



## Incorporating boundary conditions in the heat conduction model

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### ABSTRACT

This note introduces a mathematical derivation of the heat conduction model that incorporates boundary conditions. In particular, in the present approach boundary conditions are derived in parallel to the heat equation, while in the standard approach to heat conduction modelling they are appended at a later stage. Because of its peculiar mathematical formulation, this method allows modelling heat sources or sinks placed on the boundary. Furthermore, it is shown that when such heat sources depend linearly on the surface temperature and the heat flux, each of their points can be described as a point source emitting a heat wave directed into an infinitesimal volume in the neighbourhood of the surface.

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### 1. Introduction

The diffusion of heat, or heat conduction, is a subject extensively discussed both in the classic [1,2] and in the modern [3–5] scientific literature, as well as in heat transfer textbooks [6–8]. As such, one may think there is not much left to say about it. On the contrary, heat conduction is still a rich source of challenging problems for the mathematician, the physicist and the engineer. Examples are the well-known paradox of infinite propagation speed [9–12], and the relation of heat conduction with general variational theorems [13,14].

The standard derivation of any heat conduction model is based on the conservation of energy in a given material domain, which is usually chosen as a sub-set of an Euclidean space ( $\Omega \subseteq \mathfrak{R}^n$ ), surrounded by a smooth boundary,  $\partial\Omega$ . If  $\mathbf{J}$  represents the heat flux, the total heat rate going out of the domain is:

$$\int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} dS \quad (1)$$

where  $\mathbf{n}$  is the outward unit vector normal to  $\partial\Omega$ , and  $dS$  the surface measure on the boundary. Thus, defining  $q$  as the heat stored in the unit volume, one can write the conservation of heat in integral form:

$$\frac{d}{dt} \int_{\Omega} q dV = - \int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} dS \quad (2)$$

which after applying the divergence theorem to the surface integral becomes:

$$\frac{d}{dt} \int_{\Omega} q dV = - \int_{\Omega} \nabla \cdot \mathbf{J} dV \quad (3)$$

Assuming that the stored heat can be described by a sufficiently smooth function, one can move the derivative under the sign of integral and write:

$$\int_{\Omega} \frac{\partial q}{\partial t} dV = - \int_{\Omega} \nabla \cdot \mathbf{J} dV \quad (4)$$

which yields immediately the conservation equation in differential form:

$$\frac{\partial q}{\partial t} = -\nabla \cdot \mathbf{J} \quad (5)$$

The model is completed by a phenomenological constitutive equation, the well-known Fourier's law, which establishes a linear relationship between the heat flux and the temperature gradient (note that this is no longer true in hyperbolic conduction models [9,10]):

$$\mathbf{J} = -k\nabla T \quad (6)$$

Combining Eq. (5) with Eq. (6), and assuming that the stored heat is proportional to temperature (i.e.,  $q = \rho CT$ ), for a material with constant thermophysical properties one obtains the well-known parabolic equation:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T \quad (7)$$

where  $\alpha = k/\rho C$  is the thermal diffusivity.

The solution of Eq. (7) can be obtained after supplying appropriate initial and boundary conditions, which in the most general case may be a function of time. However, in most practical cases the time dependence can be neglected, so that in the heat transfer literature the following three boundary conditions are usually considered:

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**Nomenclature**

<b>C</b>	specific heat
<b>J</b>	heat flux
<b>k</b>	thermal conductivity
<b>n</b>	outward unit vector normal to the surface
<b>q</b>	thermal energy per unit volume
<b>r, r'</b>	curvilinear coordinate
<b>t</b>	time
<b>T</b>	temperature
<b>x</b>	position vector

<i>Greek symbols</i>	
$\alpha$	thermal diffusivity
$\Phi$	function representing a fictitious heat source
$\rho$	density
$\omega$	real parameter
$\Omega$	material volume
$\partial\Omega$	material volume boundary

1. Dirichlet boundary condition:  $T(\mathbf{x}, t) = f(\mathbf{x})$  for  $\mathbf{x} \in \partial\Omega$  and  $t > 0$ .
2. Neumann boundary condition:  $\frac{\partial T(\mathbf{x}, t)}{\partial \mathbf{n}} = f(\mathbf{x})$  for  $\mathbf{x} \in \partial\Omega$  and  $t > 0$ .
3. Robin boundary condition:  $\beta \frac{\partial T(\mathbf{x}, t)}{\partial \mathbf{n}} + \gamma T(\mathbf{x}, t) = f(\mathbf{x})$  for  $\mathbf{x} \in \partial\Omega$  and  $t > 0$ .

The identification of a unique solution also requires setting the initial condition,  $T(\mathbf{x}, 0) = T_0(\mathbf{x})$ , for  $\mathbf{x} \in \partial\Omega$ . Note that the debate on the classification of boundary conditions for the heat equation is still open [15].

Thus, in the standard derivation of the heat conduction model reviewed above, one finds a solution in differential form for any point within the material domain, and boundary conditions are appended at a later stage.

This paper introduces an alternative approach to heat conduction modelling, where boundary conditions arise within the mathematical model in parallel to the heat equation, generating a system of two differential equations (one which holds within the material domain and one which holds on the boundary) to be solved simultaneously. In particular, one of these equations can be reduced to any of the standard boundary conditions (named after Dirichlet, Neumann, and Robin) with the appropriate choice of one parameter. A peculiar feature of this approach is the capability of modelling heat sources or sinks placed exactly on the boundary in a formally rigorous way, which is not possible using the conventional approach.

**2. Analysis**

**2.1. Problem formulation**

The standard derivation of the heat conduction model outlined above can be re-formulated assuming ab initio the presence of a fictitious heat source on the boundary, described by a general function  $\Phi = \Phi(t, \mathbf{x}, T, DT, D^2T)$ , where the notation  $DT, D^2T$  is used to indicate the first and second derivatives of temperature.

To account for the heat source on the boundary, one can introduce the measure space  $(\bar{\Omega}, d\mu)$ , defined as the Cartesian product between the measure spaces of the region  $\Omega$  and its boundary,  $\partial\Omega$ :

$$(\bar{\Omega}, d\mu) = (\Omega, d\mathbf{x}) \otimes (\partial\Omega, dS) \tag{8}$$

The rate of change of the heat stored in the region  $\bar{\Omega}$  is now:

$$\frac{d}{dt} \int_{\bar{\Omega}} q d\mu \tag{9}$$

while the outgoing heat rate is given as usual by Eq. (1). Moving the derivative in Eq. (9) under the sign of integral and applying the divergence theorem to Eq. (1), one can write the conservation equation in integral form as:

$$\int_{\bar{\Omega}} \frac{\partial q}{\partial t} d\mu = - \int_{\Omega} \nabla \cdot \mathbf{J} dV + \int_{\partial\Omega} \Phi(t, \mathbf{x}, T, DT, D^2T) dS \tag{10}$$

Introducing the constitutive models for the heat flux ( $\mathbf{J} = -k\nabla T$ ) and the internal energy ( $q = \rho CT$ ), and decomposing the domain  $\bar{\Omega}$ , one obtains an equation containing two volume and two surface integrals:

$$\begin{aligned} \int_{\Omega} \frac{\partial}{\partial t} (\rho CT) dV + \int_{\partial\Omega} \frac{\partial}{\partial t} (\rho cT) dS \\ = \int_{\Omega} k \nabla^2 T dV + \int_{\partial\Omega} \Phi(t, \mathbf{x}, T, DT, D^2T) dS \end{aligned} \tag{11}$$

However, equating the volume integrals yields as usual Eq. (7), so that Eq. (11) reduces to:

$$\int_{\partial\Omega} \left[ \frac{\partial}{\partial t} (\rho CT) - \Phi(t, \mathbf{x}, T, DT, D^2T) \right] dS = 0 \tag{12}$$

Eq. (12) holds when the following equation is true on  $\partial\Omega$  and for  $t > 0$ :

$$\frac{\partial T}{\partial t} = \frac{1}{\rho C} \Phi(t, \mathbf{x}, T, DT, D^2T) \tag{13}$$

One can show that all of the standard boundary conditions listed above can be represented by Eq. (13), with suitable choices of the function  $\Phi(t, \mathbf{x}, T, DT, D^2T)$ . For example, one can reduce Eq. (13) to the Dirichlet boundary condition by setting  $\Phi(t, \mathbf{x}, T, DT, D^2T) \equiv 0$ : in fact, this means that  $\partial T / \partial t = 0$ , so that  $T(\mathbf{x}, t) = T_0(\mathbf{x})$  for  $\mathbf{x} \in \partial\Omega$ .

The Neumann boundary condition can be obtained by introducing an arbitrary function of time:

$$\Phi(t, \mathbf{x}, T, DT, D^2T) = \rho C g(t) \tag{14}$$

In this case, Eq. (13) yields  $\partial T / \partial t = g(t)$  for  $\mathbf{x} \in \partial\Omega$ , and taking the gradient one finds that:

$$\nabla \left( \frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial t} \nabla T = 0 \tag{15}$$

hence  $\nabla T$  and  $\partial T / \partial \mathbf{n}$  are a function of the spatial coordinate only, as required by the Neumann condition.

Finally, one can obtain the Robin boundary condition with the following choice:

$$\Phi(t, \mathbf{x}, T, DT, D^2T) = \rho C g(t) \exp(\omega r) \tag{16}$$

where  $\omega$  is a real parameter, and  $r$  is the coordinate along the line  $L$  that passes through the point  $\mathbf{x}$  and contains the vector  $\mathbf{n}$  ( $r > 0$  for points on  $L \cap \Omega$ ). With this choice, Eq. (13) becomes:

$$\frac{\partial T}{\partial t} = g(t) \exp(\omega r) \tag{17}$$

Taking the derivative with respect to the coordinate  $r$ , one finds:

$$\frac{\partial}{\partial \mathbf{n}} \left( \frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial t} \left( \frac{\partial T}{\partial \mathbf{n}} \right) = \omega g(t) \exp(\omega r) \tag{18}$$

which holds on  $L \cap \Omega$ ; introducing Eq. (17) shows that on the boundary  $\partial\Omega$ :

$$\frac{\partial}{\partial t} \left( \frac{\partial T}{\partial \mathbf{n}} \right) = \omega \frac{\partial T}{\partial t} \quad (19)$$

and one can conclude that for  $\mathbf{x} \in \partial\Omega$ :

$$\frac{\partial T}{\partial \mathbf{n}} - \omega T = f(\mathbf{x}) \quad (20)$$

In general, one can show that all of these boundary conditions can be described by means of the function defined in Eq. (16), for appropriate choices of the parameter  $\omega$ , and in particular:

- $\omega = -\infty$ : Dirichlet boundary condition.
- $\omega = 0$ : Neumann boundary condition.
- $\omega < 0$ : dissipative Robin boundary condition.
- $\omega > 0$ : non-dissipative Robin boundary condition.

While the examples listed above refer to the simplified cases of boundary conditions not dependent on time, time-dependent boundary conditions can also be described by Eq. (13) with appropriate choices of the arbitrary function.

## 2.2. Modelling heat sources on the boundary

The function  $\Phi = \Phi(t, \mathbf{x}, T, DT, D^2T)$  introduced above has been defined as a fictitious heat source on the boundary. Thus, the mathematical formulation of heat conduction introduced above can be used to study the case of a heat source placed on the boundary, which cannot be described using the standard boundary conditions. Without loss of generality, one can assume that such heat source depends linearly both on the temperature of the boundary and on the heat flux through it, so that:

$$\frac{1}{\rho C} \Phi(t, \mathbf{x}, T, DT, D^2T) = -b(\mathbf{x}) \frac{\partial T}{\partial \mathbf{n}} + c(\mathbf{x})T \quad (21)$$

where  $b(\mathbf{x}) > 0$  corresponds to a heat source, and  $b(\mathbf{x}) < 0$  to a heat sink. From Eq. (13), one can write the boundary condition on  $\partial\Omega$  as:

$$\frac{\partial T}{\partial t} = -b(\mathbf{x}) \frac{\partial T}{\partial \mathbf{n}} + c(\mathbf{x})T \quad (22)$$

For simplicity, one can start the analysis with  $c(\mathbf{x}) = 0$ , to obtain from Eq. (22):

$$\frac{\partial T}{\partial t} + b(\mathbf{x}) \frac{\partial T}{\partial \mathbf{n}} = 0 \quad (23)$$

Consider an infinitesimal region on the boundary, where for any point  $\mathbf{x} \in \partial\Omega$ ,  $B_\varepsilon(\mathbf{x})$  denotes the ball of radius  $\varepsilon$  about  $\mathbf{x}$ . Because  $\partial\Omega$  is a regular surface, one can choose a coordinate system for  $B_\varepsilon(\mathbf{x}) \cap \bar{\Omega}$  such that the boundary of  $B_\varepsilon(\mathbf{x}) \cap \bar{\Omega}$  in the transformed coordinates is flat, and the point  $\mathbf{x}$  is mapped to  $\tilde{\mathbf{x}} = (x_1, \dots, x_{n-1}, 0)$ ; in other words, in the neighbourhoods of  $\mathbf{x}$  the boundary lies in the hyperplane  $x_n = 0$ . In these coordinates, the outward unit normal to  $\partial\Omega$  in the point  $\mathbf{x}$  is the unit vector  $\mathbf{e}_n$ , which will form a certain angle with the outward unit normal vector in the old coordinates,  $\mathbf{n}$ , and  $r'$  is the coordinate along the line containing  $\mathbf{e}_n$ . In the transformed local coordinate system, the boundary condition expressed by Eq. (23) writes:

$$\frac{\partial T}{\partial t} + b(\mathbf{x}) \frac{\partial T}{\partial r'} = 0 \quad (24)$$

The well-known general solution of this equation represents a one-dimensional wave which is directed into the domain  $\Omega$  for  $b(\tilde{\mathbf{x}}) > 0$ , and is given by:

$$T(\tilde{\mathbf{x}}, t) = \tilde{f}[r' - b(\tilde{\mathbf{x}})t] \quad (25)$$

where  $\tilde{f}(\cdot)$  is a generic function. Mapping back to the original coordinate system, the solution of Eq. (23) is:

$$T(\mathbf{x}, t) = f[\mathbf{x} - b(\mathbf{x})t\mathbf{n}] \quad (26)$$

Using similar arguments, one can find the solution for Eq. (22) with  $c(\mathbf{x}) \neq 0$ , which turns out to be in the form of another travelling wave, modulated by an exponential term:

$$T(\mathbf{x}, t) = \exp[-c(\mathbf{x})t]f[\mathbf{x} - b(\mathbf{x})t\mathbf{n}] \quad (27)$$

These solutions show that in heat conduction problems a heat source placed exactly on the boundary and linearly dependent both on the boundary temperature and on the heat flux through it can be described as an ensemble of points which generate heat waves directed into an infinitesimal layer near the boundary.

## 3. Conclusions

The standard procedure to obtain the well-known mathematical model of heat conduction has been revisited to incorporate boundary conditions, which are usually introduced separately after the heat equation has been derived in differential form. In particular, the global energy balance has been re-written to include ab initio a fictitious heat source on the boundary, and decoupled into two differential equations which hold, respectively, inside the material domain and on its boundary.

The proposed formulation of the heat conduction problem allows one to describe all of the three standard boundary conditions (Cauchy, Neumann, and Robin) using the same mathematical expression, where only the value of a single parameter changes. In addition, this model can account for heat sources or sinks placed on the boundary. When such heat sources are described by functions that depend linearly on the local temperature and the heat flux on the boundary, each of their points can be represented as the source of a heat wave that propagates into an infinitesimal layer near the boundary itself.

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