Assessment of insulating package performance by mathematical modelling

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A mathematical model has been developed in the present work to describe the temperature change in a typical insulated shipping container as a function of time. The model was created by combining steady state and transient models in a 2D geometry of a typical shipping container and was subsequently validated by an ice melt test and comparison of temperature change obtained from the model and experimental measurement. An excellent agreement was obtained between the computational model developed in this work and experimental results. In addition, a parametric study was also carried out to investigate various factors in controlling the insulation performance of the packaging. It was found that the model has capability of evaluating the effect of a wide range of packaging design parameters such as thermal conductivity, surface emissivity, packaging geometry, and sounding temperature.

KEYWORDS
food packaging, mathematical modelling, insulation materials, package design

1 | INTRODUCTION

The quality of perishable goods, such as seafood goods and medicines, is strongly affected by surrounding temperature. In order to avoid deterioration during transportation and storage, the temperature of the products and the surrounding environment needs to be carefully controlled. With rising population and uneven distribution of goods across the world, there has been an increasing demand for delivering temperature-sensitive cargos over long distances. As a result, cold chain is commonly employed to preserve the quality of transported goods. Active cold chain uses shipping refrigerated containers, maintaining the required temperature during transportation. This method normally results in a high cost-to-payload ratio and is also limited by location accessibility. Passive cold chain method typically use insulated shipping containers incorporated with insulation materials and/or phase-changing materials (PCM) for sustained low temperature envi-

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ronment inside the package. Such system opens up the possibility of postal service as a mean of goods transportation, which is often much cheaper than active cold chain. The performance of a passively chilled package is influenced by multiple factors including packaging shape, insulation materials, quantity, and type of PCM used.

A number of studies have been undertaken to evaluate the performance of passively chilled packages.3-8 Burgess derived equations describing the thermal resistance (R-value) of a package based on packing material, thickness of packing walls, geometry of the container, and other design features.9 The equations were obtained after conducting multiple ice melt tests and fitting the formulas to match the observed results through linear regression. The model was then used to predict the shipment time for only selected packages and was compared with physical measurement. The difference was found within 20%. In addition, this approach presented limited utility as multiple tests were required to manipulate packaging models in order to create a database.9 A more theoretical approach was used by Choi, who created a 2D steady-state model for calculating heat penetration rate (HPR). HPR has the ability to describe the quantity of energy transferred into the box at a unit temperature difference across package walls. Although this model can evaluate the insulation performance of the package accurately, it cannot do so with time evolution.5 This issue was investigated by Terpák et al, who developed a transient model to describe the temperature variation inside the container as a function of time. The model takes into account heat flow from the surroundings to the packaging walls by considering both convection and radiation.4 Furthermore, conduction effects are also included for the packaging walls in direct contact with the goods. Despite this transient approach, simplified package geometry and construction is a limiting factor that can lead to a significant uncertainty.4 More recently, Ge et al developed a 3D transient model with the ability to predict the temperature within a package at any position and time.10 They calculated heat transfer coefficient by taking into account heat transfer from the inside through the insulation walls and from the container inside wall to its centre. The model presented only partial agreement due to the use of constant conductivities of packaging materials and air instead of actual products during the simulation. Furthermore, the model required significant computational resources because of 3D approach, especially when thick insulation or significant amount of phase-change materials were used.10 Other attempts at modelling shipping containers also include the use of finite element (FE) modelling by Wang et al or computational fluid dynamics (CFD) by Valtysdottir et al.8,11 Both incorporated detailed descriptions of the package and shipment products into their models. Despite the fact that the models neglected the heat transfer through radiation or convection, they were still able to achieve excellent correlation between experimental and simulation results. This approach showed great potential for insulated package design, although it also requires the access to expensive software and significant computational resources. This could significantly limit its accessibility for ordinary passive cold chain users.8,11

The experimental approach has also been commonly used in the past in order to design and test the performance of the shipping containers.12 However, large variety of insulated container design and a wide range of factors affecting the outcome of the measurements make it extremely difficult to compare the results from different studies.12 Nevertheless, some main techniques have been established to qualitatively assess the performance of the shipping containers. For example, both Burgess and Choi have used such test to calculate the HPR of rigid insulated packages. Although the HPR is a single numerical value used to compare the insulation performance of the packages, it cannot directly address temperature change with time evaluation.5,7 In addition, Singh has used thermocouples to constantly monitor the temperature inside containers.13 This measurement evaluated the thermal resistance of the packages and investigated insulation performance of both rigid containers as well as insulated flexible packages. In addition, the effect of different PCMs on the shipment time was also investigated. This was followed by a series of similar tests on temperature profiles of different insulated packages.14 A similar approach was also used by Ge et al who placed the thermocouples inside an EPS foam container and measured internal temperature variation over time in order to obtain desirable shipment time.10 Such approach is subject to some limitations as the temperature inside container will be strongly dependent on surrounding conditions (eg, humidity, external temperature) during the experiment. Consequently, those findings can be used only as a first approximation for the maximum shipment time provided by the container. Other more sophisticated measurement techniques were described by Childs et al and included interferometry, planar thermopile, or thin skin sensors.15 This leads to high cost and complexity of measurement implementation for investigating insulated shipping containers.15

In the present work, we have developed a transient mathematical model to assess insulation performance of passive insulated packages. In addition, the effect of various insulating materials on package insulation performance was also investigated through ice melt tests and temperature profiling. The results obtained from the model and experimental measurement were subsequently compared to validate the model. Finally, the parametric study was carried out to investigate sensitivity of the model.

2 | MATHEMATICAL MODELLING

A passively insulated package typically includes a container with single or multiple layers of insulating materials to for part of packaging wall. As a result, such package may be viewed as a heat sink with external energy attempting to travel through the container wall. It is reasonable to assume that conduction will dominate overall heat transfer in a perfectly closed container surrounded with insignificant fluid displacement. Radiation occurs both inside and outside of the container and is mainly controlled by the reflective properties of the materials used for the package inner and outer surfaces or view factors. Other thermal processes taking place in insulated packaging include phase change of coolant and accumulation of latent heat.16

The mathematical model developed in this work is based on thermal energy balance, which describes basic thermal processes such as heat transfer, conversion of heat to different forms of energy as well
as heat accumulation. It is assumed that the temperature inside the package must be known, and it is exactly the same as the temperature of the transported goods. Starting with the balance equation, we have

\[ E_{\text{in}} - E_{\text{out}} = \Delta E_{\text{st}}. \] (1)

Assuming that the direction of net energy flow is from the external environment towards the inner space of the container as shown in Figure 1, Equation (1) will be reduced to

\[ E_{\text{in}} = \Delta E_{\text{st}}. \] (2)

Assuming the temperature change of the coolant and the transported product will change at the same rate with time, the rate of energy change might be described as

\[ \Delta E_{\text{st}} = (m_1 \cdot C_{p1} + m_2 \cdot C_{p2}) \frac{dT}{dt}. \] (3)

Moreover, total heat flow entering the package can be written as

\[ E_{\text{in}} = \frac{\Delta T}{R_q}. \] (4)

The relation between HPR and the thermal resistance of the package can be described as

\[ R_q = \frac{1}{HPR}. \] (5)

HPR may be evaluated using following equation 5:

\[ HPR = \frac{1}{\frac{1}{h_{\text{out}} A_{\text{out}}} } + \frac{1}{\frac{1}{h_{\text{in}} A_{\text{in}}} } + \frac{A_2}{\frac{RW}{A_2}}. \] (6)

In order to obtain RW, the following equation was used:

\[ RW = \sum_{i=1}^{N} R_i \cdot t_i + 0.039 \cdot t_{a1} + 0.037 \cdot t_{a2} + \sum_{i=1}^{N} \frac{0.217 \cdot t_{a3}}{5.918 + t_{a3}}. \] (7)

Moreover, heat transfer coefficients of outside and inside of the package were calculated using

\[ h_{\text{out}} = 1.778 + 5.198 \cdot \varepsilon_{\text{out}}. \] (8)

\[ h_{\text{in}} = 3.557 \cdot \frac{A_4}{A_3 + A_4} + \frac{4.6 \cdot 1}{A_4} \cdot \varepsilon_{\text{in}} + \frac{1}{\varepsilon_{\text{product}}} - 1. \] (9)

Substituting Equations 3 and 4 into Equation 2 leads to below ordinary linear differential equation:

\[ R_q \cdot (m_1 \cdot C_{p1} + m_2 \cdot C_{p2}) \frac{dT}{dt} + T = T_e. \] (10)

The analytical solution to Equation 10 is in a form of Equation 11:

\[ T(t) = (T_i - T_e) e^{\frac{R_q \cdot (m_1 \cdot C_{p1} + m_2 \cdot C_{p2})}{A_2}} + T_e. \] (11)

When phase changing materials (eg, ice) are present inside the container, the latent heat of fusion of coolant must be taken into account. For instance, our model assumes that the energy transferred into the container is totally consumed to sustain the process of ice melting at a temperature of 0°C. The beginning of phase change is defined at the ice melting temperature, and the process is assumed to end when the amount of input energy equals to latent heat of coolant inside the container. Thus, before and after the phase change, Equation 11 was used in this work to determine the temperature changes inside the container. During the stage of phase change, the temperature was set to be constant, and the amount of time required to complete the phase change was calculated when total heat flow reached the sum of sensible heat and latent heat. The latter was simply determined by the amount of coolant and its specific latent heat.

This analytical model was subsequently implemented in MATLAB using a “for” loop function to calculate the package internal temperature every second of elapsed time. Amount of energy being added and total heat flow across packaging walls was also calculated by the model to identify the time when phase change should commence and finish. As a result, a temperature-time profile can be obtained for an insulated package. Such approach enables efficient evaluation of temperature-time relationship of contained product in a package as well as the impact of various packaging design parameters on this relationship.
3 | EXPERIMENTAL

In order to assess model fidelity, two experimental procedures were carried out. First, ice melt test gives the opportunity to measure HPR by quantifying the amount of latent heat needed to melt the ice. Second, tests were also carried out to measure the maximum insulation time (MIT) in a typical insulated cardboard box by monitoring the temperature inside the box using a wireless thermocouple. In the present work, MIT was defined as the time required for coolant temperature increase from \(-20°C\) to 5°C as it has been proven by the previous research that 5°C tends to be a upper limit temperature for transportation of perishable goods (eg, fish).\(^1,17\)

3.1 | Ice melt test

Ice was placed in the room at a controlled temperature (20°C) until reaching melting temperature. Five hundred grams of ice was placed inside the container whose dimension are presented in Figure 2. The sealed container was left in a temperature-controlled environment at 20°C. After 10 hours, the remaining ice was taken out of the container, and the amount of water produced in the process of ice melting was weighted. Assuming that the energy transferred into the box was entirely consumed to melt the ice, HPR may be calculated by using the following equation:

\[
\text{HPR} = \frac{\text{weight of water} \times \text{latent heat of ice}}{\text{melt time} \times (T_e - T_{ice})}.
\]

3.2 | Measurement of the maximum insulation time

This measurement was conducted in accordance with ASTM D3103. The outside conditions were kept constant with a temperature of 15°C (±1°C) and a relative humidity of 54% (±2%). The thermocouple was a Lascar Electronics EasyLog EL-USB-1 with measurement accuracy of ±0.5°C. Two 400-g ice packs were sourced in order to keep the volume and shape of the ice constant throughout all experiments. The ice packs were placed in a freezer for 48 hours before being positioned on top of the thermocouple inside. The thermocouple had been set to start recording the temperature 15 minutes after the box was sealed in order to stabilise thermocouple reading. Measurement of the temperature was terminated when it reached 5°C due to the definition of MIT.\(^1,17\) As a result, temperature change as a function time could be obtained to give the value of the MIT for the package.

4 | COMPARISON BETWEEN MODELLING AND EXPERIMENTAL RESULTS

4.1 | Heat penetration rate

Figure 3 presents a comparison between HPR calculated by the model and measured HPR using packaging boxes with different types of external surfaces. It can be found that the model gives a fairly accurate HPR with the highest discrepancy less than 10%. The difference could be caused by modelling simplification including 2D model geometry and constant temperature within the box. In addition, the model assumes the ideal initial conditions and neglect the energy stored in the walls of the package and air inside the container.

It can be also seen in the Figure 3 that the emissivity of the outer surface can have a significant effect on the HPR. The introduction of white surface elongates the transportation time by only 5% in comparison with brown surface. As expected, the box surfaced with aluminium foil showed the most decrease in the HPR (by 20%) when compared with the standard brown box.
4.2 | Maximum insulation time

Figure 4 presents temperature change inside the package as a function of time. It can be seen clearly that both the model and experimental results depicted temperature-time behaviour over three different stages. The first stage showed rapid temperature increase before it reached melting temperature of the ice packs. This was followed by a prolonged stage for ice melting with little temperature change in the container. Upon completion of this phase change, the temperature experienced fast increase towards the external temperature. It is obvious that the MIT is dominated by the second stage controlled by the phase-change material in the package.

Figure 4 also presented an excellent agreement between the modelling and the experimental results for the temperature-time relationship of the package, particularly in the first and the second stages. Nevertheless, there are still a number of areas presenting some distinctive differences. Firstly, the rate of temperature increase is steeper for calculated values than experimental results during the postmelting stage, and such temperature increase also occurs earlier in the experiment than in the modelling. This is mainly due to temperature discrepancy between the measurement and the modelling. Temperature measurement is taken from the surface of the ice packs, which have a temperature gradient from the surface to the bulk in nonequilibrium state. The model, however, assumes a uniform temperature throughout the ice packs and therefore results in a delayed phase change followed by a rapid increase in temperature after completion of the phase change. One should expect that such discrepancy can be addressed if the model takes into account temperature gradient in the coolant itself. This improvement will require greater computational resources due to the increased calculation difficulty. Since the difference in the MIT is relatively small as shown in Figure 4, the above assumption is kept for the remaining investigation in this work.

Although only a single size of container was used in the present study, previous work had showed that the HPR could be calculated with reasonably good accuracy for a wide range of containers with external sizes varying between 23.5 and 109.2 cm. As the HPR is a key parameter for the calculation of the MIT, it is reasonable to assume the model derived in this work should also be applicable to packages with different dimensions.

After obtaining a good agreement for the temperature-time relationship in a specific package, a series of experiments and simulations were further carried out to compare the MIT obtained from packages with different thermal characteristics. These conditions, together with the results for the MIT, are summarised in Table 1. In addition, Figure 5 shows packages with four different insulating liners, namely low density polyethylene, polystyrene foam, PIR board, and silica aerogel blanket.

It can be found in Table 1 that the aerogel-lined package gives a MIT nearly 2.5 times greater than that obtained from the package lined with polyethylene foam, despite the fact that the former is 5 mm thinner than the latter. This is mainly due to the extremely low thermal conductivity in the aerogel. In addition, the results for EPS-lined containers in Table 1 also clearly indicate the benefit of incorporating reflective inner surface, which gave rise to 10% increase in MIT. Furthermore, the results in Table 1 have also revealed that the model is reasonably accurate to estimate the MIT with an average difference of 10% relative to the measured values. This accuracy is

### Table 1: Maximum insulation time obtained from model prediction and measurement with various insulating liner

| Material              | Thickness, mm | Thermal Conductivity, mW/mK | Inner Surface Reflective | Outside Temperature, °C | Calculated MIT, h | Measured MIT, h | Relative Error, % |
|-----------------------|---------------|-----------------------------|--------------------------|-------------------------|-------------------|----------------|------------------|
| Polyethylene          | 25            | 61.0                        | No                       | 24.2 ± 0.7              | 17.9              | 21.3           | 15.5             |
| Polyethylene          | 25            | 61.0                        | Yes                      | 15.7 ± 0.9              | 22.8              | 24.5           | 7.0              |
| Expanded polystyrene  | 25            | 42.5                        | No                       | 24.2 ± 0.9              | 20.0              | 21.6           | 7.2              |
| Expanded polystyrene  | 25            | 42.5                        | Yes                      | 23.7 ± 0.5              | 21.1              | 24.2           | 12.9             |
| Ultra high density Polystyrene | 25       | 34.0                        | No                       | 23.5 ± 0.7              | 23.4              | 28.4           | 17.7             |
| Polysocyanurate       | 25            | 24.6                        | No                       | 22.7 ± 0.5              | 29.7              | 32.0           | 7.3              |
| Polysocyanurate       | 25            | 24.6                        | Yes                      | 15.43 ± 0.5             | 41.6              | 46.0           | 9.7              |
| Silica aerogel        | 20            | 16.2                        | No                       | 22.6 ± 0.9              | 43.3              | 39.3           | −10.1            |
| Silica aerogel        | 20            | 16.2                        | Yes                      | 16.0 ± 0.6              | 56.9              | 61.3           | 7.1              |
| Silica aerogel        | 12            | 16.2                        | No                       | 24.0 ± 0.6              | 25.2              | 21.2           | −18.9            |
| Silica aerogel        | 12            | 16.2                        | Yes                      | 22.9 ± 1.2              | 34.0              | 35.1           | 3.2              |
higher than that obtained from the models developed from previous studies. Such improvement is mainly attributed to the fact that both steady state and transient state have been utilised in our model in order to describe the behaviour of the temperature inside the container as a function of time.

Figure 6 presents the effect of external temperature on the MIT obtained from the model and the measurement. It can be seen that the calculated values are in close agreement with values obtained through the experiments especially for typical room temperatures. The discrepancy appears to increase with elevated temperatures, at which the model tends to overestimate the package performance. This is mainly caused by the way how heat transfer coefficients are calculated as shown in Equation 7 to 9, which are based on the results obtained by numerically fitting literature data on radiation and convection heat transfer coefficients in a temperature range of 0°C to 40°C. It was previously proven that both coefficients are relatively constant within the expected temperature range. Similarly, the thermal conductivity of the insulation materials is expected to rise in accordance with an increasing temperature, but thermal conductivity as a function of temperature was not introduced within the mathematical model. A decision was undertaken following comparative study presenting minor differences between constant and varying thermal conductivity for the temperature range we expect the package to be exposed to.

5 | PARAMETRIC STUDY

A parametric study was carried out to investigate the influence of design parameters of a typical insulated package on its insulation performance, which was characterised by the MIT. These parameters included surface emissivity, thermal conductivity of the material, mass of coolant, thickness of insulation layer, and external temperature. Their relation to the MIT was expressed by rearranging Equations 11 to 13 as below.

$$t = -R_q^* (C_{p1}^* m_1 + C_{p2}^* m_2)^* \ln \left( \frac{T_i - T_e}{T_i - T_f} \right)$$  \hspace{1cm} (13)$$

The package considered in the parametric study was a cardboard box that contained 1-kg ice packs with initial temperature at –20°C. The external temperature was set to be at 20°C, and as defined earlier the MIT was the time required for the ice packs to reach 5°C. 25-mm polyethylene foam was used as the insulation liner in all cases except when different insulation materials were considered for their effect on the MIT. The materials properties relevant to the investigation and their datum values were listed in Tables 1 and 2.
5.1 | Effect of surface emissivity

As shown in Figure 7, surface emissivity can significantly affect the insulation performance of a shipping container. By merely incorporating a low surface emissivity surface on the outside of the container, the MIT was increased by 12%. More increases were observed at surface emissivity below 0.8 when the inner surface was equipped with reflective foil. The maximum improvement in the MIT was found to be almost 40%. It can be also seen that in both cases the MIT increases exponentially as surface emissivity reduces and graphs converge at the surface emissivity value of 0.83.

Differences in surface emissivity are mainly attributed to the radiation part of the energy transfer, and, as described by Stefan-Boltzmann equation, decreasing surface emissivity will lead to a decrease in the energy flux through the container walls. However, the impact of such a layer will differ at different positions within the container. In the case of the inner wall, the surface with low emissivity creates conditions in which elevated surface temperature causes only a small value of radiant thermal energy being radiated towards the shipping product. On the other hand, the application of a low emissivity surface at the outside of the shipping box will also increase the reflectivity of the container. As a result, a significant part of energy radiated towards the package from the outside environment will be reflected and will not contribute towards the increase in temperature within package. Furthermore, it can be found that much better effects upon MIT are noticed when low surface emissivity material is applied to the inside surface of the container. This happens, due to the thickness of the wall which reduces the inner surface compared with the outer one. As a result, even though the outside surface area and property controls the amount of energy being absorbed by the container, it is the inside surface which limits the heat passage towards the product inside the container and enhances the effects the surface emissivity has on MIT.

5.2 | Effect of insulation material properties

Figure 8 presents the modelling results for the effect of thickness of nominal insulating materials with different thermal conductivity on the MIT. Figure 9 presents the modelling results for the effect of thermal conductivity of nominal insulation liners with different thicknesses. As expected, increasing wall thickness leads to an increase of the MIT in a linear fashion. On the contrary, the MIT experiences an exponential increase over the range of thermal conductivity presented in Figure 9. There appears to be a drastic increase in the MIT after thermal conductivity falls below a critical point as seen in Figure 9. In order to identify this critical point, the linear regression method was applied to the linear regions before and after nonlinear region for each insulation thickness. A thermal conductivity was then obtained at the intersection point of both lines. For all analysed thicknesses, the critical value falls in the vicinity of 14 mW/mK, although it is susceptible to changes if significant alterations of design parameters are introduced. Nevertheless, it is clear from Figure 9 that an attempt at increasing packaging MIT will be much more effectively achieved when the thermal conductivity of a lining material is below this critical point. In practice, such low thermal conductivity can be obtained by using materials such as aerogels. Furthermore, the effect achieved by decreasing thermal conductivity also scales with the thickness of the insulating liner. On the other hand, increasing thermal conductivity leads to convergence of the MIT approaching 20 hours as seen in Figure 9. This is expected since for a given wall thickness its insulation effect will diminish as the wall becomes more and more heat-resistant.

### Table 2

| Material          | Cardboard Box | Polyethylene Foam | Ice | Aluminium Foil |
|-------------------|---------------|-------------------|-----|----------------|
| Specific heat capacity [J/kgK] | 1400          | 2500              | 2108| 900            |
| Latent heat [kJ/kg]    | N/A           | N/A               | 335 | N/A            |
| Thermal conductivity [W/mK] | 0.061         | 0.048             | N/A | 210            |
| Surface emissivity | 0.83          | 0.90              | 0.97| 0.04           |
| Dimensions [mm]     | 272 × 210 × 254 | N/A               | 163 × 91 × 64 | N/A          |
| Thickness [mm]      | 2.78          | 25                | N/A | 0.2            |

**FIGURE 7** Modelling results for the effect of surface emissivity of package walls on the maximum insulation time

**FIGURE 8** Modelling results for the effect of thickness of insulating liner on the maximum insulation time
5.3 | Effect of mass of coolant

A common practice in transportation of perishable goods is the addition of a phase-change material (e.g., ice) inside the package in order to elongate possible shipment time by sustaining low temperature inside a container. The model derived in this work was used to investigate the effect of the quantity of ice pack on the MIT. Figure 11 shows that the addition of PCM can elongate the MIT linearly as indicated by Equation 13. This is caused by the addition of heat sinks inside the package, which effectively absorb the entering energy to transform coolant phase at the phase-change temperature before changing the temperature of the product. It should be also noted that the MIT can be adjusted by the amount of coolant as well as type of coolant. The model can help to select the optimum amount of cooling substances to keep the products refrigerated whilst minimising package weight and associated transportation costs.

5.4 | Effect of external temperature

Figure 12 shows the modelling results for the MIT as a function of external temperatures. As expected, the increase of outside temperature gives a monotonic decrease in the MIT since increasing the temperature difference across the packaging walls results in higher heat flux entering the package. It is worth mentioning that the nonlinear correlation between the external temperature and the MIT is implied by Equation 13. The external temperature affects all modes of heat transfer, although in previous study, it was shown that radiation and convection were not significantly affected by a temperature change as selected in this investigation. The results in Figure 12 also shows that the model can help to evaluate the insulation capacity of a package experiencing a wide range of temperature change during transportation.

6 | CONCLUSION

The present work presents a mathematical model capable of evaluating the insulation performance of passive insulated packages during their transportation of perishable goods. The model showed a good agreement with experimental measurement giving an average of 10% relative difference for the HPR and the MIT. In addition, a parametric study of the model was also carried out to investigate the influence of a variety of factors on the MIT of a typical delivery package. These include surface emissivity, thermal conductivity of insulation, insulation thickness, mass of coolant, and external temperature. The modelling results for all these parameters followed closely to the
expectation, and some of these results were also validated by comparing with those obtained from the experimental measurement. More importantly, it was clearly demonstrated that the model possessed the ability to provide a much wider spectrum for illustrating the effect of most key parameters for insulated packaging design. Furthermore, this analytical model can be implemented without engaging any numerical approach and resourceful computational tools. Thus, this mathematical model proved to be an excellent tool for design of insulated packaging as well as gaining a good understanding of temperature-time behaviour for a given insulated package.

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