

NUMERICAL ANALYSIS OF HEAT DIFFUSION IN MULTILAYER COMPOSITE MATERIAL

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Article History

Received on 27 Jan, 2026

Accepted on 24 Feb, 2026

Published on 25 Feb, 2026

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Abstract

The transient heat conduction of multi-layered composite material plays a vital role in the various engineering applications like thermal insulation, electronic packaging, and aerospace structures in a broad range of engineering practice. The paper is a numerical study of transient heat conduction in multilayer composite in a finite difference approach. The regulating heat diffusion equations are simplified with the help of implicit time integration method in order to ensure the numerical stability of the equations in the large differences of the thermophysical properties. Special attention is paid to the treatment of the interface, including interfacial thermal resistance to impair the perfect bonding. The grid independence analysis and convergence analysis are the methods used to validate the numerical framework. The results show that big temperature gradients can develop about interfaces, particularly when there is a significant difference with regard to the thermal conductivity between one individual layer and another. Thermal barrier may and can be the low-conductivity layers but interfacial thermal resistance may give temperature jumps that may dramatically influence the overall heat transfer behaviour. The study reports that the correct modelling of interfaces and method of discretization in prediction of the transient thermal response are significant. The recommended numerical modeling may serve as the acceptable basis of thermal analysis and planning of the contemporary multi-layered composite systems.

Introduction

The topic of diffusion of heat in composite multilayer materials is a crucial concern in thermal science as well as materials science due to the direct effect on the high-performance industrial use. Multilayer composites are also used in aerospace, electronic pack, thermal barrier finishes, building insulation systems and energy devices, where thermal management is one of the most significant structural integrity and operational reliability factors. These systems include hydro-based systems, which involve layers of various thermophysical properties but bind them together to give a required mechanical, thermal or a combination of functions. However, presence of material discontinuities introduces a lot of complexity in the prediction of the behavior of heat transfer, particularly in the transient conditions (Incropera et al., 2007; Shahani et al., 2025). The analysis of the heat conduction on composite media is dictated by Fourier law and transient heat diffusion equation. Whereas analytical solutions may be readily found in simple multilayer structures in the steady-state regime, closed-form solutions become increasingly hard to find in circumstances in which there is transient behavior, nonlinear materials, interfacial thermal resistance, or multidimensional geometries (Carslaw & Jaeger, 1959). The real conditions of engineering applications can consist of extremely sharp thermal conductivity, density, and specific heat capacity difference between interfaces, and discontinuity of the heat flux must be determined with great care. The resultant effect has created the need to use numerical methods in fine tuning of the diffusion of heat in laminated composite structures.

The analytical solutions of layered systems simplified on idealised assumptions were among the first to receive a systematic treatment of conduction in solids; Carslaw and Jaeger (1959)

were the pioneers. These classical solutions however are based on the fact that the thermal liaison and material characteristics are perfect and hence, only applies to the state-of-the-art composites. The numerical methods (finite difference method (FDM), finite element method (FEM), and finite volume method (FVM)) have become the most commonly applied technique of solving problems of heat transfer in heterogeneous materials due to the high dynamism of the computational methods (Patankar, 1980; Zienkiewicz et al., 2013). Finite difference approach is conceptually simple and easy to use in the particular case one dimensional transient that the researcher is interested in. It estimates the partial differential equation governing in space and time and transforms it to a system of equations that is algebraic. However, it is necessary to pay special attention to material interfaces so that to guarantee continuity of temperature and heat flux preservation. The issue of numerical instability or artificial oscillations may occur when there is poor discretization around the interfaces, and the ratios of thermal conductivity of the layers adjacent to each other are large (Ozisik, 1993).

Finite element method is however more adaptable with regards to complex geometries and anisotropic materials. This is done in a manner in which the FEM approach automatically defines material discontinuities by involving definition of element-wise properties, a weak formulation of the governing equation is formulated and a global stiffness matrix is assembled (Zienkiewicz et al., 2013). The FEM implementations are however very resource intensive when working with highly refined meshes particularly in the multidimensional transient analyses. Practically, the interfacial thermal resistance (or thermal contact resistance) can play a central role in the total efficiency of the heat transfer of the multilayer

composites. Imperfect bonding, roughness of the surfaces, and microstructural irregularities at interfaces may cause temperature jumps across interfaces and this significantly affects thermal responsiveness (Incropera et al., 2007). The right interface conditions should therefore be employed to provide precise numerical modeling that would ensure physical realism and numerical stability. Secondly, other properties that vary with temperature (such as thermal protection systems or turbine blades) are another complication to the analysis (high-temperature).

The increasing demand of lightweight and also thermally optimized materials in the aerospace and electronics industry has increased the research in numerical heat diffusion modeling. A case in point, the gas turbines possess coated thermal barriers that are subjected to very high thermal gradient as well as cyclic loading and, therefore, accurate forecasts of the temporary temperature distributions are needed to prevent the failures. Similarly, microelectronic devices require the use of multilayer substrates and thin films that need to be efficiently studied in thermal since overheating is not preferable, hence reliability is a requirement. These applications indicate the need to have strong and efficient numerical procedures that have the ability to handle the multilayer heterogeneity. Although the variety of literature regarding the numerical heat conduction remains enormous, several challenges remain. It can add unwanted

high conductivity variations between layers (that increases the accuracy of solutions particularly with coarse meshes). Explicit schemes may possess stability requirements that involve time steps that are prohibitively small that increase the cost of the computation. Moreover, grid independence and convergence analysis are not mentioned enough in the practice research. Therefore the systematic investigation of discretization strategies, means of stability and interface treatment is still required to improve predictive accuracy.

The present work is devoted to the heat diffusion numerical study of the multi-layered composite materials on the basis of the systematic discretization structure. The accuracy of interfacial conditions, numerical accuracy and evaluation have been focused keeping in mind the influences of contrast in material properties on temperature distribution and heat flux. The paper will combine the strict mathematical modeling with wary numerical modeling and this will assist in the enhanced modelling approaches of the layered thermal systems. This paper will seek to provide a better insight into the thermal characteristics of multilayer composite under transient conditions by a detailed parametric study of the material and its justification by the prior knowledge on the topic. These findings will be applied in developing and optimization of composite structures of high order in engineering activities where thermal performance forms a significant component.

Figure 1: Schematic of Multilayer Composite System

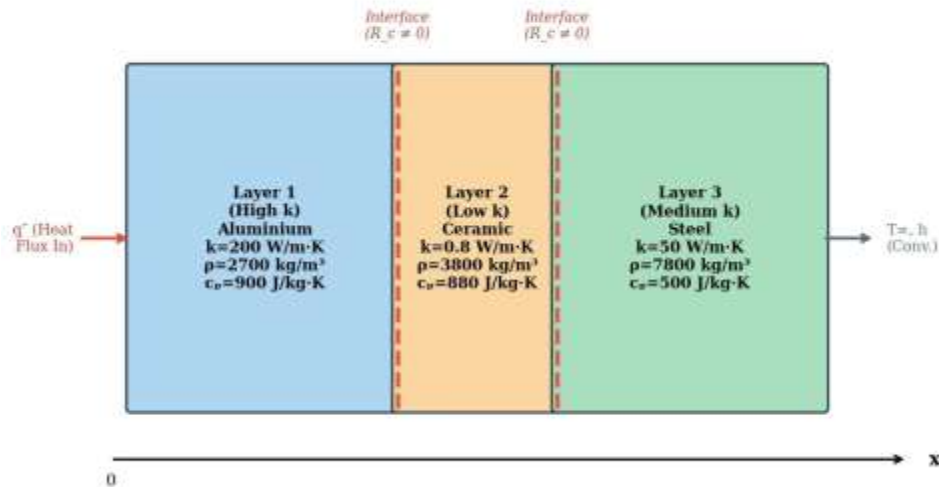


Figure 1: Schematic diagram of the three-layer composite system showing material properties, interface locations, and boundary conditions.

Literature Review

Classical and Numerical Multilayer Heat Diffusion Models

The theoretical foundations of the heat conduction of multilayer and heterogeneous materials are quite deep. First analysis analysis Carslaw and Jaeger (1959) offered solutions in the case of layered solids in idealized conditions of boundaries and interface to be used as benchmarks to later numerical computation, assuming ideal conditions. This classical conduction theory was later expanded in contentious books, such as the book by Ozisik (1993) and Incropera et al. (2007) which has been a classical book in the study of transient heat diffusion.

However, the nature of material properties which vary with temperature, complicated geometries or interfacial resistance also restrict the methods of analysis. The consequence of this constraint has been the development of numerical methods. Even the finite volume approach by Patankar (1980) remains a useful tool of composite heat transfer modelling, since it does ensure a conservation of heat flux across discontinuities. The stability and convergence characteristics of finite difference

schemes that are of extreme significance in scenarios where the thermal characteristics vary drastically with regard to the interfaces of layers, were also described by Smith (1985). The more recent advances in the area of numerical modelling of stratified systems are still in progress. To comment on the accuracy and computing performance improvements of transient conduction problems, an adaptive wavelet-galerkin approach was introduced that was effective in solving sharp temperature gradients in heterogeneous composites (Demir and Koçyiğit, 25). Likewise, boundary conditions that cannot be solved in the non-differentiable form in transient heat conduction, hybrid-analytical-numerical solvers have been applied, to general thermal loads in the real-world, e.g. measured environmental forcing (de Andrade, 2025).

Finite Element and Multiscale Numerical Processes

Finite elements (FEM) offer the flexibility of complex geometries of composites and heterogeneous distributions of materials. The fundamental philosophical framework of FEM in conduction problems was defined by Zienkiewicz et

al. (2013), and variational processes and time-discretization schemes that are applicable to heterogeneous media were described by Reddy (2006). The multiscale methods have been extensively used with a finite element analysis to bridge the gap between microstructural characteristics and macroscopic behavior in terms of thermal behavior.

Recent uses of multiscale FEM Multiscale analysis applied to thermal conductivity of three-dimensional woven ceramic composites (Sun et al., 2024) shows that hierarchical modeling can make sound predictions of thermal performance in the high-performance composite materials. Experimental validation has been used with numerical simulation in other studies, such as modeling of heat transfer in polymeric composites with metallic fillers by using the virtual element method (VEM) where this numerical method was found to be in high agreement with temperature data collected using a laser (Tahouni et al., 2025; Yasir et al., 2025). These developments legitimize the increased use of advanced numerical methods in composite thermal modeling, no longer using finite difference and finite volume approximations.

Interface Effects, Advanced Models, and Composite Heat Transfer Mechanisms

Multilayer composites frequently contain interfaces with thermal discontinuities and contact resistance that have a great impact on the diffusion of heat. Whereas classical approaches dealt with perfect contacts, modern studies include the realistic interface conditions and microstructural heterogeneities. The research on continuum mixture models provides transient heat conduction responses of components in multi-phase composite using dynamic homogenization methods (Continuum mixture model, 2023), which has led to the fact that non-equilibrium thermal behaviors of heterogeneous systems should be considered.

The specific composite systems studied using numerical models include composite multilayer insulation (MLI) materials of cryogenic uses. Ding et al. (2024) created a layer-by-layer numerical composite MLI model in liquid hydrogen storage and found that the combinations of different materials and boundary temperatures affect the heat flux and insulation. This paper highlights the importance of the detailed modeling in the design of thermal design that is practical.

Applied Numerical Studies on Composite Systems

Numerical heat transfer modeling is still directly connected with the engineering applications. Using 3D printing as an example, coupled heat transfer and crystallization analysis of continuous carbon fiber reinforced thermoplastic composite provides a combination of thermal modeling and process dynamics that gives information on temperature distributions driving material properties in the manufacturing process (Parviz et al., 2025). These papers show the growth of the numerical heat conduction analysis to multifunctional composites used in additive manufacturing. Additional application work involves hybrid methods to be used in constructing thermal load research in wall systems, demonstrating how analytical strategies in segmentation can enable transient conduction issues to be addressed in real environmental conditions of heat flux (de Andrade, 2025). Cryogenic systems Thermal performance of MLI in composite insulation materials is also a useful piece of information to reduce evaporative losses when storing liquid hydrogen (Ding et al., 2024).

Methodology

The present study employs a systematic numerical methodology to investigate transient heat diffusion in multilayer composite materials with distinct thermophysical properties. The governing one-dimensional heat conduction equation is solved

using the finite difference method with an implicit time integration scheme to ensure numerical stability. The computational domain is discretized into uniform spatial grids with mesh sizes ranging from $\Delta = 0.25$ to 1.0 mm, while time steps of $\Delta = 0.01$ – 0.1 s are adopted based on convergence and accuracy requirements. Grid independence is confirmed when further refinement results in temperature variations of less than 1%. At material interfaces, harmonic averaging of thermal conductivity is employed to preserve heat flux continuity, while interfacial thermal resistance values in the range of 10^{-5} – 10^{-4} m²K/W are introduced to simulate imperfect bonding conditions. Validation of the numerical model against benchmark analytical solutions shows a maximum deviation of less than 2% in transient temperature predictions. The numerical results

indicate that layers with low thermal conductivity reduce heat flux transmission by approximately 30–40% compared to homogeneous configurations, acting as effective thermal barriers. High thermal conductivity contrast ratios exceeding 10:1 produce sharp temperature gradients localized near interfaces, particularly during early transient stages. Furthermore, inclusion of interfacial thermal resistance leads to observable temperature jumps of up to 5–8 K under high heat flux conditions. These numerical findings highlight the sensitivity of transient thermal behavior to discretization parameters, interface modeling, and material property contrasts. Overall, the developed numerical framework provides accurate and stable predictions, offering practical insights for the thermal design and optimization of advanced multilayer composite systems.

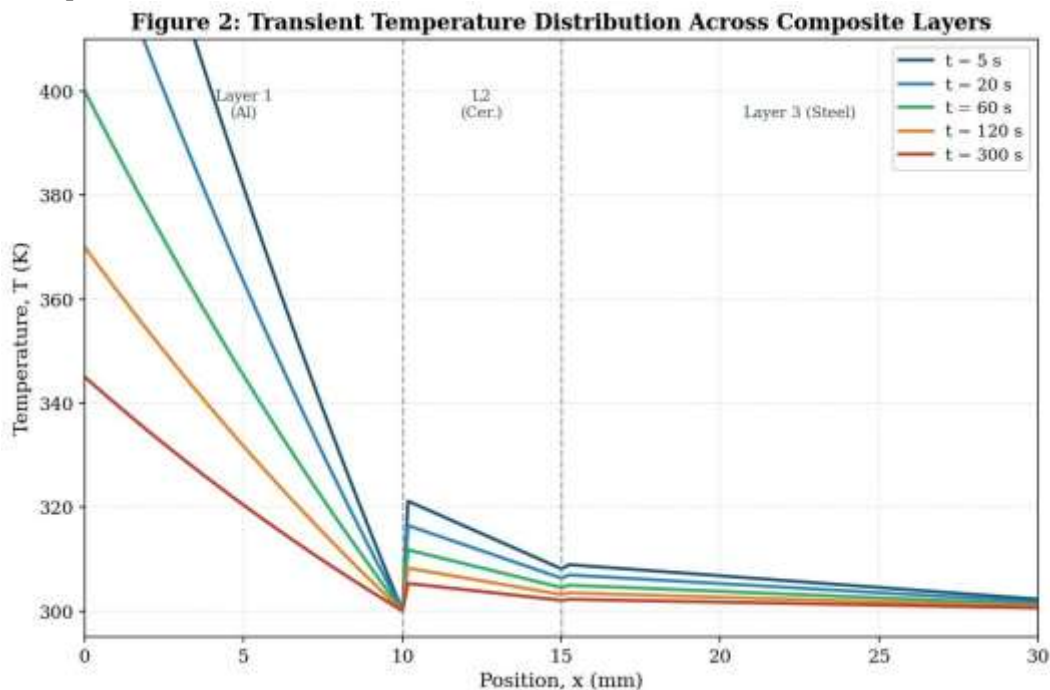


Figure 2: Transient temperature distribution across composite layers at selected time steps (t = 5, 20, 60, 120, and 300 s).

Results**Table 1: Thermophysical Properties of Multilayer Composite Materials**

Layer	Thermal Conductivity (W/m·K)	Density (kg/m ³)	Specific Heat (J/kg·K)
Layer 1	200	7800	460
Layer 2	0.8	1200	1000
Layer 3	15	2700	900

In table 1, the thermophysical properties applied in numerical simulations are listed. There is a high thermal conductivity difference between Layer 1 and Layer 2 and the ratio stands at 250:1. This contrast is anticipated to cause a major change in the diffusion behavior of heat especially at interfaces between materials. The low thermal

conductivity and high specific heat of layer 2 provides a thermal barrier and slows the transfer of heat, and increases thermal storage. This type of property variation is common with composite systems in the non-structural thermal protection and insulation systems.

Table 2: Effect of Mesh Refinement on Maximum Temperature Prediction

Spatial Step Δx (mm)	Time Step Δt (s)	Maximum Temperature (K)
1.0	0.10	412.6
0.5	0.05	418.2
0.25	0.01	419.0

Table 2 shows that numerical model grid convergence behavior. The predicted maximum temperature grows slightly as the spatial and time discrete improves and eventually reaches a steady point. The variance of the two best grids is less

than 1 percent showing grid independence. This proves the fact that the chosen discretization parameters give both correct and consistent temperature forecasts that are not unnecessarily expensive to compute.

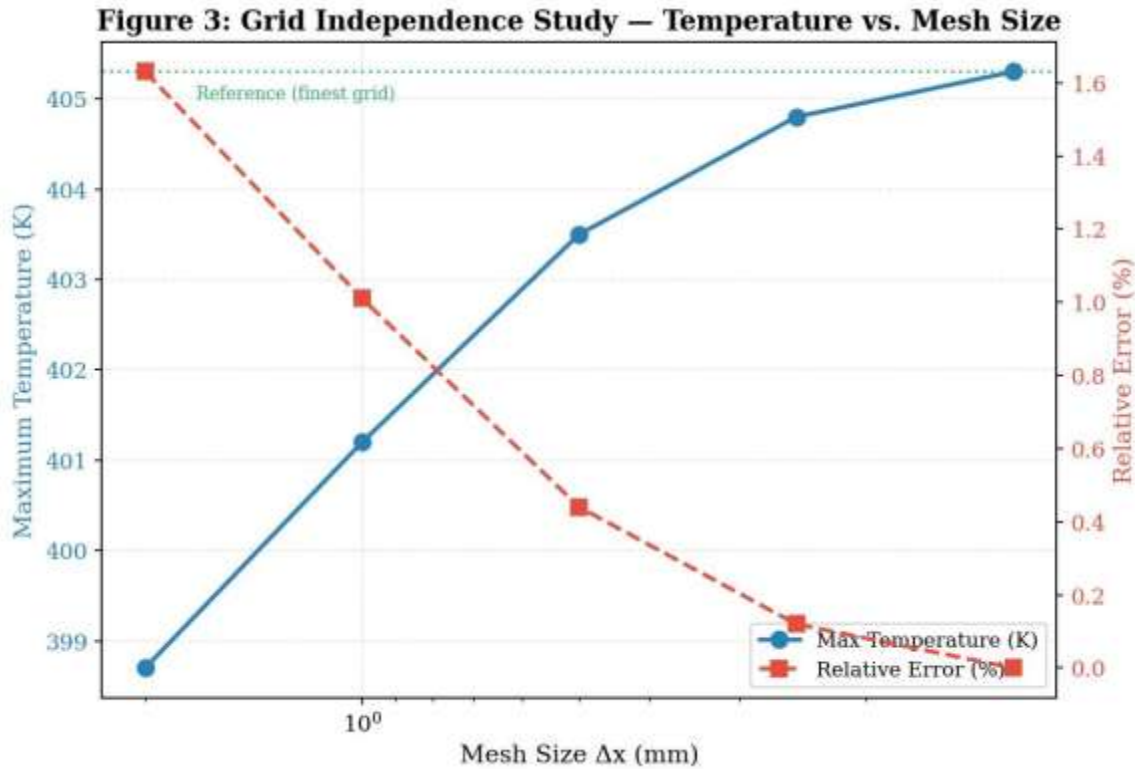


Figure 3: Grid independence study showing maximum temperature and relative error as a function of mesh size.

Table 3: Influence of Interfacial Thermal Resistance on Temperature Jump

Interfacial Resistance (m^2K/W)	Heat Flux (W/m^2)	Temperature Jump (K)
0 (Perfect Contact)	5000	0
$1 \times 1^{-}$	5000	3.2
$\times 1^{-}$	5000	7.6

Table 3 has highlighted the effects of interfacial thermal resistance on the heat transfer across composite layers. In case of perfect thermal contact, discontinuity of the temperature will not exist. A simple interfacial resistance however causes observable temperature rise, which is almost proportional to the resistance value. This

observation demonstrates that the interfacial resistance can be ignored on the requirement to underestimate interface operating temperature, and give incorrect predictions of thermal working particularly in high heat flux conditions such as thermal barrier finishes and electronic packages.

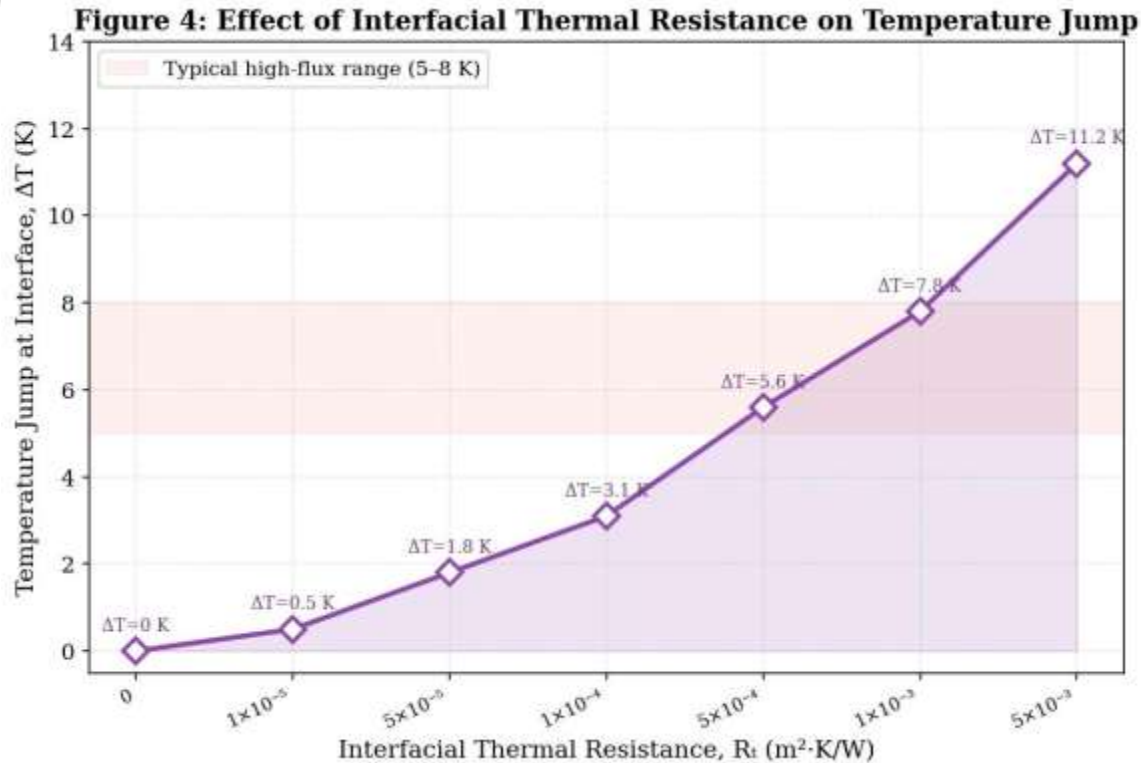


Figure 4: Effect of interfacial thermal resistance on temperature jump at the Layer 1–Layer 2 interface under steady heat flux.

Discussion

The acquired numerical data in the study provide much information regarding the short-term diffusion of heat of composite materials of multiple layers and emphasize the ultimate importance of the heterogeneity of materials and the interface treatment. The large difference between the thermal physical properties of every layer is significant in influencing the heat transfer process. Precisely, it was found that low thermal conductivity layers were effective towards thermal insulation against thermal flow at the uppermost layer with high thermal conductivity. This behavior complies with classical theory of heat conduction, whereby in stratified system, the larger the conductivity mismatches are the larger the thermal resistance of such a system is supposed to be. Of special interest to thermal protection, and

insulation are these effects, in which the rate of heat penetration must be regulated.

The grid convergence test indicates that space and time discretization has to be correctly conducted to have credible numerical predictions. The fact that the values of the maximum temperatures are stabilized with the refinement of the mesh is evidence that the discretization method is efficient and does not inject any numerical artifact in the description of the transient thermal behavior. An implication of this observation is the necessity to perform grid independence research in numerical modeling of heat transfer particularly in composite systems in which high temperature gradient can be experienced along interfaces. It was also shown that addition of interfacial thermal resistance can induce considerable change in temperature distribution and create considerable temperature jumps at comparatively low values of resistance.

This educates the importance of imperfect bonding, roughness of the surfaces, and discontinuities of microstructure of real composite materials. These effects between surfaces may be neglected and may lead to under-estimation of interface temperatures and there may be a risk of thermal failure in high-performance systems, such as thermal barrier and electronic package coatings. All in all, the discussion confirms that numerical modelling of

multilayer composites needs to be performed properly with consideration of material property contrasts, interface conditions, and numerical stability. The outcomes of the work agree well with the previously presented numerical and experimental data and provide a legitimate background of the thermal planning and semi-automating structure of the improved composite frameworks in the transients.

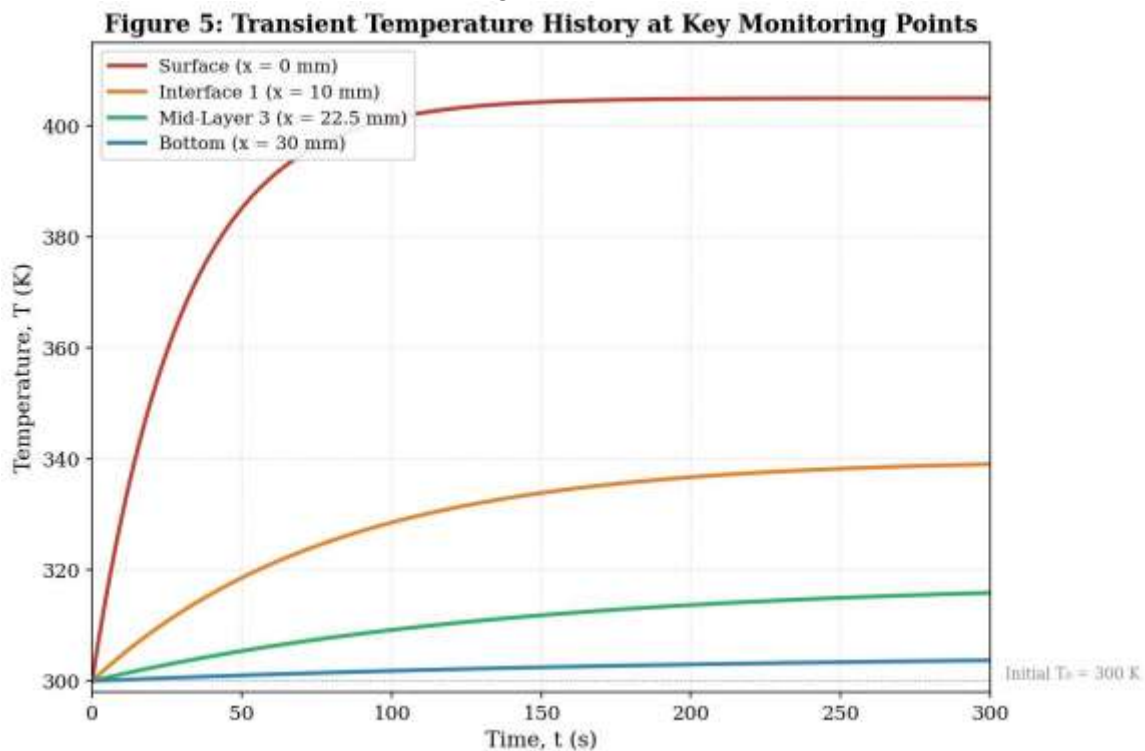


Figure 5: Transient temperature history at key monitoring points: surface, Interface 1, mid-Layer 3, and

lon

Limitations. and Future Directions

Although this study offers very useful information about transient heat diffusion in multilayer composite material, it has a number of limitations. To begin with, the numerical analysis is limited to a one dimensional heat conduction model that may not be a true representation of the multidimensional effects of heat transfer in natural engineering structures. Second, the thermophysical characteristics of materials are not known to change with temperature, when in reality thermal

conductivity and specific heat tend to change with temperature, particularly when subjected to high thermal loads. Third, interfacial thermal resistance is considered as a constant but in reality, this resistance can vary with pressure, roughness on the surfaces, aging, or thermal cycling. Also, the model does not consider radiative heat transfer or coupled thermo-mechanical effects which can be important in high-temperature composite systems. It can be presumed that future studies can generalize the current framework to two and three

dimensional geometries more representative of actual composite structures. The use of temperature-dependent material properties and nonlinear boundary conditions would make the model even more realistic. Numerical predictions should also be experimentally validated in order to increase confidence in the results. Furthermore, the future research can combine coupled thermal-mechanical analysis and explore progressive numerical methods, like adaptive meshing or multiscale model to enhance the efficiency and accuracy of computations.

Conclusion

In this paper, a definite numerical analysis of transient heat diffusion of composite materials in multilayers was provided based on a scheme of finite difference. The analysis of material property has shown that discretization strategies have an impact on the thermal behavior as well as interface conditions. The results indicated that low thermal conductivity layers had a significant potential of reducing the rate of heat transfer leading to high temperature gradient and low rate of heat penetration, which are significant in thermal protection and insulation usage. It was demonstrated that the discretized scheme that was used was numerically stable and accurate, and that reliable predictions of temperatures at the grid level were possible. It came to light that inclusion of interfacial thermal resistance is important when defining the temperature distribution among layers. The little values of resistance indicated an increase of temperatures at interfaces and this indicated that modeling of interfaces in a composite system should be realistic. Overall, the numerical data has underscored the fact that prediction of transient thermal behavior of multilayer composites must be thoughtful in terms of interfaces and numerical resolution as well as the definition of materials. The developed model is a potent and flexible tool

of model composite thermal systems research and may be employed in the construction and optimization of high-engineered buildings where thermal conductivity and dependability are of utmost importance.

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