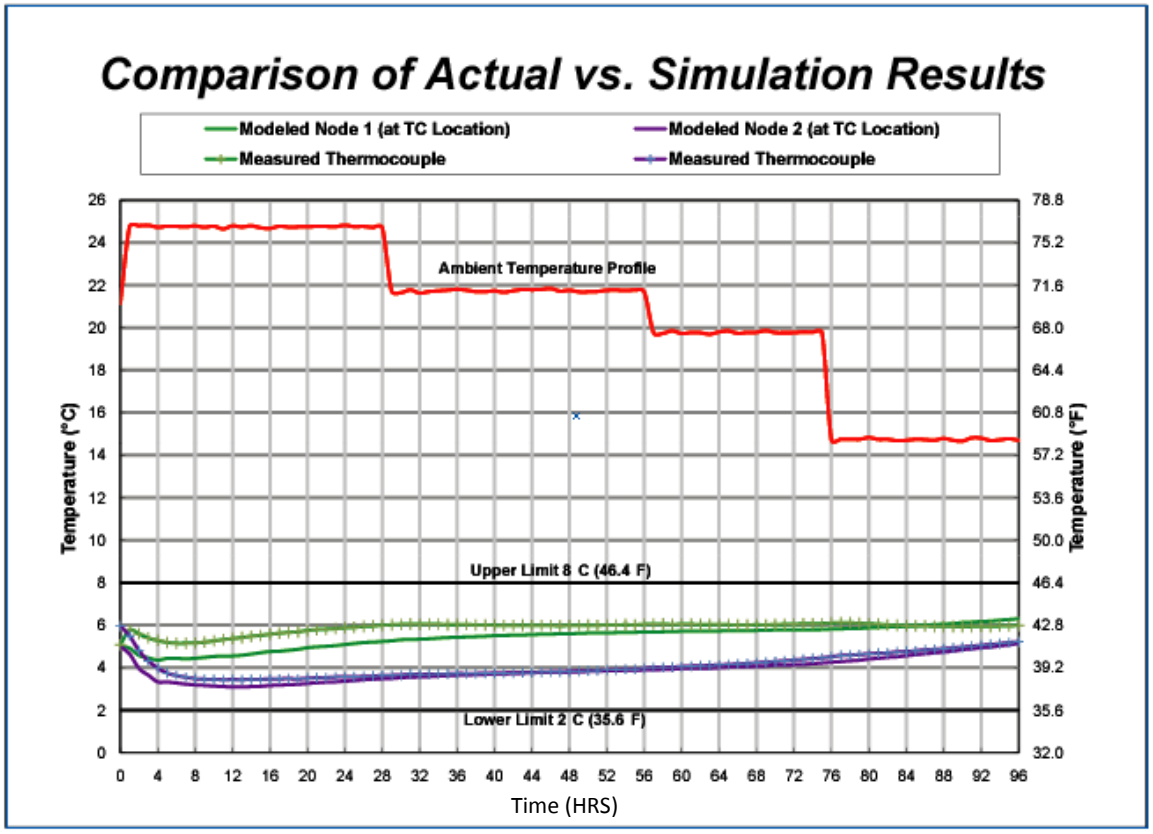

Figure 4: Shipper Product Load Temperature vs. Time: Actual vs. Simulation

Figure 5 is a graph showing how the simulated results, at identical locations in the product load, compare between a) the full thermal/fluid model and b) the conduction only model. In the conduction only simulation, all fluid elements were replaced with "solid" elements of similar size and assigned the thermal properties of air (thermally similar to insulation). As indicated in the figure, the change is dramatic. The thermal/fluid model discussed above basically replicates the actual data, and shows that this shipper design remains between 2 to 8ºC for the full 96 hour summer profile. The conduction only design, however, shows that the product load goes over the 8ºC upper limit at 28 hours at the bottom of the product (worst case) and 50 hours at the top of the product (best case). At the end of the 96 hour profile, the entire product load is between 13 and 14ºC! *These results clearly show that, for this shipper design and profile combination, a conduction only approach (no convective flow) is not a useful simulation method*. It should also be noted that each simulation was run with phase change; the only difference between the two was that the thermal/fluid model allowed free convection, while the conduction (only) did not.

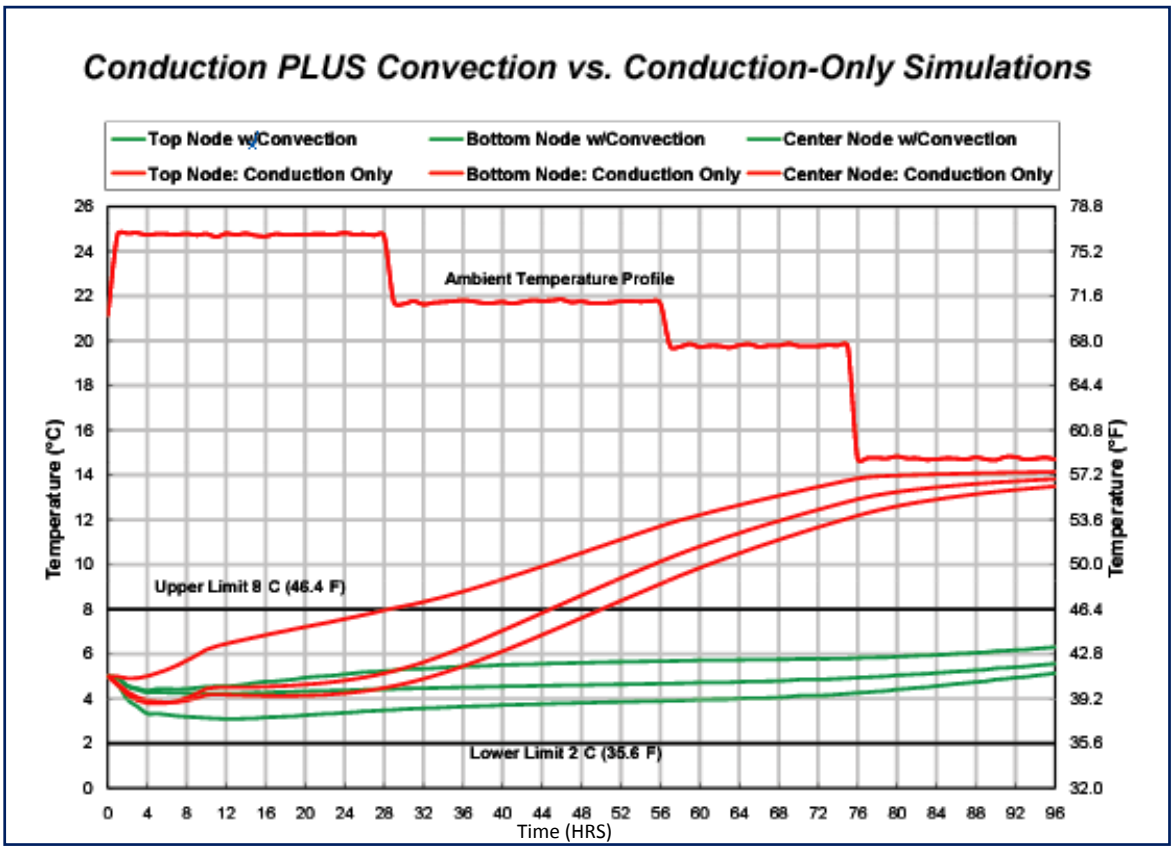

Figure 5: Product Load Temperature vs. Time: Simulation (Thermal/Fluid) vs. Simulation (conduction only)

A number of figures, that follow, show outputs from the complete (full thermal/fluid) software simulation of the PUR shipper design. These figures are presented to give the reader an indication of how the temperature of this PUR shipper design changes with both time and position.

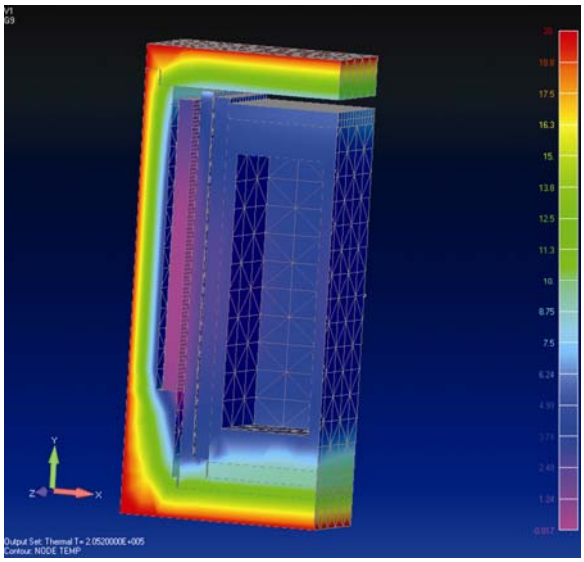

Figure 6 is the thermal profile of the shipper (¼ model) after an elapsed time of 57 hours. As expected, the shipper surface temperature is very close to the ambient temperature at ~20ºC. The figure shows the temperature gradient through the shipper, ice (still changing phase), refrigerants and the outer product box itself (3 to 6ºC).

Figure 6: PUR Shipper Design (¼ model), Thermal Profile at time = 57 hours

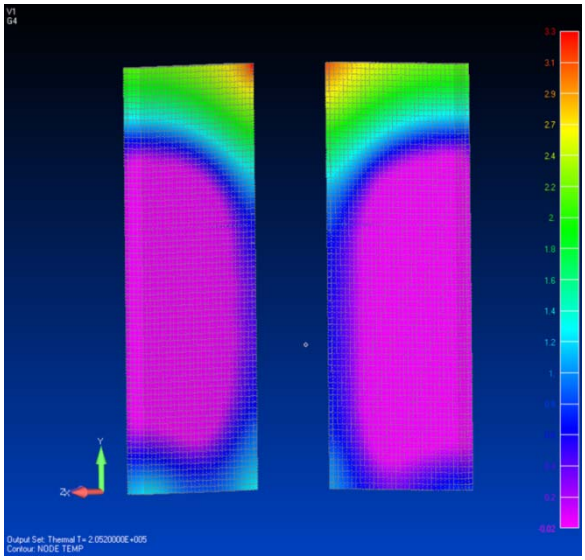

Figure 7 is the thermal profile of the ice (bricks) after an elapsed time of 57 hours. As shown in the figure, the results match the thermal profile of the shipper, in that the "corner" of the air volume closest to the outside of the shipper begins to melt first (already greater than 3ºC by this time). However, the majority of the brick is still frozen at this point, as indicated by the dark purple region that remains at 0ºC (ice to water phase change temperature).

Figure 7: Temperature Profile of (initially) frozen bricks at time = 57 hours

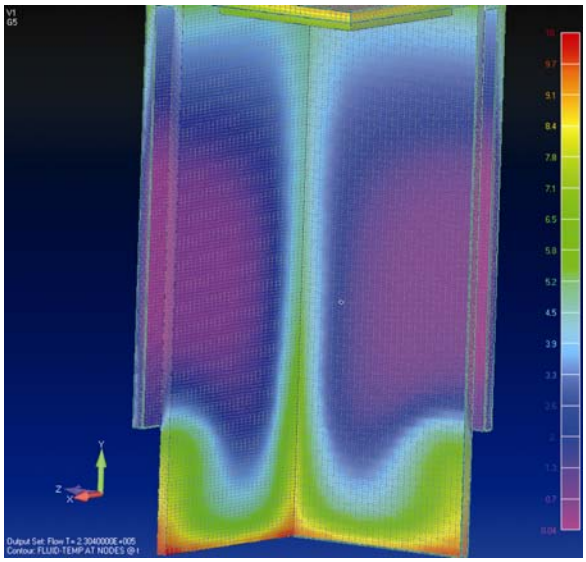

Figure 8a shows the thermal profile in the air gaps between the shipper and the refrigerated bricks after an elapsed time of 64 hours. The warmest regions of the air are located a) in the region directly above the brick/product load and b) in the region near the bottom edge of the product load. As the product load does not have any air directly below it (pure conduction), it is logical that the air is warmest (~10ºC) in this location.

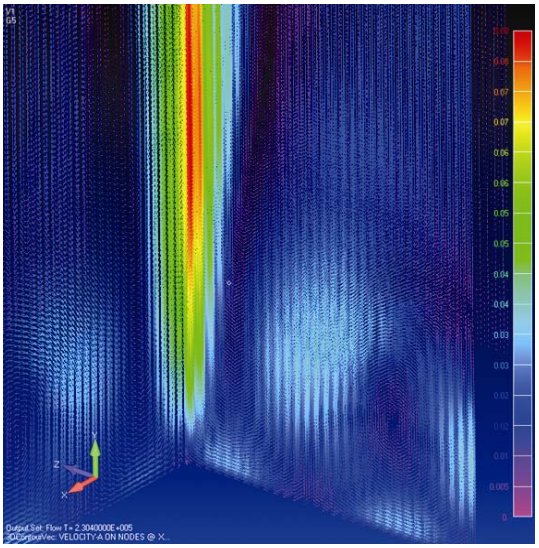

Figure 8b, shows the convective flow velocity profile in the same air gaps at an elapsed time of 64 hours. Note, per the figure, that a convective flow circuit is clearly evident. The flow, which is basically symmetric, carries the cold air down through the bulk of the air gap that is located next to the frozen (brick) and allows the warmer air to return via the "corner" of the air volume closest the outside of the shipper (location of brick that melts first). In this way, free convection acts to moderate the temperature around the product load, keeping it more uniform (tighter band) longer than the corresponding conduction (no air gap) approach.

Figure 8a: Temperature Profile of Air (gaps) at time = 64 hours

Figure 8b: Velocity Profile of Air (gaps) at time = 64 hours

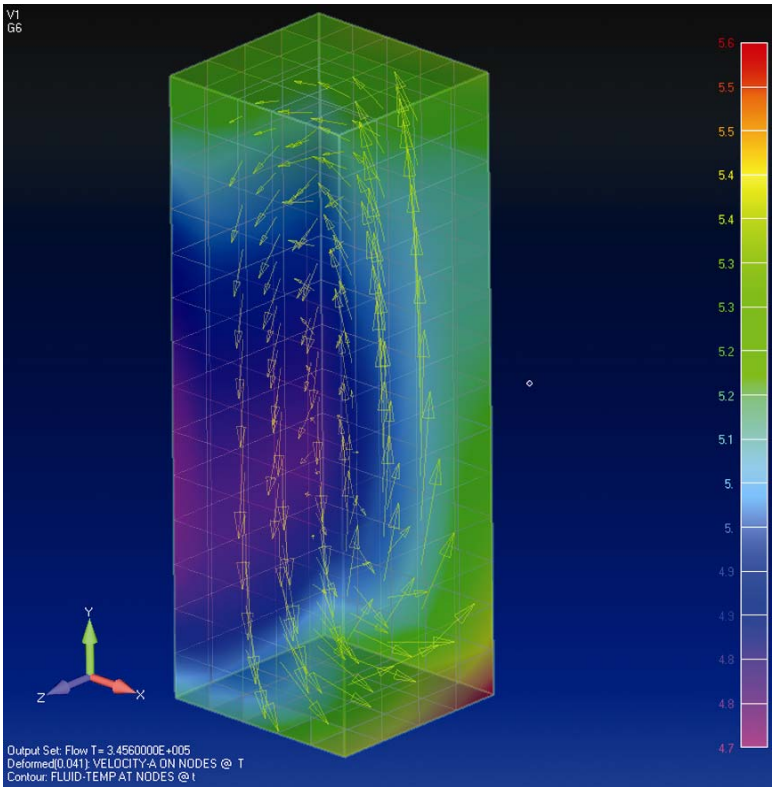

Figure 9 shows the convective flow (and outer surface temperature) inside the product box after an elapsed time of 96 hours, which is the end of the thermal cycle. As shown in the figure, the product load temperature is quite uniform, ranging from 4.7 to 5.6ºC. Figure 9 also shows that a convective flow circuit has been set-up which mirrors the one shown previously in Figure 8b. Specifically, the flow proceeds downward on the colder (brick) side and upward at the center of the product load. This flow makes the product temperature more uniform (tighter band). The results seen here also suggest that modeling the payload via conduction and/or convection must be considered on a case by case basis.

Figure 9: Temperature & Flow Profiles in Product Box at Elapsed time of 96 hours.

2.4 Summary of Results

The above simulation results have shown that, with the given 96 hour summer profile, the temperature profile versus time of this PUR shipper design can be accurately simulated using a full thermal/fluid approach. The results also show that a conduction (only) approach is not a viable method for simulation in this case. The overall benefits of this simulation method include that it is useful for a quick evaluation of initial design concepts and that it is also useful as a tool for design optimization. This approach may also be useful to predict the temperature distribution in a shipper (whose simulation has already been validated) that experiences an unexpected temperature spike during actual shipment. Certainly, this case study shows that predictive modeling can save both time and money on shipper design and development, with the overall result of reaching the market more quickly.

2.5 Acknowledgements

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