

# FINAL PUBLISHABLE REPORT

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# 1 Executive summary

## Introduction

Dissemination of measurement results and reliable decision-making require harmonised treatment of uncertainty. The current state of the art for uncertainty evaluation in metrology is provided by the Joint Committee for Guides in Metrology (JCGM) Guide to the expression of uncertainty in measurement and its Supplements, which are currently successfully applied in many but not all areas of metrology. EMRP project NEW04 developed new approaches to address uncertainty evaluation for inverse problems and for computationally expensive problems. Many industries incorporate finite element analysis in their design processes, a prime example of a computationally expensive model solved using “black box” software, and one whose results are commonly used for decision making without an associated uncertainty evaluation to support those decisions. This project aimed at facilitating the uptake of the outputs of EMRP project NEW04 by industry by providing a case study and associated freely available software.

The project’s primary supporter was Siemens, whose input ensured that the software was designed for industrial usage and that a trade journal article was written in a style appropriate for the target audience. Feedback has been collated from those who downloaded the software.

## The Problem

Thermal barrier coatings (TBCs) are used to protect expensive components, such as turbine blades and car engine parts that operate in high-temperature environments from thermal load and chemical damage. Thermal conductivity is a measure of how rapidly a material transports heat and is a key property affecting TBC performance. TBCs have a layered structure and thermal conductivity values of individual layers are challenging to measure.

Thermal conductivity is often derived from measurements of thermal diffusivity, which for homogeneous materials at high temperature is commonly measured using the laser flash technique. A method exists in the literature to derive the properties of individual materials of a layered sample from laser flash measurements. However, the uncertainties associated with these values are typically estimated using approximate methods and in practice are often overestimated to produce a “safe” uncertainty for decision-making purposes. The primary supporter of this project has stated a need to:

- improve the process of specification of TBCs and assessment of nonconforming coatings, thus reducing waste during manufacture and supporting the development of improved measurement methods for TBCs in future,
- increase the confidence in decisions made at the design stage, such as choice of thicknesses, thus reducing design time and hence cost, and
- plan their TBC development programmes and testing campaigns more efficiently, thus reducing time to market for products.

The work in EMRP project NEW04 has provided a more rigorous calculation method for uncertainties associated with thermal diffusivities and conductivities of the components of TBCs and has demonstrated this method for a simple layered system. However, it has not applied the method to a real industrial problem. Provision of software and a worked example of the method were needed to enable industrial users to apply the algorithms generated in EMRP project NEW04 to their problems without needing expert mathematical knowledge, maximising the ease of take-up.

## The Solution

This project set up to provide software and a worked example of the method to enable industrial users to apply the algorithms generated in EMRP project NEW04 to their problems without needing expert mathematical knowledge, maximising the ease of take-up.

## Impact

Lack of software is a key barrier to industry take-up of innovative mathematical methods for uncertainty evaluation. Direct impact of this project was achieved via the provision of freely available software and an associated worked example of a method for estimating the uncertainty associated with the components of a TBC system using existing laser flash thermal diffusivity data, which will be published as a trade journal article. The evaluated uncertainties will improve the primary supporter’s design, testing and assessment procedures for TBC systems, reducing material and testing costs and shortening the time to market for new products.

It is expected that the power generation and aerospace sectors will be the main beneficiaries. In the longer term the outputs of this project are expected to encourage uptake of the methodology by other industries for whom thermal characterisation is key to successful usage of advanced layered materials.

## 2 Need for the project

TBCs are used to protect expensive components that operate in high-temperature environments from thermal load, oxidation and other chemical damage. In the power generation industry TBCs are used to protect turbine blades from high temperature hot gas, which at present can reach a temperature of up to 1800 K and is likely to reach higher temperatures in future engine designs, leading to increased component lifetime and reduced down time costs. TBCs are also used to protect components in the automotive and aerospace industries.

Thermal conductivity is a key property affecting TBC performance. TBCs have a layered structure, consisting of a bond coat and a top coat applied to a substrate, and the thermal conductivity of each layer needs to be known in order to ensure that the coating will provide adequate protection. If the decisions made during the coating design process are to be reliable, the material properties used in the design process must have associated uncertainties. Thermal conductivity values of individual layers are challenging to measure and the associated uncertainties are currently estimated using very approximate, and hence conservative methods that overestimate uncertainties. Therefore, there is a need for more accurate uncertainty evaluation methods for these quantities, and this project aimed at demonstrating that the methods developed in EMRP NEW04 were suitable to solve this problem.

Thermal conductivity is often derived from measurements of thermal diffusivity. Thermal diffusivity of homogeneous ceramic materials at high temperature is commonly measured using the laser flash technique. Recent work has developed a method to derive the properties of individual materials of a layered sample from laser flash measurements, and the outputs of NEW04 extended this work to address evaluation of the uncertainties associated with the determined properties. Current methods for uncertainty evaluation estimate that the uncertainty associated with the thermal conductivity of a single layer coating is at least 5%, and a multilayer coating will have higher uncertainties than this. These values are too high for industrial usage.

The work in NEW04 provided a more rigorous calculation method, leading to less conservative uncertainty estimates. Provision of software and a worked example of the method will enable industrial users to apply the algorithms generated in NEW04 to their problems without needing expert mathematical knowledge, maximising the ease of take-up.

## 3 Objectives

The project addressed the following objectives;

1. To encourage the take-up of the outputs of JRP NEW04 by publishing a trade journal article describing a clear, well-defined method for evaluation of thermal conductivity and associated uncertainties of the components of a TBC system from laser flash measurements. The method should be applicable to any layered material that can be measured using the laser flash technique.
2. To remove a key barrier to uptake of the first objective by creating freely available software that automates the mathematically challenging aspects of the calculations, the software being promoted via the trade journal article and through other appropriate channels.

## 4 Results

*Trade journal article describing a method for evaluation of thermal conductivity and associated uncertainties of the components of a TBC system from laser flash measurements*

As part of the journal article development, a large amount of useful preparatory work was carried out. A large proportion of this focussed on the challenges of assembling an appropriate input data set, and in particular how to assign appropriate uncertainties to the input quantities when the main source of data (published literature) does not often include an uncertainty statement. The process of defining the uncertainties associated with the various input parameters led to a conference publication explaining some approaches for going from data to an uncertainty. This step is a common stumbling block that limits the application of uncertainty calculation.

The sensitivity analysis software created as part of NEW04, freely available from [here](#), was used to carry out an initial analysis of the problem, and the results were used to reduce the problem size by identifying which input quantities could be regarded as fixed, thus improving efficiency. The radius of the sample was identified as an unimportant parameter and was omitted from further consideration. Problem size, particularly regarding the number of uncertain inputs, is another barrier to the uptake of uncertainty evaluation methods.

The test data set, drawn from measurement data created as part of the EMRP project IND09, was analysed using the analysis software (see below for details) to generate results for publication in the trade journal article. The results obtained were not consistent with the primary supporter's experience of the thermal conductivity for one of the materials concerned. It was therefore decided that the journal article would not be published.

*Freely available software that automates mathematically challenging aspects of the calculations*

The project team successfully created a graphical user interface-driven software package for analysis of laser flash thermal diffusivity data from layered samples, based on guidance provided by the primary supporter. The software comprises a set of input screens for the user to supply test data files and input parameters with associated uncertainties; a central forward model of the laser flash thermal diffusivity experiment, an optimisation routine to fit the results of the forward model to the measured data; a Latin hypercube sampling routine for generation of the input value sets, and a set of post-processing and output routines. The central model of the software has been validated against other calculation approaches. The approach for layered materials (without consideration of uncertainty is shown in Figure 1.

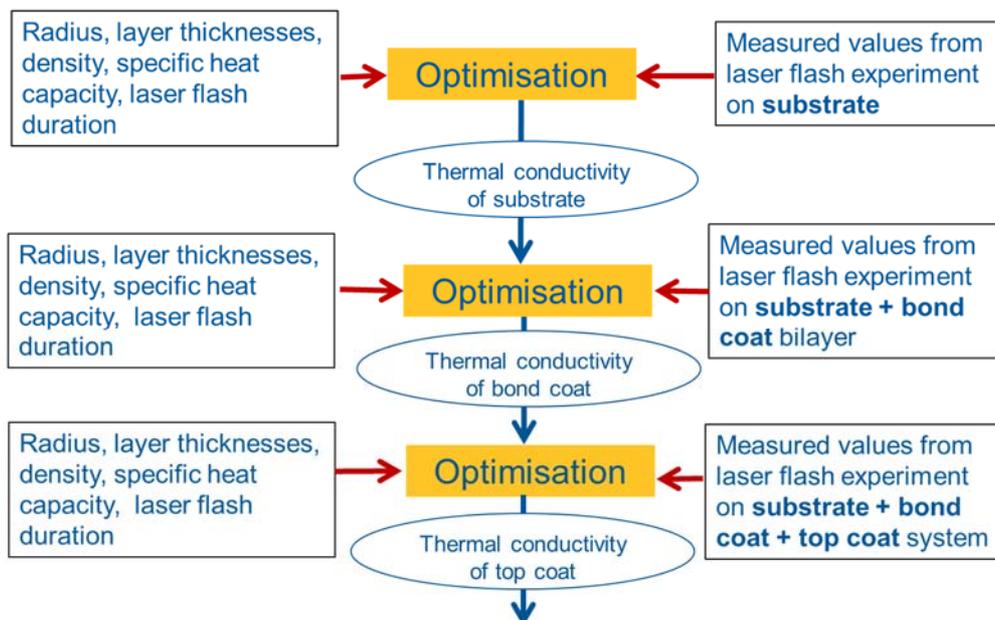


Figure 1: Sketch of parameter evaluation process for a single set of input values.

The software was made available through a dedicated website (<http://empir.npl.co.uk/tbcunc/download/software/>) as a compiled executable. The software is supplied with documentation and a test data set. The software was promoted to potentially interested parties through a webinar (for users of the COMSOL Multiphysics finite element software package), an industrial advisory group on thermophysical properties, and a presentation and associated paper at the NAFEMS World Congress.

## 5 Impact

The early outcomes of this project were disseminated to an audience from a range of industry sectors at the NAFEMS World Congress held in Stockholm in June 2017. The presentation described the project and explained how the challenges of going from information to an input distribution have been addressed for the quantities of key importance to the model. NAFEMS is an international organisation promoting good practice

in use of finite element and similar modelling techniques for engineering simulation, and has a membership drawn from most sectors of industry, international academia, and software vendors.

The software has also been promoted to users of the FE package COMSOL Multiphysics via a webinar "Simulating Heat Transfer: Knowing Your Material Properties", to attendees of a meeting of the Foundations Of Measurement working group of the German Society for Measurement and Automatic Control, and to a UK industrial advisory group on Thermophysical Properties. Key stakeholders interested in thermal barrier coating characterisation were contacted by email directly to promote the software.

The core routines in the software will be extended and reused within the EMPIR project 17IND11 Hi-TRACE. The key extension to the code will enable layered material systems with debonds and poor thermal bonds to be simulated.

## 6 Website address and contact details

<http://empir.npl.co.uk/tbcunc/>

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