THERMOPHYSICAL PARAMETER ESTIMATION OF MULTI-LAYER WALLS WITH STOCHASTIC OPTIMIZATION METHODS

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ABSTRACT

The problem of the estimation of thermal conductivities of multi-layer walls is studied using genetic algorithms and simulated annealing. Parameter estimation is shown for the cases of three- and five- layer walls, comparing the two stochastic approaches and also contrasting them with deterministic gradient-based methods. It is shown how stochastic methods permit better performances than classical ones when initial estimations of parameter values are not available or when the problem becomes complex.

1. INTRODUCTION

The estimation of thermophysical parameters of building components, in particular their thermal resistance, has important practical applications for thermal loads calculation and sizing of air-conditioning systems.

When trying to determine building thermal resistance with on-site measurements, an important role is played by the type of processing applied to temperature and heat flux data. The simplest method for thermal resistance determination is to employ a progressive average [1].

In [2] Aureli and Grignaffini proposed a method based on linear regression of experimental data. The advantage of such a method is the possibility of using a shorter data acquisition time compared to what is required by the progressive average method. A simulated extension of the test period to calculate the thermal resistance was suggested in [3]. In this way, thermal resistance estimation is possible also for walls with high heat capacity and for large temperature excursions. In both previous cases, a global value of thermal resistance is determined, even in the case of composite walls.

In this paper, we intend to analyze the problem of the simultaneous estimation of thermal conductivities of the materials composing a multilayer wall. This problem will be studied in the framework of parameter estimation in inverse heat conduction problems.

In short, it can be said that solving a direct problem describes effects obtained for the application of given causes, whereas the inverse problem has to deal with the determination of unknown causes given their effects.

From a mathematical point of view, this type of problems are usually ill-posed, because it is not assured that there is a unique solution and they are not stable under perturbations on data.

A wide range of methods has been applied in literature for thermophysical parameter estimation in the context of inverse problems. Usually, space- and/or temperature-dependent heat capacity and thermal conductivity are determined by minimizing the least-squares difference between measured and computed data [4,5], possibly with Tikhonov regularization [6]. Examples include the use of a modified Newton-Raphson method [7], of the conjugate gradient method with adjont problem [8-10], of the Levenberg-Marquardt method [11], of the Broyden-Fletcher-Goldfarb-Shanno algorithm [12], of Kalman filtering [13].

The present work is devoted to the use of stochastic optimization methods for the thermophysical parameter estimation of multilayer masonry walls. The simultaneous estimation of the values of such parameters for different media represents an inverse problem in which it may be necessary to minimize functions showing more than one minimum. In this case, deterministic optimization methods are not capable of solving the problem if a sufficiently accurate starting estimation of parameter values is not available. Even in cases in which the function to be minimized is monomodal, classical methods may not lead to convergence because the problem is ill-posed. Also, unknown parameters may be correlated and therefore be difficult to estimate through gradient-based methods using a sensitivity matrix. For all these reasons it can be useful to study the application of stochastic methods like genetic algorithms and simulated annealing to parameter estimation.

A few works exist regarding applications of genetic algorithms to thermophysical parameter estimation. Raudenský *et al.* [14] showed the possibility of using genetic algorithms and neural networks for estimating thermal conductivity and heat capacity of a steel plate by determining the coefficients of an assumed linear temperature dependence.

Garcia *et al.* [15,16] employed genetic algorithms for estimating thermophysical properties of composite materials and optimizing the experimental design of the measurement set up. Genetic algorithms have also been employed for function estimation problems in inverse heat conduction [17].

To the best of our knowledge, no application of simulated annealing to estimate thermophysical parameters has appeared in literature.

2. DIRECT PROBLEM

In all methods used for solving an inverse problem, it is necessary to solve the corresponding direct problem with guess values of the unknown parameters. This usually represents a computationally expensive task in the whole process. The direct problem we are interested in can be modeled by a monodimensional heat conduction equation

$$\frac{\partial}{\partial x}\left[\lambda(x)\frac{\partial T(x,t)}{\partial x}\right] = \rho(x)c(x)\frac{\partial T(x,t)}{\partial t} \qquad (1)$$

with the boundary and initial conditions

$$\begin{aligned} q(t) &= -\left[\lambda(x)\frac{\partial T(x,t)}{\partial x}\right]_{x=0}, \\ T(0,t) &= T_i(t), \\ T(L,t) &= T_e(t), \\ T(x,0) &= T_0(x). \end{aligned} \qquad (2)$$

The solution of the direct problem requires the determination of the temperature as a function of space

and time $T(x,t)$, and therefore also the heat flux $q(t)$ in $x = 0$, given the values of the thermophysical parameters $\lambda(x)$, $\varrho(x)$ and $c(x)$ and given initial and boundary conditions. Thermophysical parameters are here supposed to be temperature-independent and piecewise constant in space.

In a practical building application, a useful model to solve Eq. (1) is that of periodic regime. In these hypotheses, the problem presents an analytical solution in the one-dimensional case, briefly recalled in Appendix.

A numerical solution of Eq. (1), employing the control volumes method [18], has been also implemented to deal with more general transient heat conduction problems.

3. GENETIC ALGORITHMS AND SIMULATED ANNEALING

Genetic algorithms and simulated annealing are stochastic optimization methods [19], meaning that they employ a controlled degree of randomness to explore the solution space. This allows a global optimization, differently from what happens with gradient-based local search techniques.

Genetic algorithms are based on the concepts of Darwinian evolution and survival of the fittest [20,21]. They try to maximize an objective function, called fitness, by evolving a set of trial solutions through the genetic operators of selection, crossover and mutation. The trial solutions are called chromosomes or individuals and constitute a population. Chromosomes are made of genes, that are a representation of the parameters to be determined, usually realized with a binary coding. Using the genetic operators, a new generation is created from the current population. The process is iterated until a proper stopping criterion (number of generations, error tolerance) is not satisfied. Selection chooses the parents whose mating has to give rise to the next generation. There are several types of selection; in this work we used tournament selection [22]: a subset of M individuals ($M = 2$ in most cases) is chosen in a random way and their fitness is compared; the winner of the competition is inserted in the set of parents and the subset of M individuals is reinserted in the current population. The process is repeated until enough parents have been created for breeding. The latter is realized using the crossover operator, single-point crossover being the most frequently used: a random number p in the interval [0,1] is generated; if $p < p_{\text{cross}}$ (where p_{cross} is the crossover probability, usually set in the range 0.6-0.9) a random position in the string representing the chromosome is chosen and an offspring is created from the parents swapping the part of the chromosome after the crossover point; if, instead, $p > p_{\text{cross}}$ then the offspring is a copy of the parents. There also other forms of crossover in which the crossover points are more than one. After that, the mutation operator is applied to the offspring: it allows the exploration of portions of the parameter space that are not accessible with the simple crossover of the chromosomes existing in a given moment. Mutation is applied with a probability p_{mut} (usually set in the range 0.01-0.1): if a randomly generated number p is less than p_{mut}, a random location in the chromosome is chosen and the corresponding bit is negated; if $p > p_{\text{mut}}$, the chromosome remains unaltered. Also used in this work is an elitist strategy: if the best individual of current generation has a fitness lower than that of the best individual of previous generation, the latter is inserted in the present population substituting the less fit individual. This helps in not loosing good genetic material.

Simulated annealing [23] is the other stochastic optimization method employed in this work. It takes as a model the thermodynamical process of annealing of a solid. Let us consider a system with a large number of interacting particles, as atoms in a solid, at thermal equilibrium at temperature T. The configuration of the system is represented by the set of the spatial coordinates of its constituent particles. At temperature T the probability $\pi_T(s)$ that the system is in a configuration s depends on the energy of the configuration $E(s)$ and follows Boltzmann distribution law

$$\pi_T(s) = \frac{\exp\left[-\frac{E(s)}{kT}\right]}{\sum_{w \in R} \exp\left[-\frac{E(w)}{kT}\right]}. \qquad (3)$$

The behavior of the system at thermal equilibrium at temperature T is simulated with a stochastic relaxation technique, the Metropolis algorithm [24]. Suppose the system to be in the configuration s at t; a possible configuration s_1 at $t + \Delta t$ is generated in a random way and is accepted according to the difference between the energies of s_1 and s. In detail, the ratio p between the probability of the system to be in s_1 and in s is computed; if $p > 1$, that is the energy of s_1 is lower than the energy of s, then the configuration s_1 is accepted as the new configuration at $t + \Delta t$. If, instead, $p \leq 1$, then the configuration s_1 is accepted with probability p. This means that higher-energy configurations are temporarily acceptable. It is just this mechanism that allows the system to tend to a global minimum without being stuck in a local minimum. Because of Boltzmann distribution law, low-energy configurations have higher probability at low temperature. To reach low-energy configurations it is necessary to proceed as in the physical annealing process: the temperature of the system is first raised and then gradually lowered, keeping the system at each temperature enough time for it to reach thermal equilibrium. Simulated annealing steps are therefore the following:

- A starting temperature T_{ini} is prescribed so to let almost all initial configurations to be accepted.
- A temperature decrease law and the time to spend at each temperature are set.
- For each temperature and for the number of iterations selected, the Metropolis algorithm is executed on random configurations.
- The process is stopped when a given number of iterations is reached or a prescribed error tolerance is satisfied.

Critical points for the minimization effectiveness are the selection of the temperature decrease law and the way a configuration is varied. Both points depend on the problem under examination and are empirically determined.

4. RESULTS

To test the performances of the various parameter estimation methods, a known case of periodic regime will be considered: thermophysical parameters and time-dependent temperatures on the two sides of a multi-layer wall, as well as the heat flux at one side of the wall are known quantities.

Simulated values are those reported in the annex A of the PrEN 12494 [1] regulation, presenting reference cases to be employed to test estimation methods for determining building components thermal resistance. We analyze in particular a three-layer and a five-layer walls, whose characteristics are described in Tab. 1.

Table 1. Reference walls properties as reported in PrEN12494 regulation.

Layer	Material	Thickness (m)	Density (kg/m^3)	Specific heat (J/kg K)	Thermal Conductivity (W/m K)
Wall 1					
1	Covering	0.01	600	1000	0.100
2	Insulation	0.40	30	1000	0.035
3	Covering	0.01	600	1000	0.100
Wall 2					
1	Covering	0.01	600	1000	0.100
2	Insulation	0.05	30	1000	0.035
3	Masonry	0.30	1800	1000	0.700
4	Insulation	0.15	30	1000	0.035
5	Covering	0.01	600	1000	0.100

Temperature and heat flux are provided through their Fourier series expansion.
The function to be minimized for an n-layer wall is the least-squares norm

$$S(\lambda_1,\dots,\lambda_n) = [\mathbf{q}\text{-}\tilde{\mathbf{q}}(\lambda_1,\dots,\lambda_n)]^T[\mathbf{q}\text{-}\tilde{\mathbf{q}}(\lambda_1,\dots,\lambda_n)] = \\ = \sum_{i=1}^{I}[q_i - \tilde{q}_i(\lambda_1,\dots,\lambda_n)]^2 \qquad (4)$$

where $\tilde{\mathbf{q}}$ is calculated with trial values of parameters and $\mathbf{q}$ is measured (in the present case is known from data tabulated in the PrEN regulation).

4.1. Three-layer wall

The first example of parameter estimation is the determination of the thermal conductivities of the three-layer wall in Tab. 1.

Sensitivity study. Before carrying on the parameter estimation, it is useful to perform a sensitivity analysis to evaluate the possibility of success in the solution of the inverse problem and the number of parameters that can be simultaneously determined. In our problem we have to consider the variations of the heat flux with respect to thermal conductivity. A dimensionless normalized version of the sensitivity coefficient is considered to allow quantitative comparisons between coefficients

$$J_\lambda(t) = \frac{\lambda}{q_{\max}}\frac{\partial q(t)}{\partial \lambda} = \frac{\lambda}{q_{\max}} J_{0\lambda}(t). \qquad (5)$$

In the frequency domain, the expression of $\bar{J}_{0\lambda}(f)$ for a homogeneous wall in periodic regime is derived in the Appendix and is given by Eq. (A.3). As it can be seen, the sensitivity coefficient depends on λ through the dependence on $\nu = \sqrt{j2\pi f/D}$. The inverse problem is therefore nonlinear and its solution with a classical method requires a linearization and an iterative solution process. Using a stochastic optimization method to solve the inverse problem, instead, it is not necessary to go through a linearization step, because a sensitivity matrix does not have to be calculated for the solution of the problem. Nonetheless, as we said, sensitivity coefficients are usefully calculated to gain insight into the problem.
Also in the case of a multi-layer one-dimensional structure, it is possible to obtain analytic expressions of the heat flux at the edge of it (see Appendix) and therefore of the respective sensitivity coefficients.

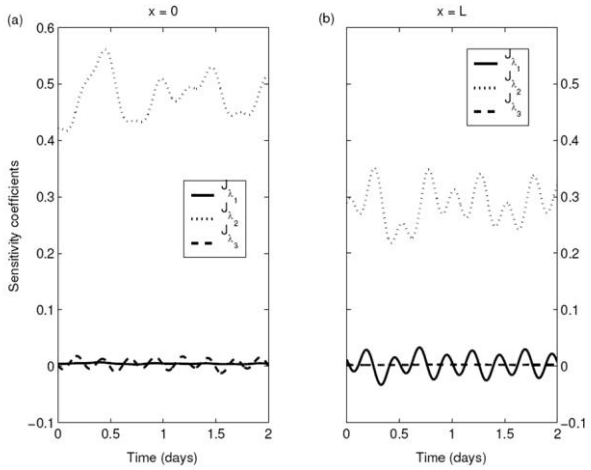

Figure 1: Sensitivity coefficients for the heat flux at $x = 0$ (a) and at $x = L$ (b) with respect to thermal conductivities of the three layers of the wall.

For the three-layer wall, their normalized values versus time are shown in Fig. 1a for the heat flux at $x = 0$. The calculation has been done by summing expressions like (6) for the various frequencies composing the temperature signals and employing the actual values of the wall's thermophysical parameters. As it can be seen, there is a difference of two orders of magnitude among the values of the three coefficients: $\text{mean}(J_{\lambda_1}) = 4 \cdot 10^{-3}$, $\text{mean}(J_{\lambda_2}) = 0.5$ and $\text{mean}(J_{\lambda_3}) = 4 \cdot 10^{-3}$. This is reflected in the different accuracy with which it is possible to determine the values of the three thermal conductivities. Parameters with sensitivity coefficients lower than 0.1 are extremely difficult to determine [25]. It is not surprising that the parameter that influences most heat flux variations is the conductivity of the intermediate insulating layer, that also has a thickness much larger than the other two layers.
The possibility of simultaneous estimation of the n parameters can be related to their correlation coefficients [26]

$$r_{ij} = \frac{P_{ij}}{\sqrt{P_{ii}P_{jj}}} \quad i,j = 1,\dots,n \qquad (6)$$

where $\mathbf{P}=(\mathbf{J}^{\mathrm{T}}\mathbf{J})^{-1}$ and $\mathbf{J} = [J_{\lambda_1} \dots J_{\lambda_n}]$ is the sensitivity matrix. As a rule of thumb, two parameters are considered correlated when the modulus of their correlation coefficient is larger than 0.9; in this case their simultaneous estimation is extremely difficult. In our case, $r_{12} = -0.99$, $r_{13} = -0.3$ and $r_{23} = 0.2$. Given the low sensitivity to its value and its high correlation with λ_2, λ_1 is therefore the most difficult parameter to determine.
We can also consider the other point of the wall which is accessible to measurements, that is $x = L$ (see Fig. 1b). It is seen that the roles of J_{λ_1} and J_{λ_3} are swapped in the sense that in this case the most difficult parameter to be determined simultaneously with the other two is J_{λ_3}. Indeed, we have: $\text{mean}(J_{\lambda_1}) = 2 \cdot 10^{-3}$, $\text{mean}(J_{\lambda_2}) = 0.3$

and mean$(J_{\lambda_3}) = 2 \cdot 10^{-3}$, and $r_{12} = 0.2$, $r_{13} = -0.3$ and $r_{23} = 0.99$.

Deterministic methods. In order to motivate the need to go beyond classical optimization methods, a few estimation tests for the three-layer wall problem have been performed with conjugate gradient and Levenberg-Marquardt algorithms. Being optimization methods that are capable of detecting local minima, they are sensitive to the starting values of the unknown parameters.

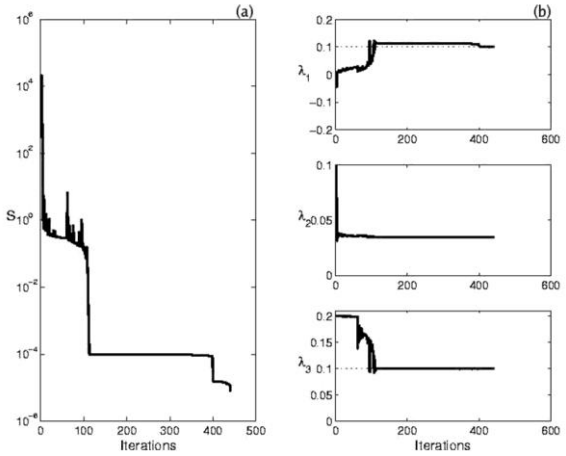

Figure 2: Evolution of least-squares norm S (a) and thermal conductivities (b) with the conjugate gradient method. Dotted lines indicate actual parameter values.

Fig. 2 shows the result of the application of the conjugate gradient method: the evolution during the optimization process of residuals (a) and of parameters (b) when the starting point is given by $\lambda_1 = 0.01\,\mathrm{W/m\,K}$, $\lambda_2 = 0.1\,\mathrm{W/m\,K}$ and $\lambda_3 = 0.2\,\mathrm{W/m\,K}$. The expression used for the conjugation coefficient has been that of Polak-Ribiere [27]. Even if λ_1 gets also negative values, which is physically meaningless, after a quite large number of iterations parameter values tend to converge to actual values. The different convergence speed of the three parameters is expected given the values of their sensitivity coefficients. A slight variation in the starting point (*e.g.* $\lambda_1 = 0.3\,\mathrm{W/m\,K}$, $\lambda_2 = 0.1\,\mathrm{W/m\,K}$ and $\lambda_3 = 0.2\,\mathrm{W/m\,K}$) has the consequence that convergence to the actual parameter values is not achieved.
The application of Levenberg-Marquardt method has proven to be even more critical because it is more sensitive to the inverse problem ill-conditioning ($|\mathbf{J}^{\mathrm{T}}\mathbf{J}| \approx 0$).

Genetic algorithms. As it has been shown, there are cases where convergence to actual parameter values is not achieved, in particular when the starting point is too far from the solution. It makes sense, therefore, to apply stochastic methods to the considered problem as it is the very stochastic nature of the procedure that allows a certain degree of independence on the starting point in the parameter space.
Since genetic algorithms employ a binary coding of parameters, there are optimal values uniquely determined, toward which the algorithm has to go, which are the best approximation obtained of the actual parameter values, given the number of bits in the coding. In our example, therefore, there are bit sequences representing the optimal values of thermal conductivities.

The calculation amount can be roughly quantified by estimating how many times the fitness function has to be evaluated by solving the direct problem, since this requires the larger part of the calculation. For populations of 100 individuals and with 100 generations, the fitness function has to be evaluated 10000 times, that is much larger than what is required by classical optimization methods. On the other side, as already said, stochastic methods can be the only solutions when tackling complex problems. They can also be employed to provide a first rough parameter estimation, to be improved afterwards with the use of classical optimization methods (hybrid genetic algorithms [28]) or through the synergy with other heuristic methods [29].
To apply genetic algorithms, each one of the three unknown conductivities has been coded with 10 bits (giving rise to a chromosome with 3 genes and 30 bits) and different combinations of crossover type and mutation probability have been evaluated. The algorithm parameters which are common to the various examples have been synthesized in Tab. 2.

Table 2. Parameters of the genetic algorithm employed for the three-layer wall problem.

$\lambda_{\min}$	$\lambda_{\max}$	n_{bit}	n_{ind}	n_{gen}	**selection**	p_{cross}
0.01	1	10	100	100	tournament	0.9

Since genetic algorithms are used to maximize functions, the fitness function has to be chosen as the opposite of Eq. (4).
The sensitivity analysis showed that the simultaneous estimation of the three conductivities is a hard task to be performed. To allow a wide exploration of the parameter space, two options have been tested to differentiate the genetic material: multipoint crossover and high mutation probability.

Table 3. Parameter estimation with genetic algorithms for three-layer wall. Heat flux at $x = 0$.

Crossover	p_{mut}	**Parameter**	**% mean error**	**% std error**
Single-point	0.1	λ_1	127.8	284.6
		λ_2	1.8	4.5
		λ_3	94.9	215.7
Single-point	0.5	λ_1	1.9	7.1
		λ_2	0.0	0.0
		λ_3	0.3	0.9
Three-point	0.1	λ_1	90.9	229.2
		λ_2	0.1	0.6
		λ_3	16.1	39.1
Three-point	0.5	λ_1	131.9	322.0
		λ_2	0.3	0.8
		λ_3	9.0	23.8

As it is shown in Tab. 3, the algorithm with best performances proved to be that using single-point crossover and mutation probability equal to 0.5. In this case, the error in the determination of λ_2 equal to zero means that the algorithm always converges to the optimal value of the parameter in the 10 bit coding. All results in Tab. 3 are average values for 20 runs of the program. The difference in the errors on the three parameters clearly reflects the diversity of their sensitivity coefficients seen in the previous paragraph. In particular, the thermal conductivity of the first layer is extremely difficult to determine, because of the low sensitivity coefficient J_{λ_1} and of the high correlation between λ_1 and λ_2.

It is interesting to analyze the convergence behavior in the four cases considered. The convergence to the optimal values is never reached in the first case shown in Tab. 3, is reached 17 times out of 20 in the second case, 4 out of 20 in the third case, and 16 out of 20 in the fourth case. This means that, even if the errors obtained in the third and fourth cases are comparable, a larger mutation probability seems to be beneficial for the convergence effectiveness of the algorithm.

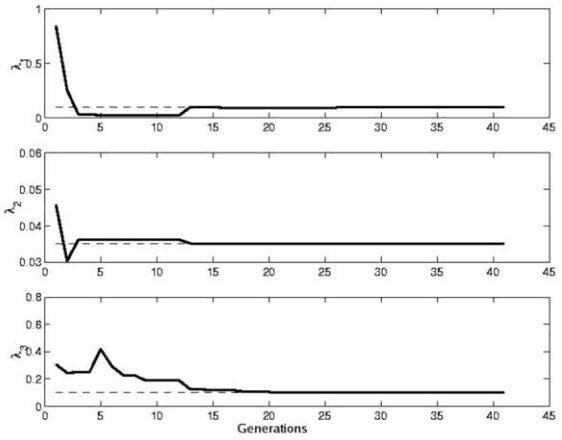

Figure 3: Convergence to the optimal values (dashed lines) of the thermal conductivities for the three-layer wall using genetic algorithms.

Fig. 3 shows the evolution toward the optimal values of the parameters in a typical example of the third case. What is shown is the result for the best individual in each generation.
The genetic algorithm parameters that provided the best estimation results have been employed in a second example of solution of the inverse problem. In this case the simulated heat flux is that at the $x = L$ edge of the wall. Tab. 4 shows the results of the estimation (average on 20 runs) for this case. The performances are similar to those obtained in the previous case. We can say, therefore, that, for the considered problem, a proper combination of crossover and mutation allows a quite accurate determination of parameters.

Table 4. Parameter estimation for three-layer wall with genetic algorithms. Heat flux at $x = L$.

Crossover	p_{mut}	**Parameter**	**% mean error**	**% std error**
Single-point	0.5	λ_1	0.6	1.2
		λ_2	0.0	0.0
		λ_3	0.5	1.0

To further characterize the performances of genetic algorithms, we realized some tests of robustness against noise. In this case, however, given the very high correlation r_{12} between λ_1 and λ_2 and the extremely low sensitivity of the heat flux at $x = 0$ with respect to λ_1, the presence of the noise makes almost impossible to determine simultaneously the three parameters. Therefore, the attention has been concentrated on the estimation of just λ_2 and λ_3. Different amounts of Gaussian white noise have been added to heat flux and temperature data to simulate measurement errors. Wavelet denoise, as implemented in the Wavelet Toolbox of Matlab®, has been used to filter data before applying the estimation. The results are shown in Tab. 5 and refer to ten runs for each case.

Table 5. Estimation of the parameters λ_2 and λ_3 for three-layer wall with genetic algorithms and noisy data. Heat flux at $x = 0$.

σ_t **(K)**	σ_q **(W/m^2)**	**Parameter**	**% mean error**	**% std error**
0.1	0.1	λ_2	0.0	0.0
0.1	0.1	λ_3	27.3	0.6
0.5	0.1	λ_2	0.0	0.0
0.5	0.1	λ_3	24.4	0.4
0.5	0.5	λ_2	1.1	1.4
0.5	0.5	λ_3	58.3	18.2

It is seen that genetic algorithms provide quite good results also in this case for the insulator thermal conductivity. They are less effective in the estimation of the covering thermal conductivity, but this is not surprising given the very low value of the corresponding sensitivity coefficient.

Simulated annealing. As it has been said in section 3, critical points in the use of simulated annealing are the selection of the temperature variation law and of the criterion to modify trial values of parameters. Regarding the first point, we selected the following temperature law [30]:

$$T_j = 2^{-\frac{j-1}{2}} T_{\text{ini}} \qquad j = 1,2,\dots,N_T \tag{7}$$

In the examples seen in this paragraph $T_{\text{ini}} = 3000$. The value of T_{ini}, clearly, has no meaning from a physical point of view, but it has been chosen so that, in the first part of the process almost all configurations are accepted, even if they entail a considerable energy increase, so that the parameter space is sampled extensively. In this way it is possible to avoid the algorithm to 'freeze' in a state with an energy not sufficiently low, or, in other terms, to avoid it to be trapped in a local minimum.
The variation of parameter values has been realized by adding or subtracting to the current value a random quantity comprised within a given percent of it. The new value of the thermal conductivity can then be expressed as a function of the old one as:

$$\lambda = [1 + \text{sgn}(-0.5 + \text{rnd}_1)\text{rnd}_2\varepsilon]\lambda_{\text{old}} \tag{8}$$

where sgn(.) is the signum function, that is sgn(x)=1 for $x > 0$, sgn(x)=-1 for $x < 0$ and sgn(x)=0 for $x = 0$, while rnd_1 and rnd_2 are random numbers uniformly distributed between 0 and 1. ε is the percentage of which the current value is changed and has been varied with the temperature with the law:

$$\varepsilon = \frac{\alpha}{\beta + i\gamma} \tag{9}$$

where α, β and γ are proper constants and i is the index associated to the temperature variation. The starting temperature and the constants that appear in (10) have been empirically selected. Each run performs 500 temperature steps and 40 iterations for each temperature.
The first part of Tab. 6 shows the results obtained when the heat flux is simulated at $x = 0$. The second part of Tab. 6 shows instead the results obtained for heat flux at $x = L$. All the errors obtained are statistical values for 20 program runs. As happens for sensitivity coefficients, in the latter case the roles of λ_1 and λ_3 are interchanged and

λ_3 becomes the parameter whose determination presents the larger error. If it is possible to acquire heat flux measurements both at $x = 0$ and at $x = L$, the two estimations can be performed together to provide accurate values for all three parameters.

Table 6. Parameter estimation for three-layer wall with simulated annealing.

Heat flux at $x = 0$.

T_{ini}	Eq. (10) constants	Parameter	% mean error	% std error
3000	$\alpha = 3$, $\beta = 1$, $\gamma = 0.1$	λ_1	20.2	16.3
		λ_2	0.2	0.2
		λ_3	1.3	1.2

Heat flux at $x = L$.

T_{ini}	Eq. (10) constants	Parameter	% mean error	% std error
3000	$\alpha = 3$, $\beta = 1$, $\gamma = 0.1$	λ_1	0.3	0.5
		λ_2	0.8	0.4
		λ_3	43.2	17.4

Figs. 4a-b show the evolution of the energy and of the parameters in a typical run. It is seen that in the first part of the process large energy oscillations are allowed. It is just this mechanism that provides a way to escape from local minima.

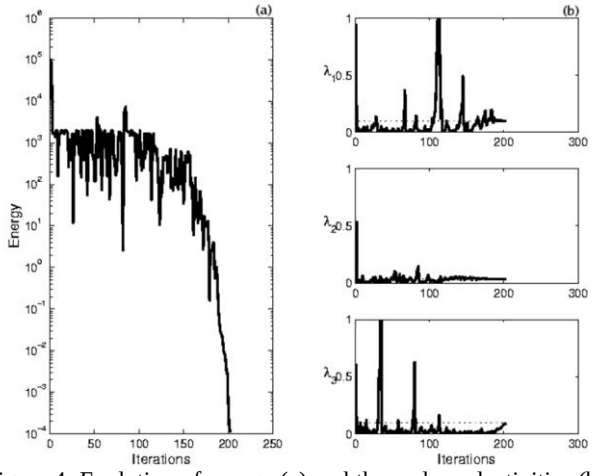

Figure 4: Evolution of energy (a) and thermal conductivities (b) in the three-layer wall problem for the estimation with simulated annealing.

4.2. Five-layer wall

The problem of the determination of thermal conductivities of a five-layer wall (wall 2 in Tab. 1) is now presented.

Sensitivity coefficients. Fig. 5 shows the sensitivity coefficients of the heat flux with respect to variations of the five thermal conductivities at $x = 0$ (upper row) and at $x = L$ (bottom row). As in the case of the three-layer wall, they present a trend that is specular in the two situations. This property can be exploited to obtain accurate estimations. They differ by orders of magnitude: the sensitivity analysis suggests that the simplest parameters to be determined should be λ_2 and λ_4 in both cases. Almost completely correlated parameters are λ_1 and λ_2 for measurements at $x = 0$, λ_4 and λ_5 for measurements at $x = L$ (correlation coefficients almost 1 in both cases).

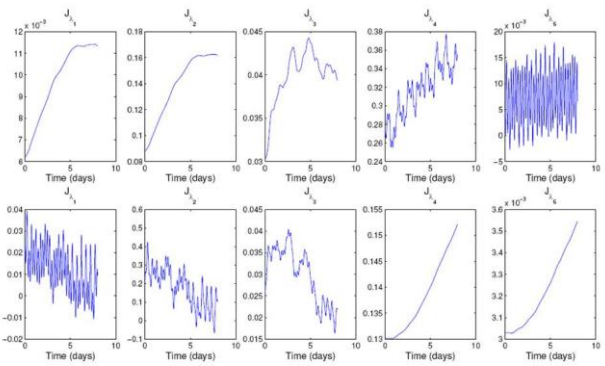

Figure 5: Sensitivity coefficients of the heat flux at $x = 0$ (upper row) and at $x = L$ (bottom row) with respect to thermal conductivities.

Genetic algorithms. To employ genetic algorithms, the unknown parameters have been represented with 10 bit genes, for a whole chromosome length of 50 bits. The other parameters of the genetic algorithm are reported in Tab. 7.

Table 7. Parameters of the genetic algorithm employed for the five-layer wall problem.

λ_{min}	λ_{max}	n_{bit}	n_{ind}	n_{gen}	selection	p_{cross}
0.01	1	10	100	300	tournament	0.9

Different options regarding mutation probability and crossover type have been tested. The best results, that however are not satisfying, are reported in Tab. 8. The values shown refer to 10 runs of the genetic algorithm.

Table 8. Parameter estimation for a five-layer wall with genetic algorithms.

Crossover	p_{mut}	Parameter	% mean error	% std error
Single-point	0.5	λ_1	465.6	403.8
		λ_2	400.2	601.2
		λ_3	50.0	45.8
		λ_4	16.4	18.8
		λ_5	16.8	21.4

Simulated annealing. For this application, 500 temperature steps (with the variation criterion in Eq. (7)) and 40 iterations for each temperature have been considered. The results are shown in Tab. 9. Satisfactory estimations are obtained for λ_3, λ_4, and λ_5 at $x = 0$ and for λ_1, λ_2, and λ_3 at $x = L$. This is not in complete agreement with the sensitivity study and the difference is probably due to the nonlinear character of sensitivity coefficients.

Also in this case, as in the three-layer wall problem, it is possible to achieve an accurate estimation of all parameters if a supplementary heat flux measurement is performed at $x = L$. Moreover, the overall results show an improvement compared to those obtained with genetic algorithms. This means that, when problems become complex, simulated annealing appears more efficient in avoiding premature convergence, that is one of the typical inconveniences of genetic algorithms.

Table 9. Parameter estimation with simulated annealing for a five-layer wall problem. Statistical values for 10 runs.

Heat flux at $x = 0$.

T_{ini}	Eq. (10) constants	Parameter	% mean error	% std error
3000	$\alpha = 3, \beta = 1, \gamma = 0.1$	λ_1	69.3	64.2
		λ_2	67.7	75.9
		λ_3	3.3	2.3
		λ_4	0.3	0.3
		λ_5	1.0	1.4

Heat flux at $x = L$.

T_{ini}	Eq. (10) constants	Parameter	% mean error	% std error
3000	$\alpha = 3, \beta = 1, \gamma = 0.1$	λ_1	0.8	1.0
		λ_2	0.2	0.2
		λ_3	1.4	1.7
		λ_4	15.9	9.5
		λ_5	76.6	21.5

5. CONCLUSIONS

We investigated the problem of determining the unknown thermophysical parameters of multilayer walls starting from temperature and heat flux measurements on the edge walls.

Two stochastic optimization methods have been employed with this aim: genetic algorithms and simulated annealing. It has been shown that both methods are capable of providing solutions of the problem when classical methods fail. With both types of stochastic algorithms it is necessary to empirically select a few parameters to tailor the performances of the optimization method to the problem under examination. For more complex problems, as the five-layer wall, simulated annealing seems to provide better performances, in particular when supplementary measurements at the outer edge of the wall can be acquired.

Hybrid methods could be applied where a first rough parameter estimation is performed with a stochastic method and a second, more accurate estimation is realized using conjugate-gradient like methods. This would combine global optimization and accuracy.

Future work should take into account the temperature dependence of thermophysical parameters. The estimation methods can be easily extended to this case if known functional forms of temperature dependence are assumed. Thermophysical and functional parameters should be therefore determined. However, the computational burden would increase due to the solution of the direct problem which becomes non linear.

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APPENDIX

For a homogeneous wall subject to heat conduction in periodic regime, solutions of Eq. (1) can be assumed in the form $T(x,f,t) = \bar{T}(x,f)\exp(2\pi j f t)$, which, inserted in eqs. (1) and (2), gives the solution

$$\bar{T}(x,f) = \frac{\bar{T}_L \sinh(\nu x) - \bar{T}_0 \sinh[\nu(x-L)]}{\sinh(\nu L)} \qquad (A.1)$$

where $\nu = \sqrt{2\pi j f/D}$. The heat flux at x is therefore:

$$\bar{q}(x,f) = -\frac{\lambda\nu}{\sinh(\nu L)}\{\bar{T}_L \cosh(\nu x) - \bar{T}_0 \cosh[\nu(x-L)]\} \qquad (A.2)$$

At frequency f, the non-normalized sensitivity coefficient of the heat flux $\bar{q}(f)$ with respect to variations of the thermal conductivity λ results from Eq. (A.2)

$$\begin{aligned}\bar{J}_{0\lambda}(f) &= \frac{\partial \bar{q}(f)}{\partial \lambda} \\ &= -\frac{\nu}{2}[\nu L \coth(\nu L) \\ &+ 1]\frac{\bar{T}_L \cosh(\nu x) - \bar{T}_0 \cosh[\nu(x-L)]}{\sinh(\nu L)} \\ &+ \frac{\nu^2}{2}\frac{x\bar{T}_L \sinh(\nu x) - (x-L)\bar{T}_0 \sinh[\nu(x-L)]}{\sinh(\nu L)} \qquad (A.3)\end{aligned}$$

To obtain the spatial temperature distribution and the heat flux at $x = 0$ for an N-layer wall, it is useful to start from the homogeneous case and evaluate Eq. (A.2) at $x = 0$ and at $x = L$ as

$$\begin{aligned}\bar{q}_0 &= a\bar{T}_L + b\bar{T}_0 \\ \bar{q}_L &= -b\bar{T}_L - a\bar{T}_0 \qquad (A.4)\end{aligned}$$

where $a = -\lambda\nu/\sinh(\nu L)$ and $b = \lambda\nu \coth(\nu L)$. Rearranging terms in Eq. (A.4), we can set

$$\mathbf{G}_L = \begin{bmatrix}\bar{q}_L \\ \bar{T}_L\end{bmatrix} = \begin{bmatrix}-b/a & b^2/a - a \\ 1/a & -b/a\end{bmatrix}\begin{bmatrix}\bar{q}_0 \\ \bar{T}_0\end{bmatrix} = \mathbf{A}_{10}\mathbf{G}_0 \qquad (A.5)$$

For an n-layer wall with lengths $L_1, \ldots, L_n$, Eq. (A.5) can be extended as

$$\mathbf{G}_{L_n} = \begin{bmatrix}\bar{q}_{L_n} \\ \bar{T}_{L_n}\end{bmatrix} = \mathbf{A}_{n0}\mathbf{G}_0 = \mathbf{A}_{n\,n-1}\mathbf{A}_{n-1\,n-2}\cdots\mathbf{A}_{10}\mathbf{G}_0 \qquad (A.6)$$

Summing over all the frequencies, it is therefore possible to obtain $q_{L_n}(t)$ and $T_{L_n}(t)$ as a function of $q_0(t)$ and $T_0(t)$ (or $q_{L_n}(t)$ and $q_0(t)$ as a function of $T_{L_n}(t)$ and $T_0(t)$).

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Nomenclature

c	specific heat	J / kg K
D	thermal diffusivity	m^2 / s
E	energy of a configuration	J
f	frequency	Hz
I	number of measurements	
$J_{o\lambda}$	sensitivity coefficient	K / m
J_λ	dimensionless sensitivity coefficient	
$\mathbf{J}$	dimensionless sensitivity matrix	
k	Boltzmann constant	J / K
L	wall length	m
M	number of individuals in tournament selection	
N_T	number of temperature levels	
p	probability	
q	heat flux	W / m^2
$\mathbf{q}$	heat flux vector	W / m^2
r	correlation coefficient	
R	set of all possible configurations	
s	configuration in solution space	
S	least-squares norm	W^2 / m^4
t	time	s
T	temperature	K
x	space	m
Greek symbols		
ε	percent variation of parameter value	
λ	thermal conductivity	W / m K
ν	spatial frequency	1 / m
π_T	probability of a configuration at temperature T	m
ϱ	density	kg / m^3
σ_q	std deviation of noise on heat flux	W / m^2
σ_t	std deviation of noise on temperature	K
Superscripts		
$\bar{}$	frequency domain	
$\sim$	calculated with trial parameter values	
Subscripts		
cross	crossover	
e	external	
i	internal	
ini	Initial	
max	maximum value	
mut	mutation	
old	old value	