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Determination of the thermal conductivity and the volumetric heat capacity by genetic algorithm

Theses Booklet

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1. Introduction

Problems appear in almost every branch of mechanical engineering where differences in temperature between or within structural elements also influence physical processes. (e.g.: during the production and heat treatment of metallic and non-metallic materials in materials technology, during forming procedures in machine production, as a result of friction in machine design, or in the case of heat engines during energy transformation and transport processes.) In such cases thermodynamic calculations (and measurements) have to be performed to obtain a detailed understanding of the problem and assure proper reliability and quality of the machines involved. The majority of thermodynamic calculations pertain to heat conduction problems. When dealing with heat conduction, knowledge of the geometry and material properties of the structural elements examined as well as the boundary conditions is required. In connection with a transient problem volumetric heat capacity (density multiplied by specific heat) and thermal conductivity should both be available. These material properties may be considered constant (temperature independent) in case of certain materials and temperature range, in turn, however, there are numerous cases where they significantly vary with temperature. Due to the constant development in materials technology there is a permanent need for the determination of the thermophysical properties of materials. One of the most dynamically growing branches of materials technology is polymer technology, where the temperature dependence of thermophysical material properties is rather significant with a great proportion of materials.

Material properties are determined by measurement. Over the last decades a large number of measurement methods have become available; however none of these may be considered universal. A given method may usually be applied to measure the material properties of a specimen of strictly defined shape and size on a specific scale and in a specific temperature range. The mapping of temperature dependence may in many cases be done by measurements repeated at different temperatures, which is usually quite time consuming. Based on this the need emerges to increase the universality of measurement methods (e.g. determining thermal conductivity and volumetric heat capacity with the same device, probably even simultaneously, a faster and more simple measurement of temperature dependence, the capability to determine an ever increasing scale of properties, the extension of measurable temperature range, independence of the specimen’s geometry). Another motivating factor behind the continuous development of measurement methods is the relatively large deviation between measurements done on identical materials at different laboratories employing different methods.

The commonly used thermophysical property measurement methods are almost without exception based on mathematical models with an analytical approach. The reason for this being, that the material properties sought may be easily expressed based on measurement data (temperature, geometry, heat power etc.), thus making it simple to evaluate measurement results. However, the great many limitations faced when planning the measurement (primarily one-dimensional, simple geometry, homogenous initial and boundary conditions, constant material properties) do quite adequately characterize the disadvantages involved in the analytical approach. The universality of the measurement may be increased by letting go of the limitations of the analytical approach and planning a measurement that can only be treated by a numerical mathematical model (numerical approach). In this case there are almost no restrictions involved (arbitrary geometry, arbitrary time- and location dependent boundary conditions, arbitrary temperature dependent material property functions), measuring technicalities may be given priority (increased simplicity of equipment, increased accuracy of boundary conditions, increased accuracy of temperature measurements, reduction of the quantity measured), furthermore the possibility arises to simultaneously measure multiple material properties as well as directly determine temperature dependence.

2. Research history

László Kiss' research on thermal properties is summarized in his candidate's thesis [Kiss, 1983]. Therein he proposes the following measurement method with numerical approach (BICOND): the sample shall be a long, thick walled cylinder ($L / D \approx 4$) featuring, by good approximation, radial one-dimensional heat conduction. The sample shall be set up in accordance with the measurement arrangements shown in Figure 1. The core-sample-shield assembly shall be heated to a predefined (isothermal) temperature and then cooled by forced air flow to ambient temperature. During cooling the temperatures of the inner and outer sensors together with the temperature of the air flow should be continuously registered. Temperature dependent thermal conductivity ($k(T)$) and volumetric heat capacity ($\rho c_p(T)$) shall be determined based on the transient temperature readings of the inner and outer sensors (evaluation). This method needs the solution of a rather complicated inverse heat conduction problem, and could consequently not be fully realized given the limitations of computer technology available in the 1980s.

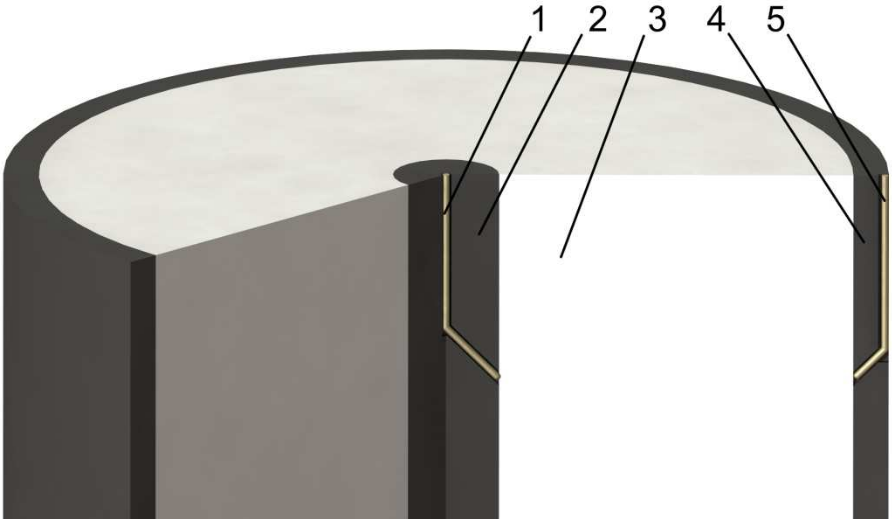


Figure 1 Design of the measurement arrangement
(1 – inner sensor, 2 – core, 3 – sample, 4- shield,
5 – outer sensor)

In connection with the above problem I, based on the literature available, took stock of the principles related to the measurement of thermophysical material properties and the physical - mathematical models to be applied. Based on this, I also examined the methods applicable to solve the differential equation describing the problem. I surveyed the methods for solving inverse heat conduction problems, paying special attention to artificial intelligence based methods. I also compiled a summary of the scientific achievements made in the field of inverse heat conduction by the latter methods. Introducing new classification (analytical and numerical approach) I presented the methods most frequently employed in engineering practice to measure the thermophysical material properties of solid materials in the low to medium thermal conductivity range. Briefly I also surveyed the typical instances of material properties' temperature dependence.

3. Objectives

The main objective of this thesis is to devise an automatized, reliable and universal, genetic algorithm based evaluation procedure in connection with the BICOND thermophysical property measurement method. (The measurement method may be applied to low to medium thermal conductivity solid, porous or powder based materials.) The aim of the evaluation is to simultaneously determine both, temperature dependent thermal conductivity and volumetric heat capacity based on a single transient measurement. To achieve this I defined the following subtasks:

- Finding a fast and accurate numerical solution to the direct heat conduction problem defined on the basis of the BICOND measurement method.
- Examining the convergence of the genetic algorithm based inverse solution with simulated measurement data assuming the linear temperature dependence of material properties.
- Solving the inverse problem and analyzing its accuracy with simulated measurement data, assuming arbitrary temperature dependence of material properties.
- Restoring the measuring device made in the 1980s and supplementing it with modern appliances as well as using it for measurements. Testing the new evaluation procedure with real measurement data. Comparing the material properties evaluated with those measured on identical material with different methods as well as data derived from literature, which essentially amounts to validating the evaluation procedure.

4. Examination methods

The solution of the following inverse problem is required for the evaluation of the BICOND measurement: the geometry of a three-layered (core – sample – shield) infinite (1D) cylinder, the homogenous initial and boundary conditions, the material properties of two layers (core and shield) as well as transient temperature readings registered during a cooling process by 1 or 2 sensors considered to be known the volumetric heat capacity and thermal conductivity of the second layer (sample) have to be determined simultaneously with arbitrary temperature dependence.

When devising a numerical solution to the direct heat conduction problem the main aim was to find a compromise between the contradicting requirements of performing the fastest possible calculation and producing the most accurate result possible. This was quintessential for it also determined the time required to calculate the inverse solution. I solved the direct heat conduction problem by finite difference method, for which I also developed a software application of my own. I found the optimal solution to the direct problem by a series of accuracy and verification tests.

Employing finite difference method I performed the sensitivity analysis of the parameters assumed to be unknown in the inverse solution with regard to both, function based and parametric representation.

I first solved the inverse problem using simulated measurement results. The advantage of this being that the material properties sought are precisely known, thus making it possible to easily calculate the accuracy of the method, examine the convergence and exclude eventual errors in modeling resulting from differences between the mathematical model and reality. I solved the inverse problem in 3 cases: when establishing the material properties simultaneously according to a linear function, individually according to an arbitrary function, and simultaneously according to an arbitrary function. In the most complicated case I was searching for 42 unknown parameters. In the inverse solution I also examined the impact of random errors or regularization on the solution's accuracy, as well as when it was sufficient to use only one sensor and when there was a need for two sensors to produce a solution. I developed a software application of my own to solve the inverse problem. (Figure 2).

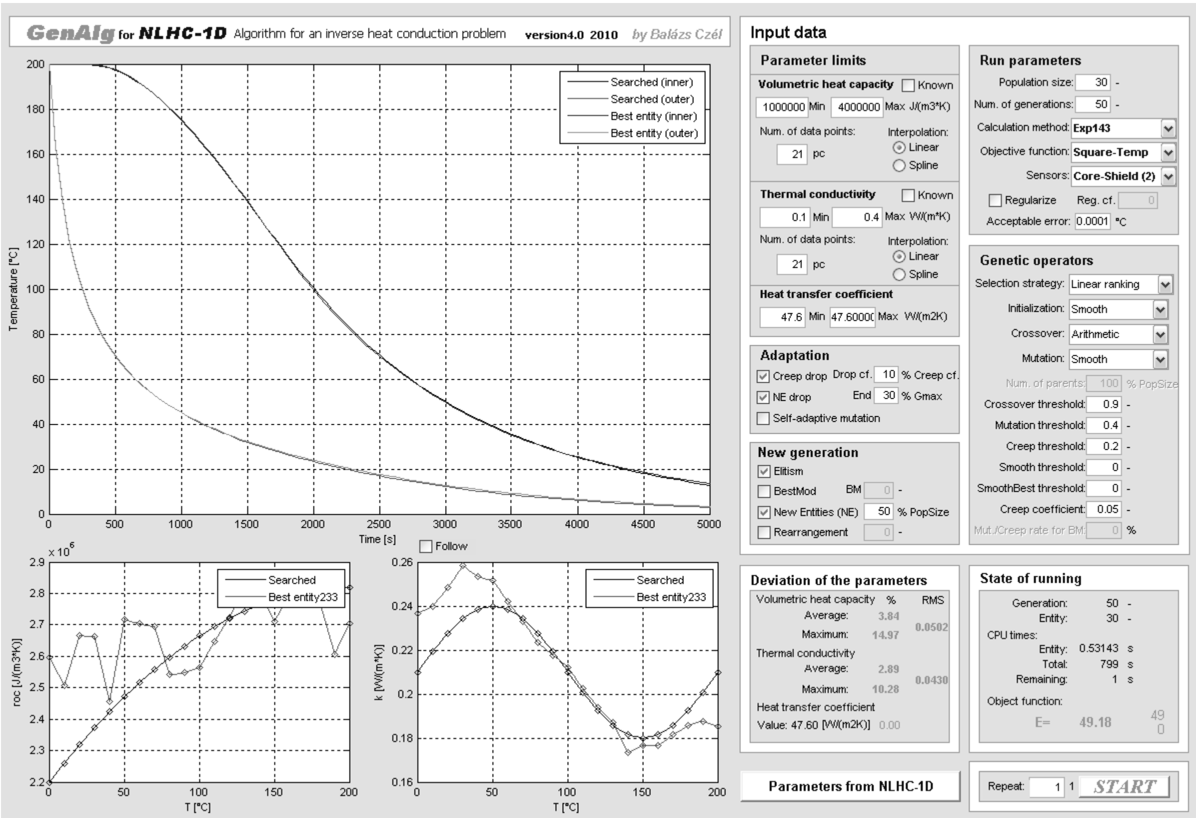
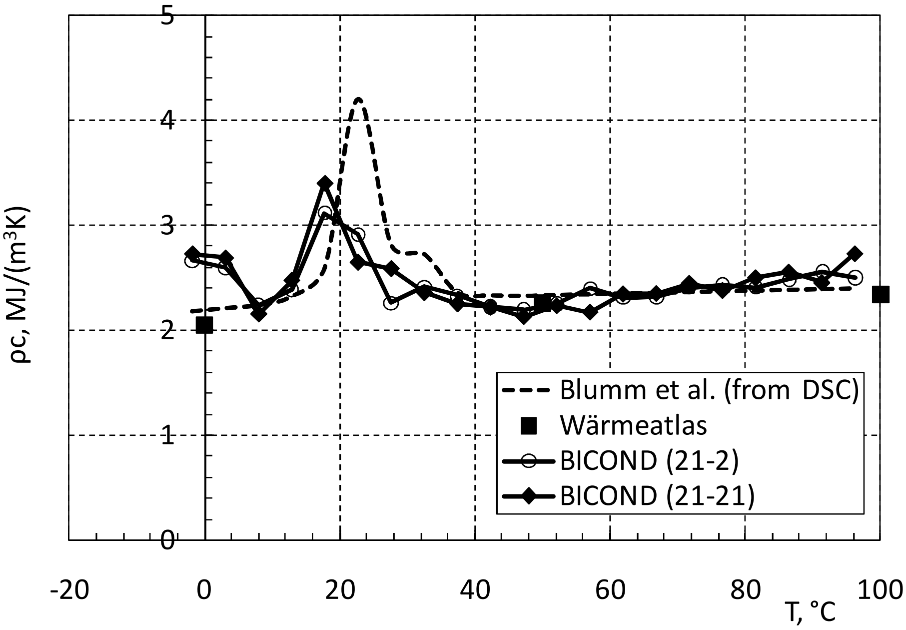


Figure 2 User interface of the application developed to solve the inverse problem

I performed measurements according to the BICOND measurement method on polyamide (PA) and teflon (PTFE) samples, which I then evaluated by the genetic algorithm based evaluation procedure I had devised. I determined the material properties parallely as a linear function of temperature in the case of PA and parallely as an arbitrary function of temperature in the case of PTFE. In the case of PA I compared the results of evaluation with the results of verification measurements done by different methods whereas with PTFE I compared them with data from literature. The results of the measurements performed on the PTFE sample are shown in Figure 3.

a)



b)

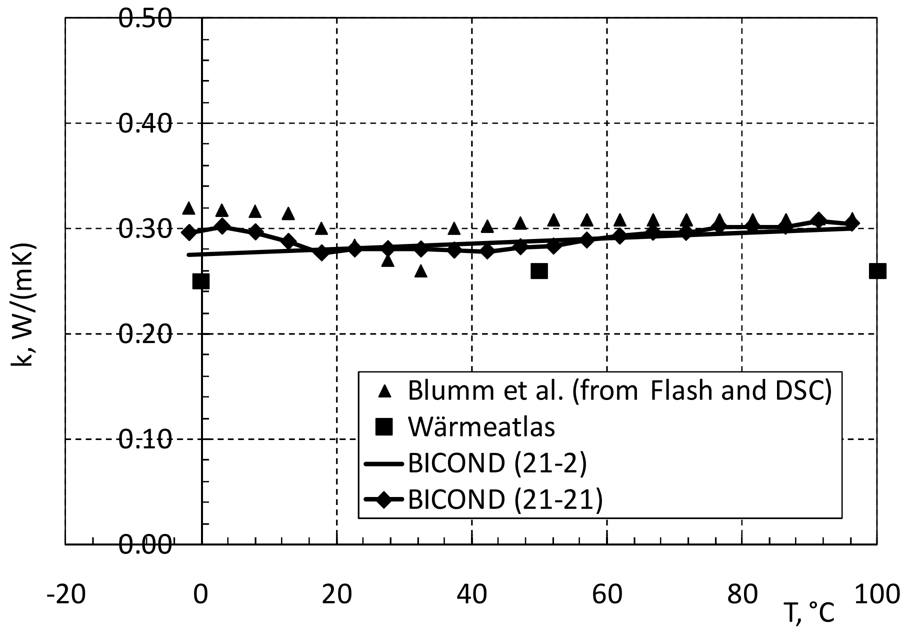


Figure 3 Results of the measurements performed on the PTFE sample and data from literature (a) volumetric heat capacity, b) thermal conductivity) ([Blumm, 2008], [Wärmeatlas, 2006])

5. New scientific results

Thesis 1 ([1])

I have made the following conclusions based on the sensitivity analyses connected to the inverse heat conduction problem arising from the evaluation of the BICOND measurement method:

a) I have shown by sensitivity analyses that it is more feasible to use the inner sensor for the one-sensor-based evaluation as the temperatures measured with the inner sensor (at $r = R_1$) are 3 to 5 times more sensitive to changes in material properties than the temperatures measured with the outer sensor (at $r = R_2$).

b) When establishing the material properties according to an arbitrary function the relative sensitivity coefficients of the material properties pertaining to the lower and upper 10% of the measurement's temperature range ($\left[T_\infty, T_0\right]$) are low, thus making their determination unreliable. Material properties may be dependably established in the evaluation's temperature range. Knowing the measurement's temperature range I suggest the following interval for the evaluation's temperature range: $\left[T_\infty + 0{,}1 \cdot \left(T_0 - T_\infty\right), T_0 - 0{,}1 \cdot \left(T_0 - T_\infty\right)\right]$.

Thesis 2 ([1], [2], [3])

When modeling the transient heat conduction of a one-dimensional three-layered cylindrical geometry by finite difference method, defining the thermal conductivity ($k\left(T\right)$) function of the second layer by chart with linear interpolation between the data points, the surge (breaking point) in the gradient of the function at the data points causes oscillation at $r = R_2$ (at the interface closer to the outer shield, outer sensor) in the transient temperature. This oscillation may as well result in the instability of the solution. Oscillation may be reduced by increasing the grid's density.

Thesis 3 ([4], [5], [6])

By calculations performed with the application of the genetic algorithm based evaluation procedure using simulated measurement results I have made the following conclusions:

a) the accuracy of the inverse solution remains immune to random errors in simulated measurement results even with regard to the most general search of the material properties,

b) if only one of the $k(T)$ and $\rho c_p(T)$ functions is considered unknown, even the application of one sensor is sufficient for the inverse solution,
c) with the material properties determined according to an arbitrary function, regularization improves the accuracy of the inverse solution if there is no second order phase transition in the evaluation's temperature range.

Thesis 4 ([4], [5])
By calculations performed with the application of the genetic algorithm based evaluation procedure using simulated measurement results I have shown that estimating the material properties simultaneously as linear function of the temperature the original material properties may be estimated by arbitrary accuracy. For the establishment of the final estimated values I propose that the results of multiple genetic runs be taken into account, a so called "comet diagram" be drawn up and based on this one of 3 methods (limit curve method, average method, best entity method) be applied. When determining the material properties simultaneously as linear function of the temperature the use of the absolute objective function allows for a more simple establishment of the final estimated values.

Thesis 5 ([6])
By calculations performed with the application of the genetic algorithm based evaluation procedure using simulated measurement results I have shown that with the material properties determined individually ($\rho c_p(T)$ or $\lambda(T)$) or simultaneously ($\rho c_p(T)$ and $\lambda(T)$) according to an arbitrary (non-linear) function the inverse problem may be solved without any prior information on the functions and special computational apparatus in acceptable calculation time with satisfactory accuracy for the engineering practice.

Thesis 6 ([7], [8])
a) The modeling errors affecting the genetic algorithm based evaluation procedure devised for the BICOND measurement method do not demonstrably influence the accuracy of the evaluation. The basis of this statement being that when evaluating the results of the BICOND measurement performed on a PA sample by the genetic algorithm based evaluation procedure with the material properties searched simultaneously as linear function of the temperature and comparing them with the results of verification measurements and data from literature the deviation I encountered did not exceed 10% in the case of thermal conductivity and fell

between 10 to 15% in the case of volumetric heat capacity, which is considered to be good correspondence with regard to the measurement of thermophysical properties.

b) Repeating BICOND measurements and their evaluations I have found reproducibility to be within 5%, which is satisfactory in engineering practice.

c) When evaluating the BICOND measurement with the material properties searched simultaneously as arbitrary function of the temperature the genetic algorithm based evaluation is suited for detecting second order phase transition in solid material. Evaluating the results of the BICOND measurement performed on a PTFE sample by the genetic algorithm based evaluation procedure with the material properties searched simultaneously as arbitrary function of the temperature and comparing them with data from literature I found the deviation to be within 10% with respect to both material properties in most parts of the evaluation's temperature range. In line with data from literature, I have by evaluating the BICOND measurement succeeded in expressly demonstrating the second order phase transition occurring at around 20°C and manifested in the substantial increase of volumetric heat capacity in a narrow temperature range.

6. Utilization of results

As a result of my research I succeeded in devising a universal and automated evaluation procedure for the BICOND measurement method by which results of satisfactory accuracy may be obtained for engineering practice in acceptable computational time without the need for special computational apparatus. By this, a measurement method has become available to engineering practice that allows for significantly more information to be derived from a single measurement than has been the case with prevalent methods. (Based on a single transient measurement the volumetric heat capacity and the thermal conductivity may be simultaneously determined as an arbitrary function of temperature without any prior information on the function.) In addition, the measuring device does not require any special measuring technology, so it may be constructed relatively cheaply, while the measurement procedure itself is also significantly less time consuming than has been the case with prevalent methods.

Another advantage of the proposed evaluation procedure is that changing the calculation module of the direct problem connected to the measurement method the inverse module needs only slight modifications. Such a way the evaluation procedure can be easily adapted to apply it with other measurement methods.

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