

# Heat-Kernel Parametric Model of Heat Transfer through Layered Materials

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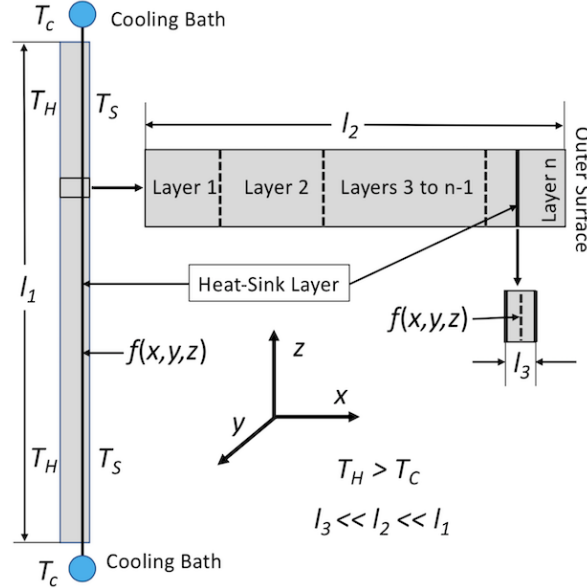
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## Introduction

The control of heat transfer through multilayer materials is significant for many applications, ranging from heat treatment of materials to thermal management of systems. Optimizing heat transfer through multilayer materials requires estimating the thermal response of layered composite materials. This can be achieved using parametric models that combine heat transfer characteristics of a specified layered system and thermal material properties, enabling prediction of temperature fields. These models should be conveniently adaptable for estimating the thermal response of different types of layered materials. This study presents a parametric model of heat transfer through a layered material system. The parametric model is motivated by welding processes [1,2], where workpiece temperatures are controlled by material composition and thermal contact to base plates. The control of heat transfer through multilayer materials can also utilize heat sinks. The general physical character of heat sinks is that their thermal diffusivities are substantially greater than those of the workpieces whose temperature fields are to be controlled [3,4]. Accordingly, thermal coupling of heat sinks to adjacent layers can be represented parametrically by phenomenological negative heat sources [5].

Parametric modeling of temperature fields follows the approach of inverse analysis [6], i.e., inverse thermal analysis [7-12], which is for estimating optimal parameter values for a given system specification. The parameter values (e.g., effective thermal diffusivities) should be achievable for realistic system design. For complex material systems, the determination of material response functions is well posed in terms of inverse analysis. The multiscale character of layered materials poses an inverse analysis problem, which follows from the realization that layered-material thermal properties are not the same as those of bulk materials. In addition, for layered materials there is typically influence on thermal transport due to advection at bounding surfaces of the layered system. Accordingly, parametrization should be extended to include effective diffusivities, which are based formally on replacing the advection-diffusion operator with an effective-diffusion operator. Physically, advection is not expected to manifest as influencing thermal transport locally within a layered-material system, but rather as influencing thermal transport over the its entire length of the layered system. Accordingly, the phenomenological influence of advection, which is associated with ambient environments at surface boundaries of a layered-material system, again poses a problem of inverse thermal analysis for determination of effective diffusivities. Finally, heat transfer across interfaces of layers making up a layered material system can be effectively singular with respect to heat transfer trend characteristics because of thermal contact resistance and possible large differences of thermal diffusivity. Accordingly, with respect to parametric modeling, an interface may be represented by a layer having singular characteristics with respect to heat transfer. Heat transfer through a characteristically singular layer from adjacent layers of material will depend on the characteristic thermal coupling of layer interfaces, which again is a complex material property, not known *a priori*, and thus appropriately posed for inverse thermal analysis.

There exists different types of configurations for heat sink coupling to a heated system. The parametric model considered here, for heat sink coupling to a heated layered system, is described schematically in Figure 1, where coupling occurs at edges of the system. This configuration poses a specific problem with respect to inverse thermal analysis.



**Figure 1.** Schematic representation of parametric model defined by Eqs. 1-5 described below. for layer and heat sink controlled heat transfer in layered materials, where  $T_H$  and  $T_S$  are temperatures of heated surface and surface at ambient atmosphere.

This study presents a parametric model for heat transfer through layered material systems, formally based on the heat kernel solution of the heat conduction equation [5], which includes effects of multiple layers with varying thermal diffusivities, interface effects (e.g., large changes in thermal properties), contact resistance, and the effects of singular heat sinks (represented by negative heat sources). This model is structured for analysis of both steady state and time-dependent heat transfer, in thin layered materials. In addition, this model is combined with another parametric model of heat sink cooling, which is based on a specific interpretation of Rosenthal equation for a moving heat source [2]. This interpretation is discussed elsewhere. Organization of subject areas presented are as follows. First, a parametric model of temperature fields for layer controlled heat transfer in layered materials is presented. Second, prototype analyses using the parametric model are described. Finally, a discussion and conclusion are given.

## Parametric Model

Presented in this section is a parametric model for heat transfer through a thin layered material heated at one surface, with transfer of heat to an ambient environment at the other surface by means of radiation and convection, with the possibility of heat sink channel cooling, at steady state. This model is based on formal extensions and approximations of analytical solutions to the heat conduction equation [3,6], and is given by

$$T(x, y, z) = T_H \exp \left[ -\frac{1}{4\tau_H} \left( \frac{x - x_n}{\sqrt{\kappa_n}} + \sum_{k=0}^{n-1} \frac{x_{k+1} - x_k}{\sqrt{\kappa_k}} + \sum_{j=1}^{N_j} \frac{u(x - x_j)}{\sqrt{h_j}} \right)^2 \right] - f(x, y, z) \quad \text{Eq. 1}$$

$$f(x, y, z) = g(y, z) \exp \left[ -Q_x \frac{|x - x_{hs}|}{g(y, z)} \right] \quad \text{Eq. 2}$$

$$g(y, z) = h(z) \exp \left[ -Q_y \frac{|y - y_{hs}|}{h(z)} \right] \quad \text{Eq. 3}$$

and

$$h(z) = \Delta T_c \exp[-Q_z |z - z_{hs}|] \quad \text{Eq. 4}$$

The quantities  $h_j, j = 1-N_j$ , are the interface contact-diffusivity parameters (analogous to contact conductance) whose units are 1/s, where locations of layer-layer interfaces are at  $x = x_j$ , and  $u(x)$  is the Heaviside unit step function. The source function  $f(x, y, z)$  is the 3D cooling field of the heat sink. The quantities  $\tau_H, Q_x, Q_y$ , and  $Q$  which are formally a delay time and cooling fluxes, specify heat flux at the heating boundary (parameter  $\tau_H$ ) and strength of coupling of heat sink layer to a cooling bath (parameter  $Q_z$ ) to adjacent material layers (parameters  $Q_x$  and  $Q_y$ ). Note that physically, for a given location  $(x, y, z)$ , heat sink cooling is formally for all  $x, y$  and  $z$ . Our goal, however, is parametric modeling of heat transfer to the surface of the layered system, and therefore the region  $x > x_{hs}$  is of most interest. The function  $f(x, y, z)$  assumes a model representation that is, in principle, based on either physical assumptions, i.e., materials having known thermal properties or phenomenological parameters adjusted with respect to measurements. Specifically, the parametric model is defined in terms of adjustable parameters,  $\tau_H, Q_x, Q_y, Q_z$  and  $\Delta T_c$  which are determined in principle according to experimental measurements, i.e., inverse thermal analysis. Similarly, contact conductances  $h_j$  are adjustable parameters to be determined by measurements.

Referring to Eqs. 3 and 4, note that  $0 < y - y_{hs} < L_y$  and  $0 < z - z_{hs} < L_z$ . The quantity  $L_z$ , which for present simulations has arbitrary units, is scaled according to the transverse length  $l_l$  coupled to cooling bath as shown schematically in Figure 1. The quantity  $L_y$  (not considered here), together with  $L_z$ , represent two-dimensional coupling to a cooling bath.

Next, given a surface boundary at  $x = x_s$ , and letting  $T_S = T(x_s, y, z)$ , defined by Eq. 1, for  $x > x_s$ ,

$$T(x, y, z) = \min[T_A, T_S] + (T_S - \min[T_A, T_S])e^{-\frac{Q_s(x-x_s)}{T_S}(\frac{x-x_s}{k_A})} \quad \text{Eq. 5}$$

where

$$Q_s = h_c(T_S - \min[T_A, T_S]) + \varepsilon\sigma(T_S^4 - (\min[T_A, T_S])^4) \quad \text{Eq. 6}$$

The quantities  $h_c$ ,  $\varepsilon$ ,  $\sigma$ , and  $T_A$  are the convective heat transfer coefficient, emissivity of the outer surface, Stefan-Boltzmann Constant ( $5.6704 \cdot 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$ ) and the ambient temperature at the outer surface, respectively. Equations 1-6 define a parametric model for heat transfer through a layered material, from a hot body to a ambient environment external to the outer surface, with cooling due to an embedded heat sink.

### Structure of Parametric Model

This section examines the formal structure of the parametric model defined by Eqs. 1-6, which is for heat transfer through a thin layered material, heated at one surface, with transfer of heat to an ambient environment at the other surface by means of radiation and convection, with the possibility of heat sink channel cooling. Heat transfer is assumed either at steady state or time dependent. Time dependency of heat transfer is assumed to be measured and represented parametrically by means of time-delay parameters according to inverse thermal analysis. This model is based on formal extensions of heat-kernel solution to the heat conduction equation [5], given by

$$T(x, t) = \frac{C_o}{\sqrt{4\pi\kappa_0 t}} \exp\left[-\frac{(x - x_0)^2}{4\kappa_0 t}\right] \quad \text{Eq. 7}$$

Before proceeding with application of the model, there are key aspects of the type of layered system considered (see Figure 1), and its parameteric-model representation Eqs. 1-6, that should be emphasized for model-parameter interpretation. These are:

1. The heat-kernel Eq. 7 is a convenient ansatz for parametric representation of time evolution, i.e., time-dependent heat transfer.
2. For both steady state and time-dependent heat transfer, the time-delay and cooling-flux parameters can be given physical interpretations.
3. The parametric model assumes that contact conductance between layers is dominant with respect to influencing heat transfer through the layered material system, relative to the influence of changes in thermal properties across an interface.
4. The parametric model Eqs. 1-6 is convenient for parameter adjustment with respect to boundary conditions on the system shown in Figure 1.
5. The thermal diffusivities can be either measured quantities (i.e., material properties), or adjustable phenomenological parameters.
6. The delay-time  $\tau_H$  is a parameterization of the heat flux from the heating body, while cooling fluxes  $Q_x$ ,  $Q_y$  and  $Q_z$  are parameterizations of heat sink cooling, which include influence of thermal properties, and heat sink coupling to cooling bath and adjacent layers.

The time-delay parameter  $\tau_H$  may be interpreted by considering heat transfer to first order. Specifically, that the heat flux  $Q_H$  given by

$$Q_H = -k \frac{dT}{dx}, \quad \text{Eq. 8}$$

for conductance  $k$ , integrated over interval  $(x, x_s)$  for a surface at  $T_H$ , gives

$$T(x) = T_H - \frac{Q_H(x - x_o)}{k}. \quad \text{Eq. 9}$$

Next, Eq. 7 is reformulated to satisfy two boundary conditions, which are temperatures at the heating and outer surface boundaries of the layered material, and is thus

$$T(x) = T_H \exp \left[ -\frac{(x - x_o)^2}{4\kappa_0\tau_H} \right] \quad \text{Eq. 10}$$

Next, assuming  $(x_s - x_o)$  is small, consistent with the condition of a thin layered material, it follows that

$$T(x) \approx T_H \left[ 1 - \left( \frac{\rho C_p (x_s - x_o)}{4\tau_H} \right) \frac{(x - x_o)}{k} \right] \quad \text{Eq. 11}$$

Comparing Eqs. 9 and 11,

$$Q_H = \frac{T_H \rho C_p (x_s - x_o)}{4\tau_H} \quad \text{Eq. 12}$$

It follows from Eq. 12 that the delay-time parameters, for “thin” layered materials (systems of our consideration) are inversely proportional to heat fluxes (or cooling fluxes), and accordingly, are physically consistent parameterizations of these fluxes.

An important property of Eq. 1 is that, although it is structured for convenient encoding of time-dependence, based on the underlying heat-kernel ansatz, its mathematical property is that of tending toward piecewise linearity, i.e., formally Eq. 12. This is a manifestation of the underlying system, which is a “thin” layered material. This same property, tending to linearity, applies to Eqs. 2-4, representing heat sink coupling. The ansatz for these equations is the Rosenthal steady-state solution of the heat conduction equation, which is formally structured for heat transfer over extended spatial regions, as occurring in welding processes. Equations 2-4 are structured, however, for convenient inverse thermal analysis of heat sink coupling to thin layered materials.

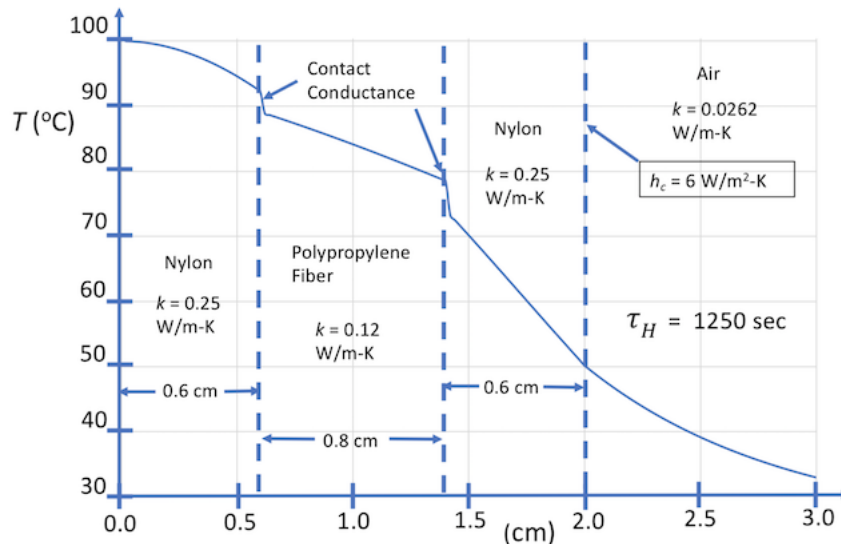
Temperature fields associated with both time-dependent and steady state heat transfer over an extended spatial region, as in welding processes, based on their spatio-temporal characteristics, may be modeled parametrically using linear combinations of weighted heat-kernel solutions, i.e., sums of heat-kernel puffs. This type of representation requires adjusting sets of weight coefficients according to evolving temperature fields extending over space as a function of time, and eventually achieving steady state. The property of Eq. 1, tending towards piecewise linearity, implies that a single heat-kernel puff is sufficient for parametric representation.

## Prototype Analyses

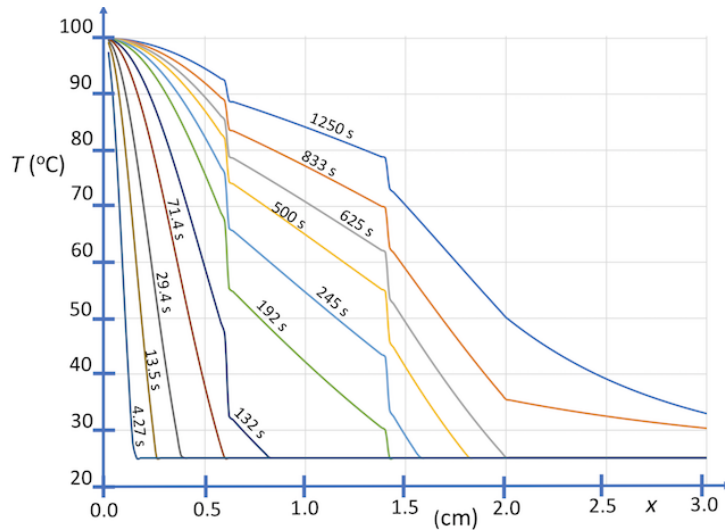
This section presents computational experiments describing parametric modeling of layer-configuration and heat sink controlled thermal transport within a layered material system. The design of these experiments, using physically realistic thermal properties and phenomenologically adjustable parameters, was not to demonstrate optimal layer-configuration and heat sink thermal control, but rather general characteristics of the parametric model for modeling and simulation of such control, as well as demonstrating feasibility of such control using multilayer and heat sink materials. The computational experiments described in this section represent both prototype inverse thermal analyses and simulations, which are both the goal of parametric modeling.

Our first prototype simulations are of heat transfer from a hot body at 100 °C through a layered system, using the parametric model defined by Eqs. 1-6, which are shown in Figures 2 and 3. These simulations assume contact conductance between layers, represented by equivalent contact diffusivities, which have been determined by inverse thermal analysis. The temperature fields shown in Figures 2 and 3 are modified in computational experiments that follow. Shown in Figure 2 is the temperature field of the layered system at steady state. Shown in Figure 3 is the time-dependent temperature field for evolution of this system to steady state.

Referring to Figure 4, it is shown that the model system represented by Eqs. 1-6 is two dimensional and associated with four boundary conditions, which are specified at the heated and outer-surface boundaries, and at the boundaries  $z = 0$  and  $L_z$ . Again, the quantity  $L_z$ , which for present simulations has arbitrary units, is scaled according to the transverse length  $l_l$  coupled to cooling bath as shown schematically in Figure 1. The time-delay parameter  $\tau_H$  is equivalent to the hot-boundary heat flux, is scaled with respect to measurements.

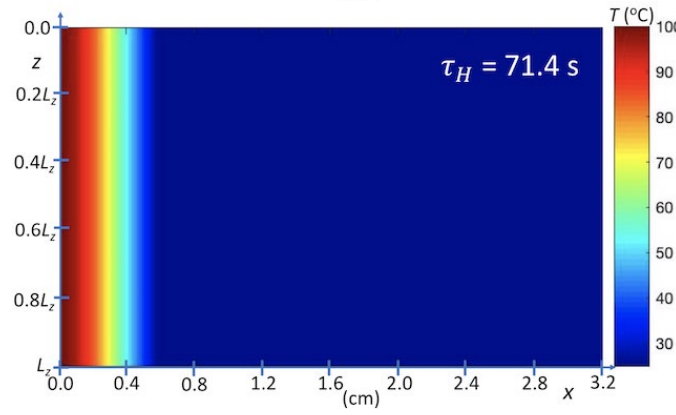
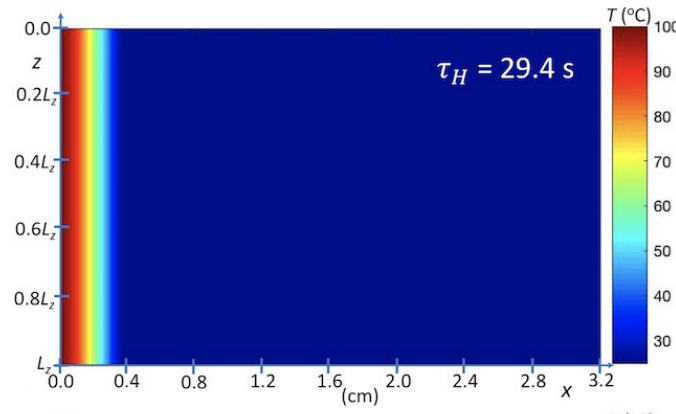
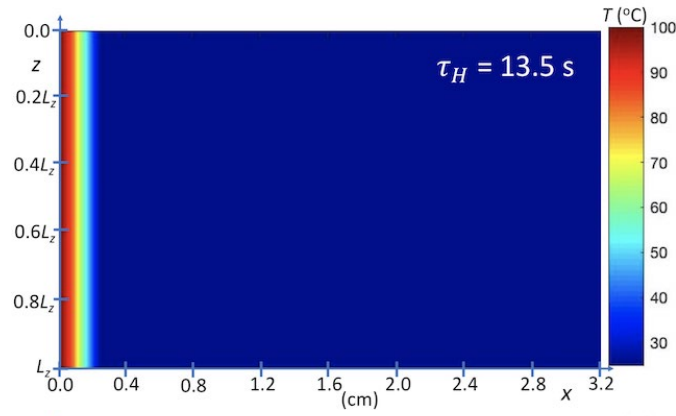
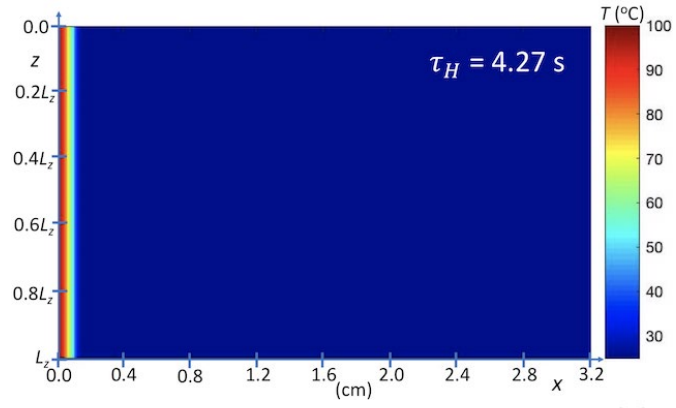


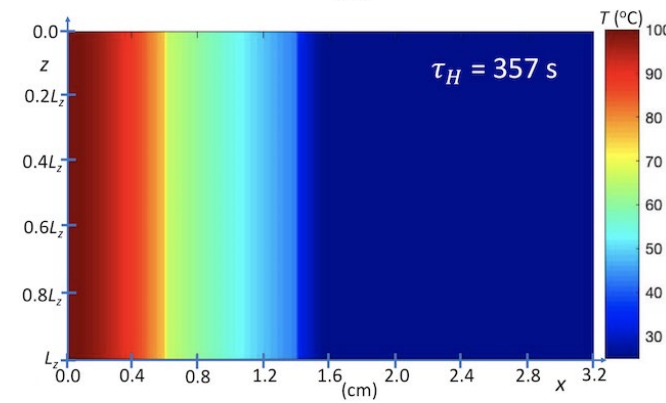
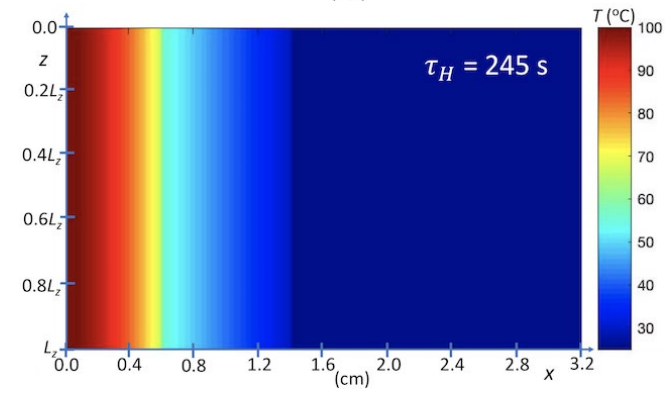
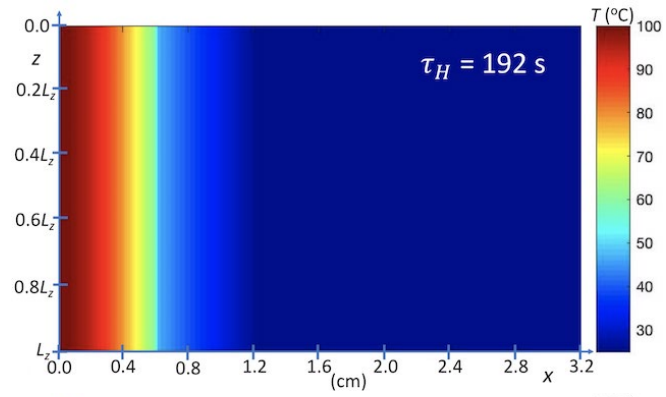
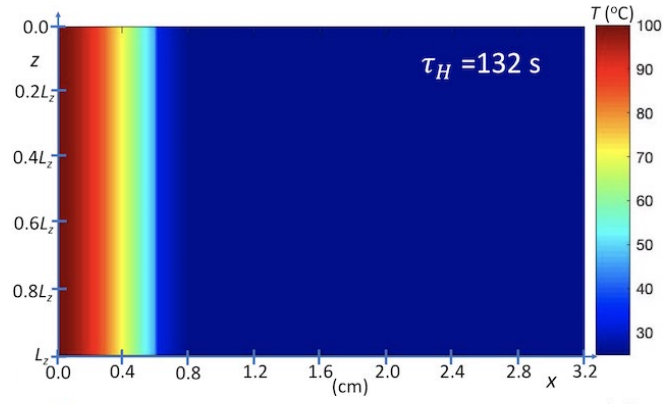
**Figure 2.** Temperature field of basic layered system, at steady state, adopted for prototype analyses.

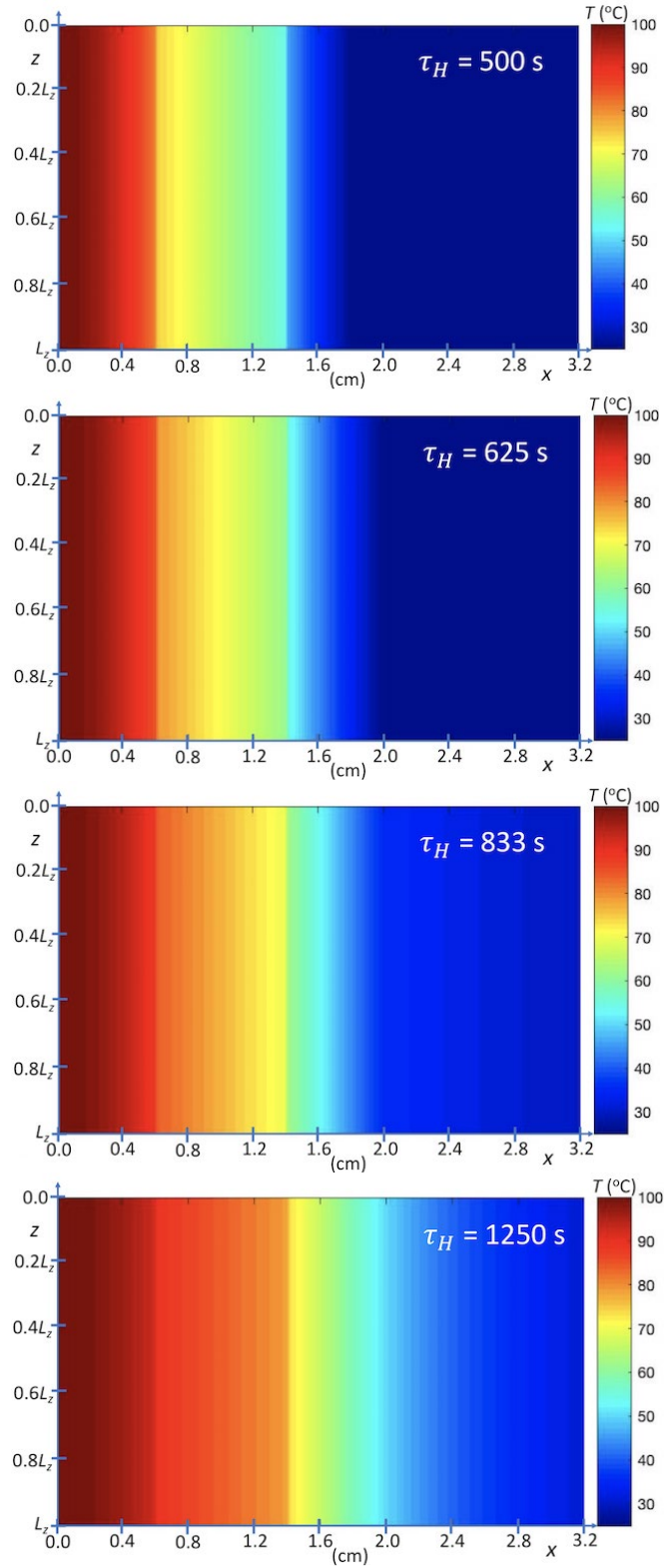


**Figure 3.** Time-dependent temperature field of basic layered system, evolving to steady state, adopted for prototype analyses

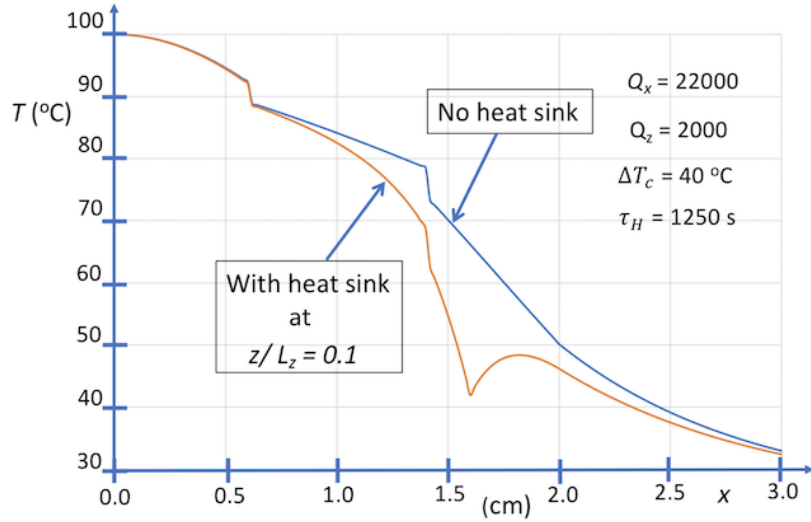
Our second prototype simulations are of heat transfer from a hot body through a layered system, where there is coupling of a highly conductive layer to a cooling bath (shown in Figures 5, 6, 7 and 8), using the parametric model defined by Eqs. 1-6. We note that the cooling layer is not represented explicitly, but phenomenologically. These simulations assume contact conductance between layers, and that heat sink coupling occurs at one or two of the boundaries along  $z$ , as shown in Figures 7 and 8, respectively. As indicated above, the model system, which is 2D, is defined by four boundary conditions. Referring to Figure 5, heat sink boundary conditions at steady state are those of an ambient cooling bath at 42 °C. Referring to Figure 6, heat sink boundary conditions for time-dependent evolution to steady state are those of an ambient cooling bath at 0 °C.



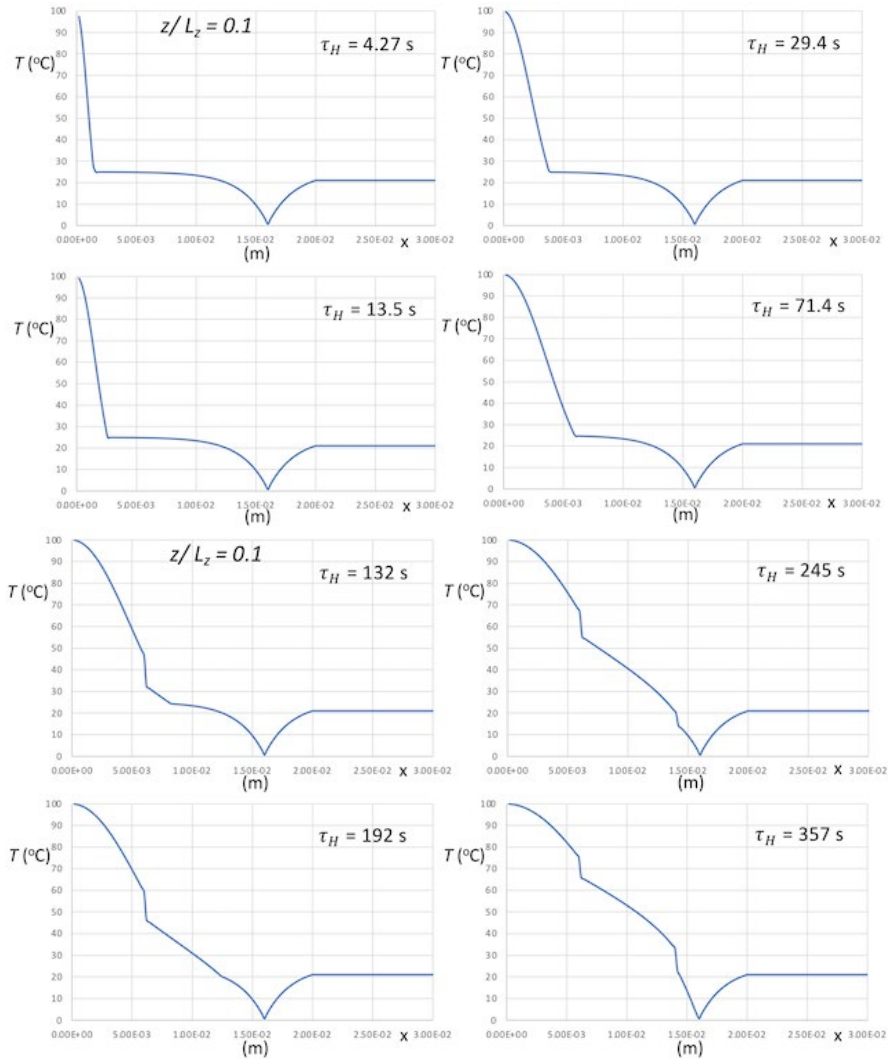


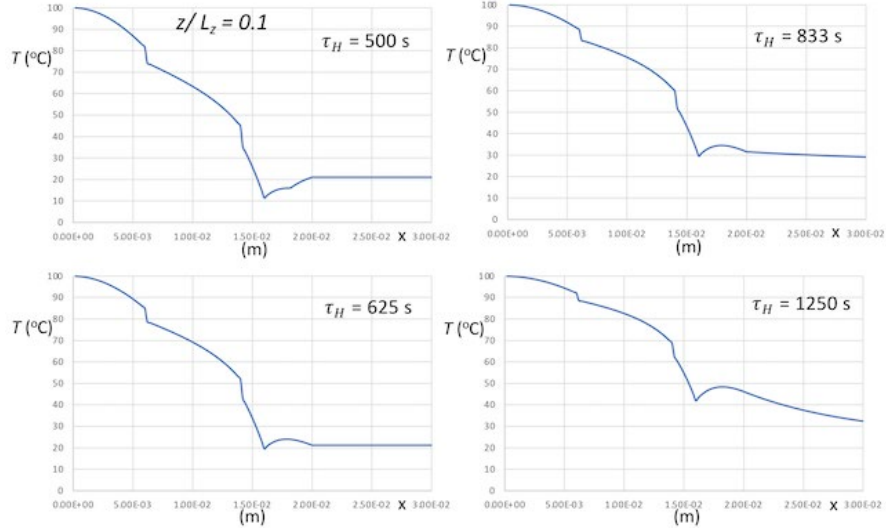


**Figure 4.** Two-dimensional time-dependent temperature field of basic layered system, evolving to steady state, adopted for prototype analyses.



**Figure 5.** Temperature field of layered system, with heat sink at location  $z$  near cooling bath, at steady state.

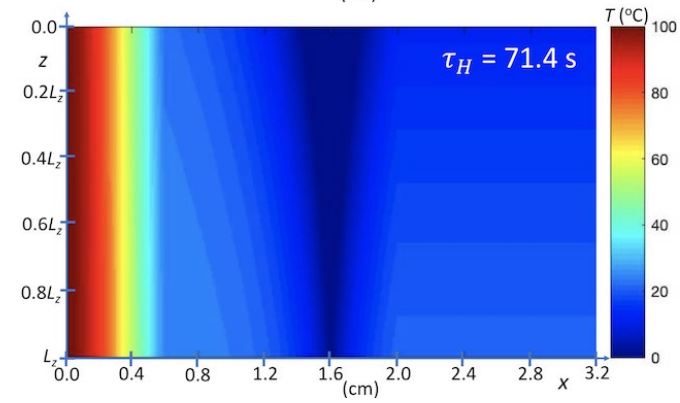
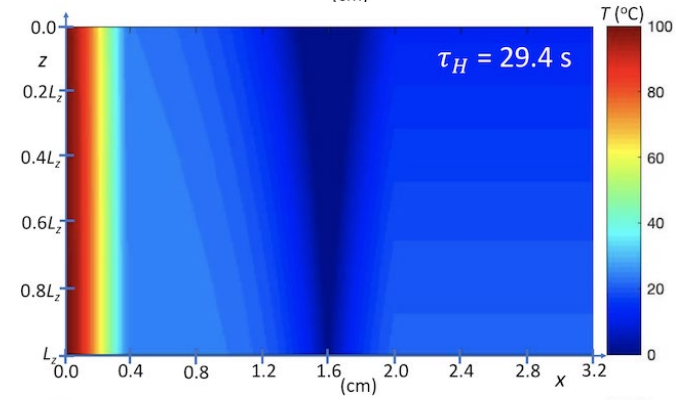
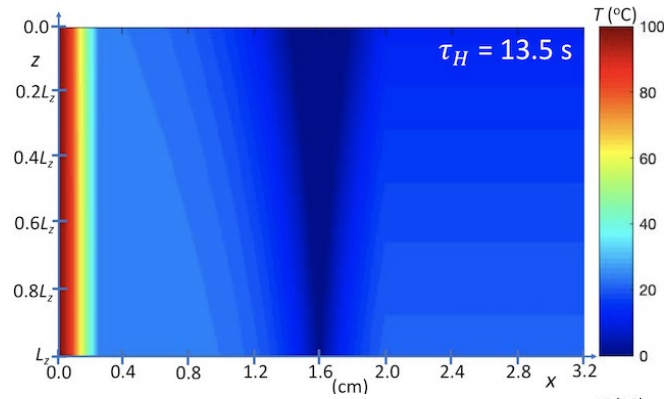
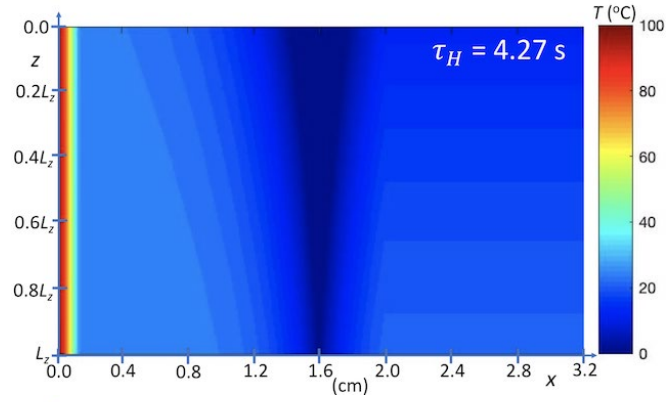


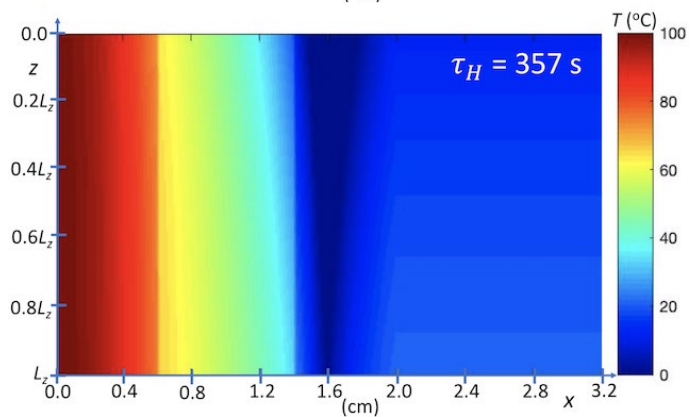
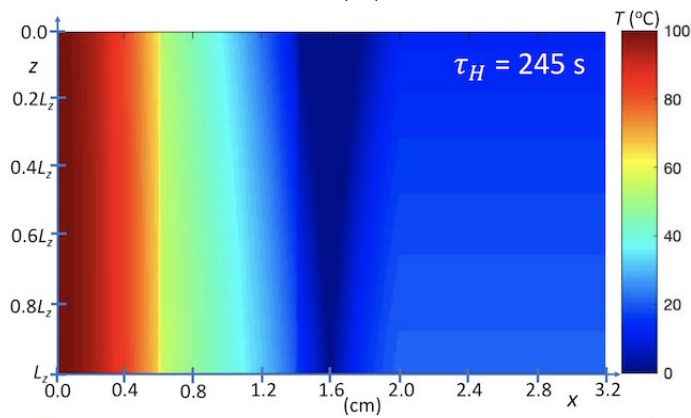
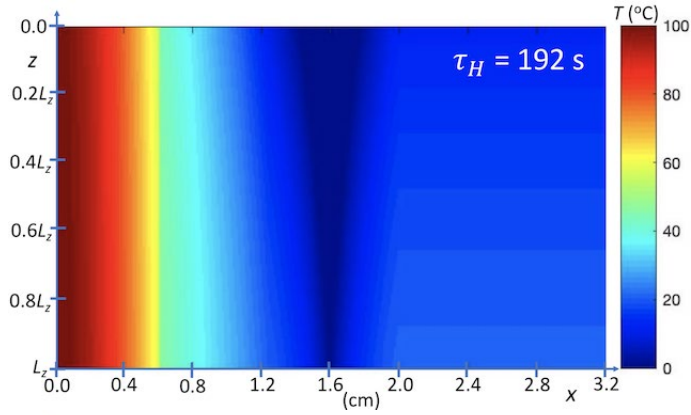
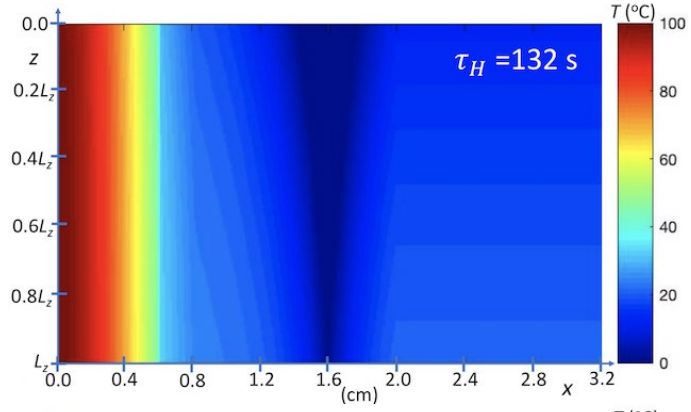


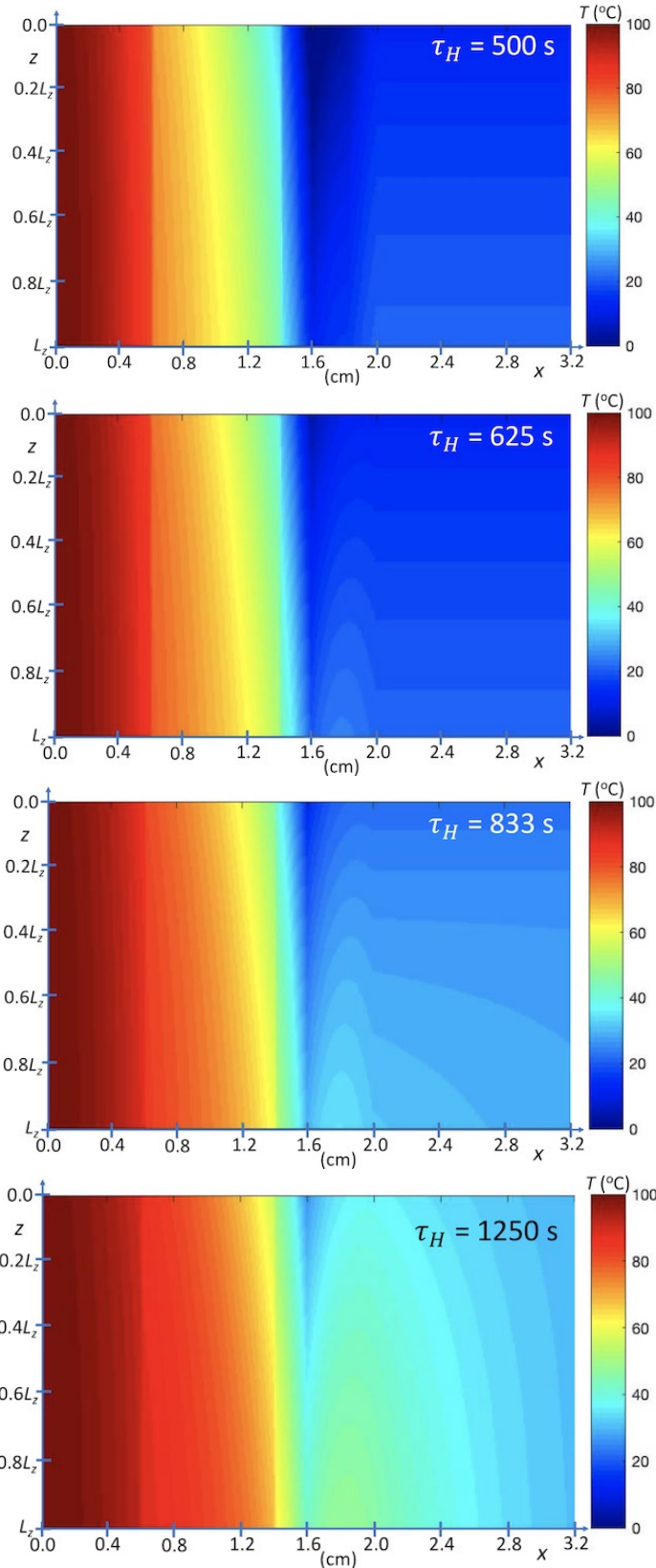
**Figure 6.** Time-dependent temperature field of layered system, with heat sink at location  $z$  near cooling bath, at steady state.

Referring to Figures 7 and 8, it is shown that the model system represented by Eqs. 1-6 is two dimensional and associated with four boundary conditions, which are specified at the heated and outer-surface boundaries, and at the boundaries  $z = 0$  and  $L_z$ . Again, the quantity  $L_z$ , which for present simulations has arbitrary units, is scaled according to the transverse length  $l_l$  coupled to cooling bath (see Figure 1) and the parameter  $\tau_H$ , is equivalent to the hot-boundary heat flux, is scaled with respect to measurements.

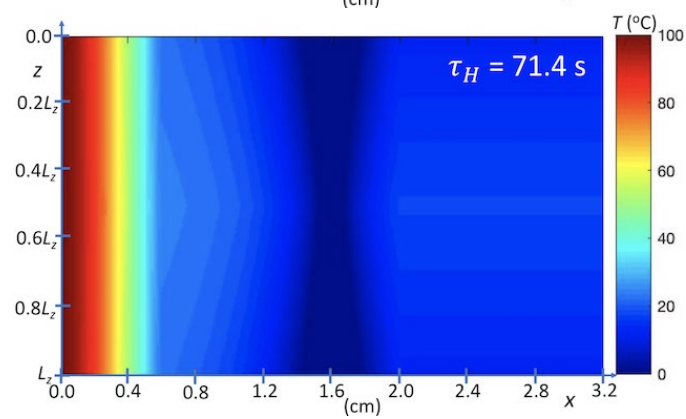
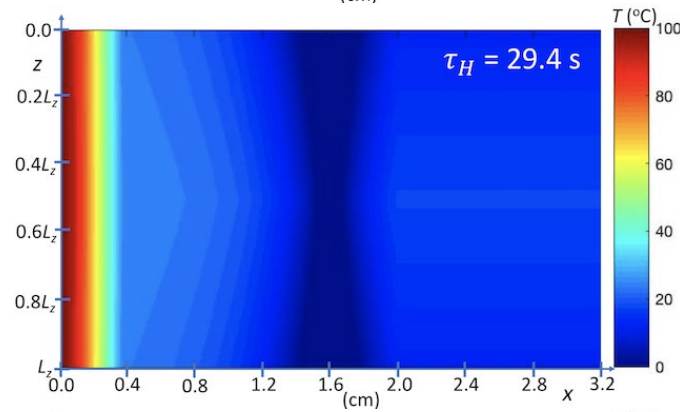
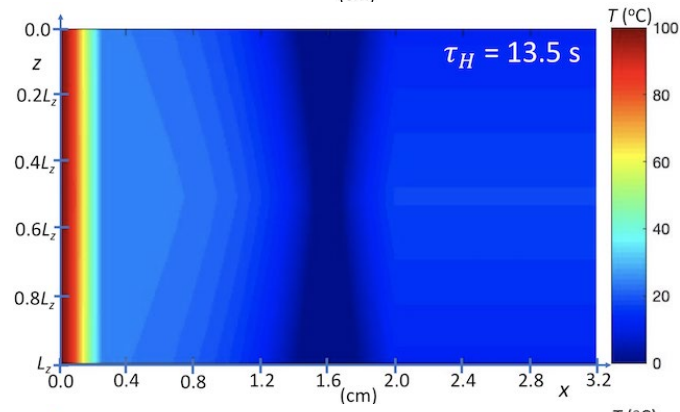
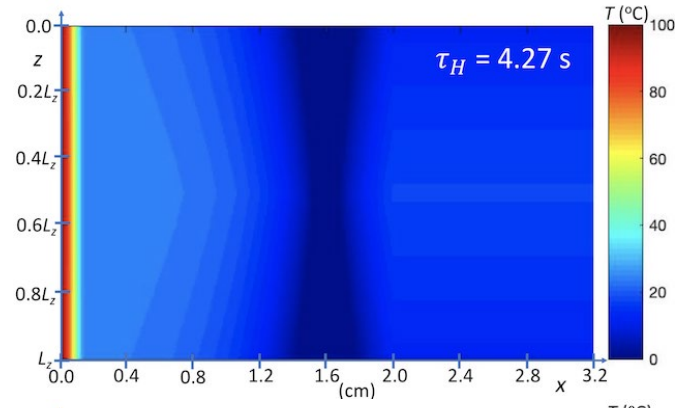
The prototype simulations, whose results are shown in Figures 5 and 6, demonstrate the general procedure for inverse thermal analysis using the parametric model Eqs. 1-6. In reality, a layered material system, where a heat sink is coupled to a cooling bath, is characterized by contact conductances at interfaces between layers (a function of the process used for layering) and anisotropic cooling along and transverse to the embedded heat sink channel. This anisotropic cooling depends on the nature of heat sink-layer coupling to adjacent layers and the cooling bath. Accordingly, design of a heat sink-cooled layered material requires quantification of heat sink coupling that is convenient with respect to inverse thermal analysis. Equations 1-6 define a parametric model requiring a relatively small number of parameters to be adjusted for encoding thermal response characteristics of embedded heat sinks. In essence, the parametric model defined by Eqs. 1-6 adopts an ideal layered system, having no contact conductance, as an initial ansatz to be further adjusted according to inverse thermal analysis of heat sink coupling, where delay-time  $\tau_H$ , cooling fluxes  $Q_x$ ,  $Q_y$  and  $Q_z$ , heat sink coupling parameter  $\Delta T_c$ , are adjustable parameters, and contact diffusivities are determined by inverse thermal analysis. The parametric model Eqs. 1-6 is structured for 3D representation, and thus for the model system considered here, which is 2D, the parameter  $Q_y = 0$ .

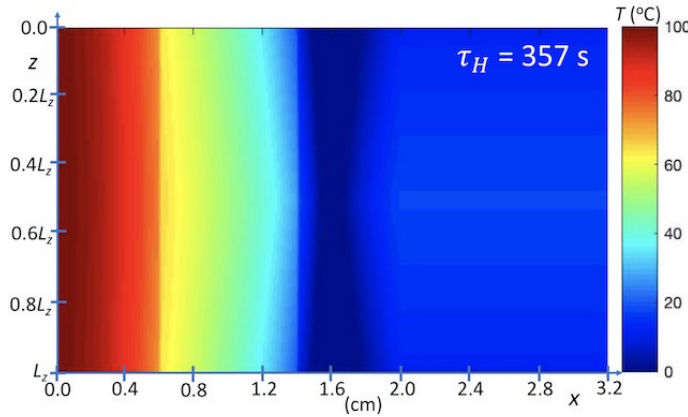
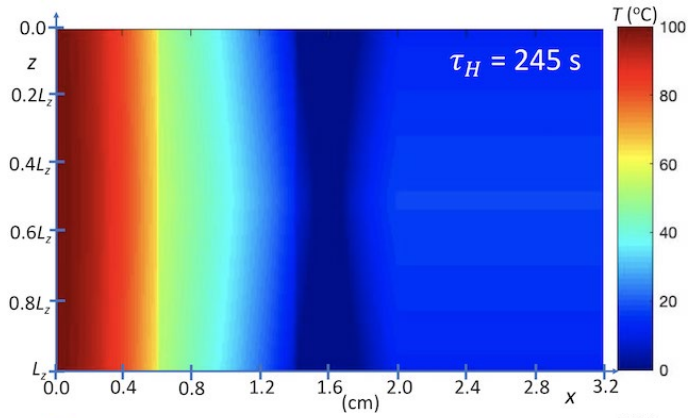
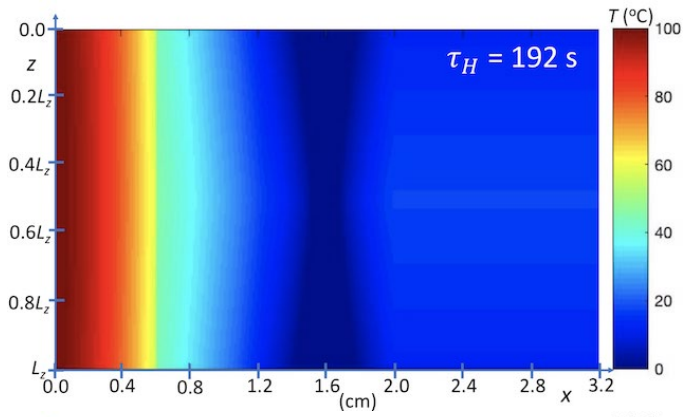
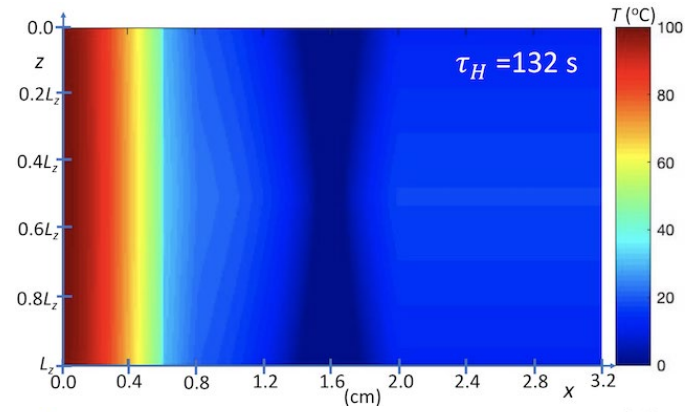


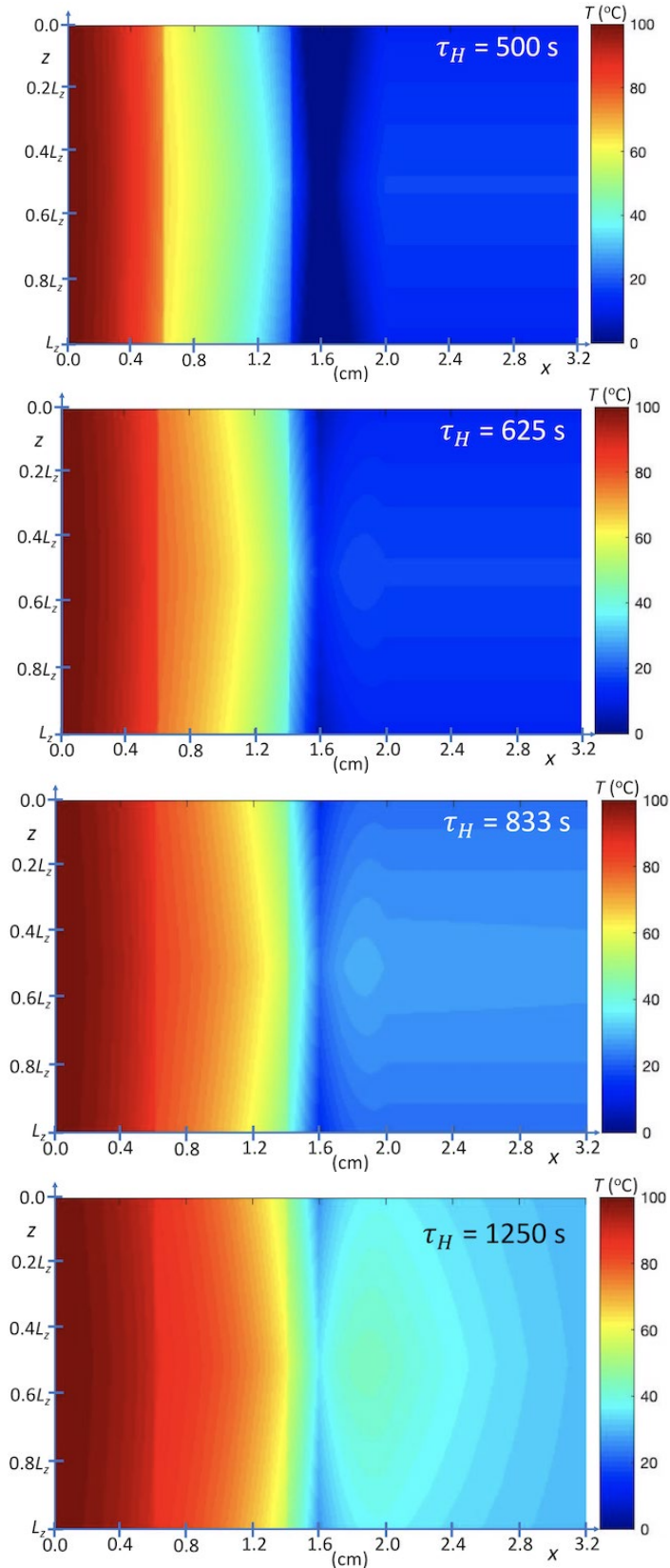




**Figure 7.** Two-dimensional time-dependent temperature field of layered system, with heat sink coupled to cooling bath at one side, evolving to steady state.







**Figure 8.** Two-dimensional time-dependent temperature field of layered system, with heat sink coupled to cooling bath at two sides, evolving to steady state.

## Discussion

The parametric model defined by Eqs. 1-6 is a formal adaptation of the heat-kernel solution of the heat conduction equation for simulation of heat transfer in layered materials, which are coupled to heat sinks at edge boundaries. As described schematically in Figure 1, the model is of a three-dimensional system that approximates heat sink cooling of a heated layered material. The parametric model combines both energy transport through an ideal system of layered materials, not having contact conductance, representing the model ansatz, and phenomenological parameterization for the influence of contact conductance and embedded heat sinks. The parametric model, whose construction is according to physical theory, includes the phenomenological source function  $f(x,y,z)$  representing multiscale coupling of embedded heat sinks, where cooling baths are located at edges of the system. Formulation of the source function  $f(x,y,z)$  is based the Rosenthal equation for a moving heat source [2], which is formally reinterpreted with respect to heat flux at a boundary. This function is structured for encoding of thermal response associated with anisotropic heat transfer at steady state. Determination of anisotropic heat diffusion characteristics poses a problem for inverse thermal analysis. In the spirit of inverse analysis, parameterization of the model is not unique, but adapted for convenience.

The parametric model Eqs. 1-6 poses the problem of generating a parameter space that is sufficiently dense, expansive and bounded, for extraction of estimated parameter values for a given target layered system. Given a parameter space, estimation of target parameter values may be achieved by observation of parameter trends as a function of quantities characterizing a class of layered materials, e.g., material combinations, thickness, contact conductance, and heat sink properties. Estimation of target parameter values can also be achieved using algorithms for searching within parameter spaces. Selection of appropriate parameter-search algorithms poses a problem itself, which should depend on the form of the parameter space.

## Conclusion

Determination of optimal process parameters for achieving a given target temperature field for heat transfer through a layered material using material-layer configurations and heat sinks poses a specific problem. The results of this study demonstrate use and general features of a parametric model, which can provide estimation of heat transfer characteristics for layered materials coupled to heat sinks for both time dependent and steady state systems.

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