Numerical study of the inverse heat conduction in composite material

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Abstract

In this work, the objective of the control optimized problem is to determine the conduction coefficient in a heterogeneous solid for heat transfer conduction, by the inverse method using the conjugate gradient method. The finite differences method is employed to determine the temperature field in a solid flat plate, for given model of thermal conductivity. The obtained results for a discretization scheme of 300 knots for the time and 20 knots for the space show that the calculated values of thermal conductivity and temperature coincide perfectly with the corresponding exact values. The difference is about 2.5% for temperature and 0.7% for thermal conductivity.

Keywords : Composite material, numerical simulation, Inverse problem, thermal conductivity

1. Introduction

Recent advances in materials processing technology allowed design and manufacturing of new materials systems which can withstand high temperatures and large temperature gradients. Composite materials like functionally graded material or FGM are a new generation of composites where the volume fraction varies gradually, which gives a micro structural non-uniformity on the surface.

In an ideal composite material, the properties of the material may vary in a one dimension. A region of smooth transition between a pure metal and a pure ceramic may lead to a multifunctional material that combines high desirable properties of temperature and thermal resistance of a ceramic, with the hardness of fracture and strength of metal [1]. Numerical analysis can be a perspective method for the design of these materials and the understanding of their behavior.

In the case of exponentially graded materials, the Green's function (GF) is expressed as the superposition of the Green's function (GF) for homogeneous material and additional terms due to the graded material [2]. The numerical implementations are performed using a Galerkin (rather than collocation) approximation. A number of examples have been carried out. The results of some specific test problems agree within plotting accuracy with available analytical solutions.

For a broad range of functional material variation (quadratic, exponential and trigonometric) of thermal conductivity and specific heat, the non-homogeneous problem can be transformed into the standard homogeneous diffusion problem. A three-dimensional boundary element implementation (BEM), using the Laplace transform approach and the Galerkin approximation, is studied by A. Sutradhar et al. [3].

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Some studies have been conducted for continuously non homogeneous functionally graded materials (FGM), by using the meshless local boundary integral equation method [4].
The inverse methods combined to iterative methods such as Newton technique are also a part of tools for identifying thermophysical properties such as thermal conductivity [5].
The main objective of this study is to determine the conduction coefficient in a heterogeneous solid for heat transfer conduction, by the inverse method using the conjugate gradient method. The finite differences method is employed to determine the temperature field in a solid flat plate, testing different models of thermal conductivity suitable for their applications.

2. Formulation of the direct problem

The considered direct problem concerns the research of temperature profile in a heterogeneous solid wall submitted to conditions imposed on its surfaces.
The Heat conduction, modeled by the phenomenological law of Fourier, involves the intrinsic properties of the material such as thermal conductivity which is variable and the specific heat considered as constant ($\rho c = 1$).
In order to build the coefficient of heat conduction $\lambda(x)$, the solid is subjected to a heat flux $\phi(x,t)$ on two walls, at an initial temperature of the surface.
The dimensionless equation of heat conduction in a heterogeneous solid is given by:

$$\frac{\partial}{\partial x}\left(\lambda(x)\frac{\partial T(x,t)}{\partial x}\right)=\frac{\partial T(x,t)}{\partial t} \qquad 0<t<t_f \text{ et } 0<x<l \tag{1}$$

Where :
T(x,t) : dimensionless temperature
x : dimensionless coordinate
t : dimensionless time
t_f : final time
$\lambda(x)$: dimensionless thermal conductivity

3. Optimization method and sensitivity problem

The inverse problem can be formulated into an optimization problem, where the unknowns are determined by minimizing the difference between the measurements from the observation of the physical system (exact solution) and the direct model. The objective of the control problem is to determine the conduction coefficient in a heterogeneous solid for heat transfer conduction, by the inverse method using the conjugate gradient method.
The least squares criterion $J(\lambda(x))$ is introduced to minimize the difference between the calculated temperature $T(x,t)$ (simulated solution) and the temperature calculated by the exact model.

$$J(\lambda(x))=\int_0^1\int_{ti}^{tf}\left(T(x,t)-T_m(x,t)\right)^2 dtdx \tag{2}$$

The objective here is to minimize the criterion so that it converges to the desired solution, i.e. $\lambda(x)$ approximates the real value (desired) such that: $J(\lambda) = \inf J(\lambda)$
The directional derivative of Gâteau in the direction of $\lambda(x)$ is defined in the linear case by [6]:

$$D_{\delta\lambda} J(\lambda) = \left. \frac{J(\lambda + \delta\varepsilon\lambda) - J(\lambda)}{\varepsilon} \right|_{\varepsilon \to 0} = \int_0^1 \int_{ti}^{tf} J'(x,t)\delta\lambda dxdt \tag{3}$$

J' : Gradient of the criterion J

The sensitivity problem is obtained by differentiating the direct problem (Eq. 1) with respect to Temperature $T(x,t)$ and thermal conductivity $\lambda(x)$:

$$\frac{\partial \delta T(x,t)}{\partial t} - \frac{\partial \lambda(x)}{\partial x}\frac{\partial \delta T(x,t)}{\partial x} - \lambda(x)\frac{\partial^2 \delta T(x,t)}{\partial x^2} - \frac{\partial \delta\lambda(x)}{\partial x}\frac{\partial T(x,t)}{\partial x} - \delta\lambda(x)\frac{\partial^2 T(x,t)}{\partial x^2} = 0 \tag{4}$$

With boundary conditions :

$$\delta T(x,0) = 0 \tag{5}$$

$$\delta\lambda(0)\frac{\partial T(0,t)}{\partial x} + \lambda(0)\frac{\partial \delta T(0,t)}{\partial x} = 0 \tag{6}$$

$$\delta\lambda(1)\frac{\partial T(1,t)}{\partial x} + \lambda(1)\frac{\partial \delta T(1,t)}{\partial x} = 0 \tag{7}$$

δT is the solution of the sensitivity equation. It is used to calculate the depth of descent

4. Adjoint problem and gradient equation

Adjoint problem and gradient equation are obtained by multiplying sensitivity equation (4) by Lagrange multipliers (or adjoint functions) P(x,t), and adding the criterion equation (3), to yields the following result :

$$\Delta J(\lambda) = \int_{ti}^{tf}\int_0^1 \left[\frac{\partial \delta T(x,t)}{\partial t} - \frac{\partial \lambda(x)}{\partial x}\frac{\partial \delta T(x,t)}{\partial x} - \lambda(x)\frac{\partial^2 \delta T(x,t)}{\partial x^2} \right] P(x,t)dxdt - \int_{ti}^{tf}\int_0^1 \left[\frac{\partial \delta\lambda(x)}{\partial x}\frac{\partial T(x,t)}{\partial x} + \delta\lambda(x)\frac{\partial^2 T(x,t)}{\partial x^2} \right] P(x,t)dxdt$$
$$+ 2\int_0^{tf}\int_0^1 \left[T(x,t) - Y(x,t) \right] \delta T dxdt \tag{8}$$

Involving the integration by parts and putting $t_i = 0$, we obtain after some simplifications:

$$
\begin{aligned}
&-\int_0^{tf}\int_0^1\left[\frac{\partial P(x,t)}{\partial t}+\frac{\partial\lambda(x)}{\partial x}\frac{\partial P(x,t)}{\partial x}+\lambda(x)\frac{\partial^2 P(x,t)}{\partial x^2}\right]\delta T(x,t)dxdt+\int_0^{tf}\int_0^1\left[\frac{\partial T(x,t)}{\partial x}\frac{\partial P(x,t)}{\partial x}\right]\delta\lambda(x)dxdt+\int_0^1\delta T(x,tf)P(x,tf)dx\\
&-\int_0^1\delta T(x,0)P(x,0)dx+\int_0^{tf}\lambda(1)\frac{\partial P(1,t)}{\partial x}\delta T(1,t)dt+\int_0^{tf}\int_0^1\left[\frac{\partial T(x,t)}{\partial x}\frac{\partial P(x,t)}{\partial x}\right]\delta\lambda(x)dxdt+\int_0^1\delta T(x,tf)P(x,tf)dx\\
&-\int_0^1\delta T(x,0)P(x,0)dx+\int_0^{tf}\lambda(1)\frac{\partial P(1,t)}{\partial x}\delta T(1,t)dt-\int_0^{tf}\lambda(0)\frac{\partial P(0,t)}{\partial x}\delta T(0,t)dt-\int_0^{tf}\lambda(1)P(1,t)\frac{\partial\delta T(1,t)}{\partial x}dt\\
&+\int_0^{tf}\lambda(0)P(0,t)\frac{\partial\delta T(0,t)}{\partial x}dt-\int_0^{tf}\frac{\partial T(1,t)}{\partial x}P(1,t)\delta\lambda(1)dt+\int_0^{tf}\frac{\partial T(0,t)}{\partial x}P(0,t)\delta\lambda(0)dt\\
&+\int_0^{tf}\int_0^1 2.\left[T(x,t)-Y(x,t)\right]\delta T dxdt=0
\end{aligned}
\tag{9}
$$

Other simplifications are also possible dealing with the initial and boundary conditions such as:

$$\delta T(x,0)=0 \tag{10}$$

$$\delta\lambda(0)\frac{\partial T(0,t)}{\partial x}+\lambda(0)\frac{\partial\delta T(0,t)}{\partial x}=0 \tag{11}$$

$$\delta\lambda(1)\frac{\partial T(1,t)}{\partial x}+\lambda(1)\frac{\partial\delta T(1,t)}{\partial x}=0 \tag{12}$$

4.1. Adjoint equation

By imposing the boundary conditions of the adjoint equation, we obtain the adjoint equation and the gradient criterion:

$$-\left[\frac{\partial P(x,t)}{\partial t}+\frac{\partial\lambda(x)}{\partial x}\frac{\partial P(x,t)}{\partial x}+\lambda(x)\frac{\partial^2 P(x,t)}{\partial x^2}\right]+2\sum_{i=1}^{\mathrm{Im}}\left[T(x,t)-Y(x,t)\right].\delta(x-x_i)=0 \tag{13}$$

Conditions of the adjoint equation are derived from the simplification of equation (9):

$$P(x,t_f)=0 \tag{14}$$

$$\lambda(0)\frac{\partial P(0,t)}{\partial x}=2\times\left(T(0,t)-Y(0,t)\right) \tag{15}$$

$$\lambda(1)\frac{\partial P(1,t)}{\partial x}=2\times(T(1,t)-Y(1,t)) \tag{16}$$

4.2. Gradient equation

Equation (9) provides the variation of the criterion:

$$\nabla J(\lambda)=\int_0^1\int_0^{tf}\left(\frac{\partial T(x,t)}{\partial x}\times\frac{\partial P(x,t)}{\partial x}\right)\delta\lambda(x)dxdt \tag{17}$$

The identification with equation (3) gives the gradient of the criterion::

$$J'(x,\lambda) = \frac{\partial P(x,t)}{\partial x}\frac{\partial T(x,t)}{\partial x} \tag{18}$$

4.3. Conjugate gradient method

The iteration process based on the conjugate gradient method is used for estimation of $\lambda(x)$ by minimizing the functional J [6, 7]:

$$\lambda^{n+1}(x) = \lambda^{n}(x) - \theta^{n} \times d^{n}(x) \qquad \text{for n} = 0,\ 1, 2, \ldots\ldots \tag{19}$$

Where θ is the step size defined by [7] :

$$\theta = \frac{\int_{ti}^{tf}\int_{0}^{1} \delta T\left(T(\lambda) - Y\right).dxdt}{\int_{ti}^{tf}\int_{0}^{1} (\delta T)^{2}.dxdt} \tag{20}$$

And d^n (x) the direction of descent given by :

$$d^{n}(x) = J'^{n}(x) + \left(\gamma^{n} \times d^{n-1}(x)\right) \tag{21}$$

The conjugate coefficient is determined from [5, 6] :

$$\gamma^{n} = \frac{\int_{x=0}^{1}\int_{t=0}^{t_f}\left(J'^{n}\right)^{2} dtdx}{\int_{x=0}^{1}\int_{t=0}^{t_f}\left(J'^{n-1}\right)^{2} dxdt} \qquad \text{with} \qquad \gamma^{0} = 0 \tag{22}$$

To perform the iterative calculation of the equation (19), we have to solve two equations, the adjoint equation which determines the direction of the descent and the sensitivity equation involving the determination of step size.

5. Numerical Resolution

The numerical resolution based on discretization by finite difference scheme can approach direct, adjoint and sensitivity equations.

Direct problem**:**

$$T_{i+1}^{\ j+1}\left(-A_i - B_i\right) + T_i^{\ j+1}\left(1 + 2\times B_i\right) + T_{i-1}^{\ j+1}\left(A_i - B_i\right) = T_{i+1}^{\ j}\left(A_i + B_i\right) + T_i^{\ j}\left(-1 - 2\times B_i\right) + T_{i-1}^{\ j}\left(-A_i + B_i\right) \tag{23}$$

with : $A_i = \left(\dfrac{\Delta t \times \left(\lambda_{i+1} - \lambda_{i-1}\right)}{8 \times \Delta x^{2}}\right)$

$$B_i = \left(\frac{\Delta t \times \lambda(i)}{2 \times \Delta x^2} \right)$$

This is a tridiagonal system of equations (TDMA), which is solved by the Thomas algorithm based on Gaussian elimination [6].

Adjoint equation**:**

$$P_{i+1}{}^{j+1}(A2+B2) + P_i^{j+1}(1-2\times B2) + P_{i-1}{}^{j+1}(-A2+B2) = P_{i+1}{}^{j}(-A2-B2) + P_i^{j}(1+2\times B2) + P_{i-1}{}^{j}(A2-B2) + \sum_{1}^{im}(2\times Er(i))\times \Delta t \quad (24)$$

with :

$Er = [T(x,t) - Y(x,t)].\delta(x - x_i)$: difference between estimated and exact temperatures

The boundary conditions are:

$$P(x,tf) = 0$$
$$\lambda(0)\frac{\partial P(0,t)}{\partial x} = 2\times(T(0,t) - Y(0,t))$$
$$\lambda(1)\frac{\partial P(1,t)}{\partial x} = 2\times(T(1,t) - Y(1,t))$$

Sensitivity equation :

$$\delta T_{i+1}{}^{j+1}\left(-A1-B1\right) + \delta T_i^{j+1}\left(1+2.B1\right) + \delta T_{i-1}{}^{j+1}\left(A1-B1\right) = \delta T_{i+1}{}^{j}\left(A1+B1\right) + \delta T_i^{j}\left(1-2.B1\right) + \delta T_{i-1}{}^{j}\left(-A1+B1\right) + C1 + D1 \quad (25)$$

with:

$$A1 = \frac{\Delta t \times \left(\lambda_{i+1} - \lambda_{i-1}\right)}{8\times \Delta x^2} \qquad B1 = \frac{\Delta t \times \lambda(i)}{2\times \Delta x^2}$$
$$C1 = \frac{\Delta t}{8\times \Delta x^2}\left(\delta\lambda_{i+1} - \delta\lambda_{i-1}\right)\left(T_{i+1}{}^{j+1} + T_{i+1}{}^{j} - T_{i-1}{}^{j+1} - T_{i-1}{}^{j}\right)$$
$$D1 = \frac{\Delta t \times \delta\lambda(i)}{2\times \Delta x^2}\left[\begin{array}{l}\left(T_{i+1}{}^{j+1} + T_{i+1}{}^{j}\right) - 2\left(T_i{}^{j+1} + T_i{}^{j}\right) \\ + \left(T_{i-1}{}^{j+1} + T_{i-1}{}^{j}\right)\end{array}\right]$$

The boundary conditions are:

$$\delta T(x,0) = 0$$
$$\delta\lambda(0)\frac{\partial T(0,t)}{\partial x} + \lambda(0)\frac{\partial \delta T(0,t)}{\partial x} = 0$$
$$\delta\lambda(1)\frac{\partial T(1,t)}{\partial x} + \lambda(1)\frac{\partial \delta T(1,t)}{\partial x} = 0$$

6. Results and discussion

To validate the numerical model, we use the exact solution given by:

$$T(x) = -\left(ax^2 + bx + c\right) \times \exp\left(-\alpha \times t\right)$$

$$\lambda(x) = \frac{\alpha}{6}\left(-x^2 - \frac{b}{a}x + \frac{b^2 - 6a \times c}{2 \times a^2}\right)$$

with : a= -0.45 b=-5 c=5.5 α=0.05

$$\begin{cases} T(x,0) = ax^2 + bx + c \\ -\lambda(0)\dfrac{\partial T(0,t)}{\partial x} = q_1 \\ -\lambda(1)\dfrac{\partial T(1,t)}{\partial x} = q_2 \end{cases}$$

The obtained results for a discretization scheme of 300 nodes for the time and 20 nodes for the space show that the calculated values of thermal conductivity and temperature coincide perfectly with the corresponding exact values (Figures 1 and 2). The difference is about 2.5% for temperature (Figure 3) and 0.7% for thermal conductivity (Figure 4).

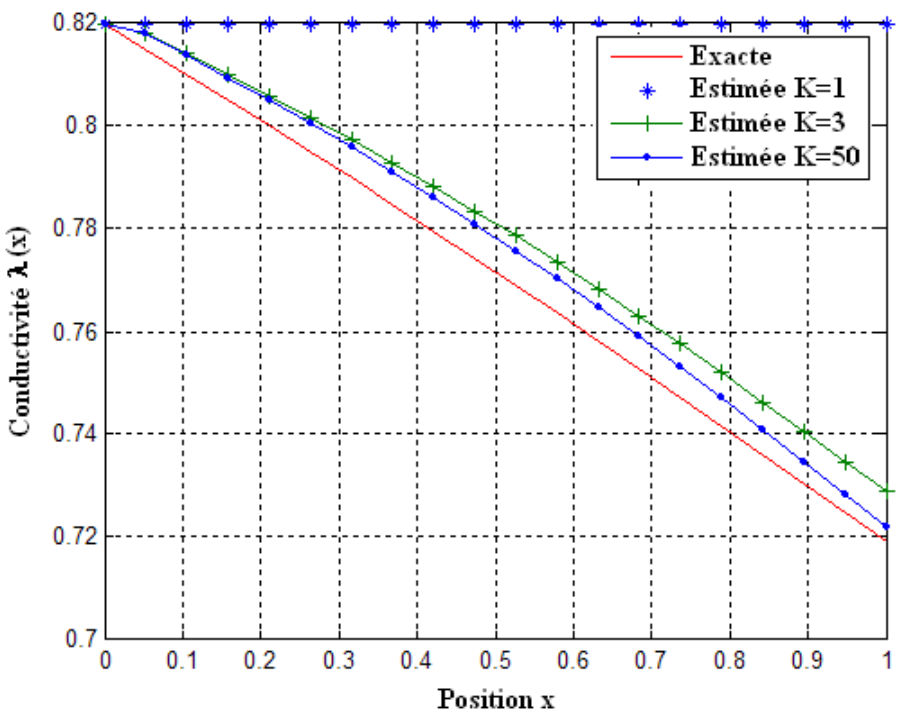

Figure 1. Exact and calculated thermal conductivity

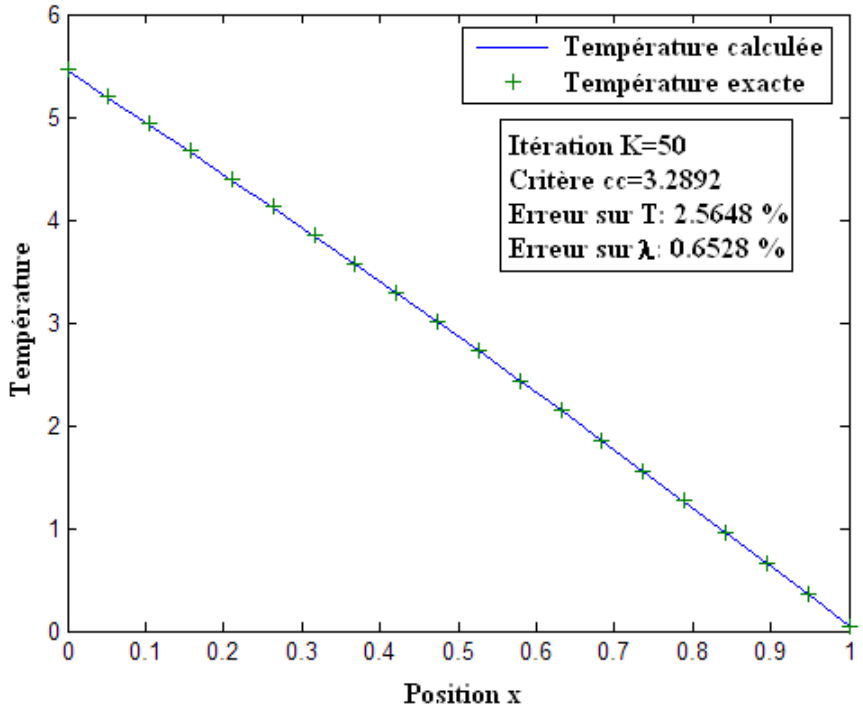

Figure 2. Exact and calculated temperature

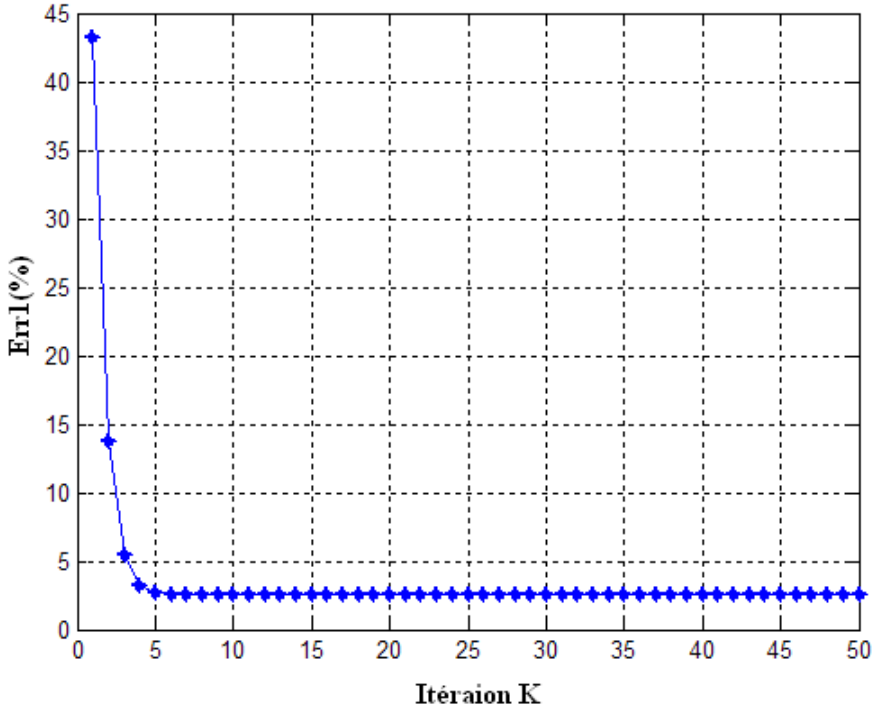

Figure 3. Evolution of temperature difference according to the number of iterations

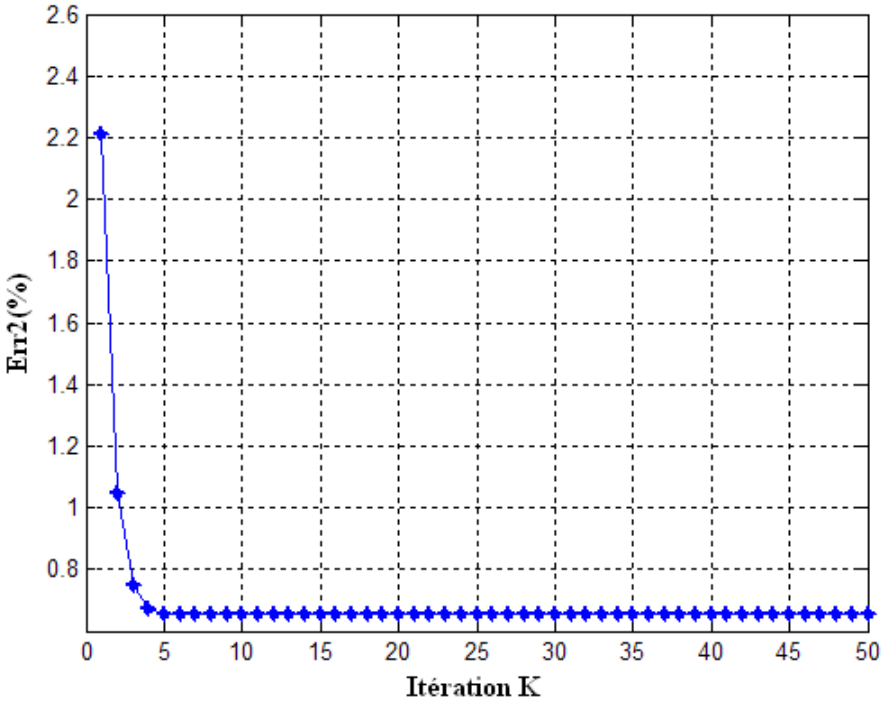

Figure 4. Evolution of thermal conductivity difference according to the number of iterations

Conclusions

The results validated by comparing the profiles of exact temperature with those of estimated solution, were used to support the reliability of this approach that allows, through a technique based on the inverse problem, of estimate the thermal conductivity.

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