NPL Report CISE 35/99

Report
to the National
Measurement System
Policy Unit, Department
of Trade & Industry

INTERIM STATUS REPORT
ON THE THERMAL AREA
FROM THE SOFTWARE SUPPORT
FOR METROLOGY PROGRAMME

BY G LORD,

NPL

September 1999

Software Support for Metrology

Interim Status Report on the Thermal Area

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Abstract

This report describes the status of the mathematics and software used to support the Thermal area of metrology, particularly as used within the NMS Thermal programme. This is one of a set of status reports produced for the NMS Software Support for Metrology (1998-2001) programme mid-way through the current programme to inform the formulation of the next SSfM programme (2001-2004). The different aspects of mathematics and software are reviewed under the headings of the themes and project topics of the current SSfM programme. The SSfM programme is identifying best practice where it exists and disseminating guidance on that best practice to other metrology areas. The outputs of the SSfM programme will be generic, applicable to more than one metrology area. This report, therefore, not only identifies problems to be tackled and best practice to be disseminated by the SSfM programme, but also if appropriate possible future Thermal programme projects applying SSfM outputs to specific problems in the Thermal area.

ISSN 1361-407X

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Contents

1. Introduction

The purpose of this status report is to inform the NMS Software Support for Metrology (SSfM) programme (1998-2001) about the status of the mathematics and software used to support the **Thermal** area of metrology, particularly what is used within the NMS **Thermal programme**. This and the companion status reports for the other metrology areas will inform the formulation of the next SSfM programme (2001-2004). It may also lead to appropriate linkage between the Thermal programme and the SSfM programme.

The SSfM programme is an underpinning programme that provides generic support in the use of software and mathematics to the NMS Programmes for each metrology area. For details of the programme, its expected deliverables and the results already produced, see the SSfM web site: http://www.npl.co.uk/ssfm/.

The NMS Programmes for specific metrology areas provide metrological support to industry. The SSfM Programme has some direct impact upon industry, as evidenced by the SSfM Club membership. This relationship is depicted in Figure 1. It is because of this relationship that the Status Reports concentrate primarily on the use of software and mathematics in the other NMS Programmes.

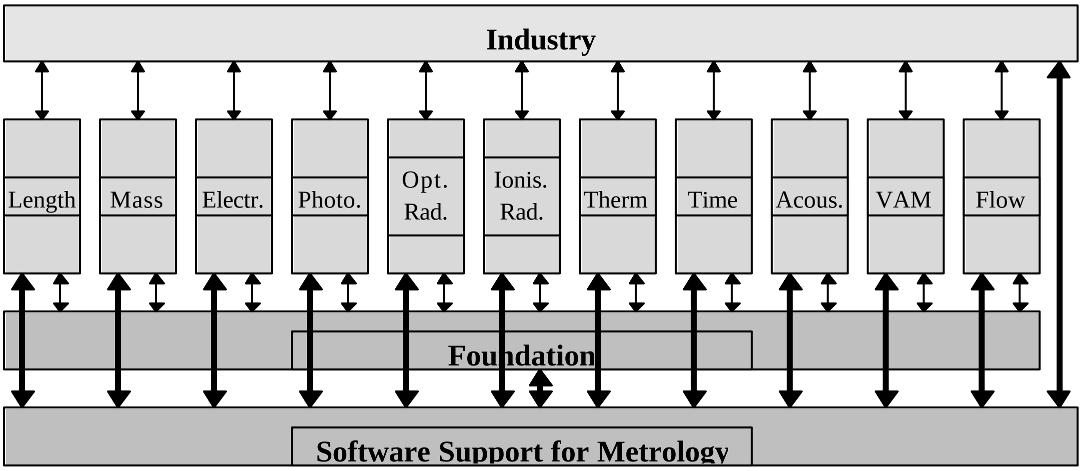

Figure 1. Relationship of SSfM to other NMS Programmes and Industry

In particular, this report addresses each of the themes within the SSfM programme and describes the status concerning the topics covered by each of the relevant projects. It also considers whether there are any important software or mathematics issues in the Thermal area which are not addressed by the current SSfM programme or which need to be taken further in the next SSfM programme.

This report is an update of an initial restricted status report produced in December 1998. That initial report was one of a set of restricted status reports which were synthesised into an overall status report for all metrology areas [8]. A summary of the differences from the initial Thermal status report is provided at the end of this report.

2. Scope of the Area Covered

The NMSPU Thermal programme covers the following themes

a) Temperature and Humidity

b) Thermophysical properties.

Thermal metrology at NPL is based on the following services

i) Maintenance of primary standards

ii) Development of new techniques

iii) Calibration and bespoke measurement services.

Typically, the DTI and/or EC act as proxy customers for i) and parts of ii); the remaining parts of ii) and iii) are offered directly to customers, in the UK and elsewhere.

Software is used extensively, from data acquisition and instrument control of digital voltmeters (DVMs) and resistance bridges, through data manipulation in spreadsheets and similar packages, to production of certificates (using WordPerfect and Word) to mathematical problem solving, e.g.,

a) data approximation (discrete modelling),

b) finite element analysis (continuous modelling) for problems in heat flow and designing black bodies (in particular, for predicting the performance of a guarded hot plate).

New techniques (e.g., using lasers) for accurate measurement of thermal properties of gases are being developed, which will require extensive software development both at the design (mainly continuous modelling) and implementation (mainly discrete modelling) stages.

In the temperature measurement services area, the main emphasis is on data approximation (discrete modelling), particularly when realising the ITS-90 temperature scale. Most of this work is fixed-price and fairly routine, but there are exceptions. The Thermophysical Properties Section's work is more likely to take the form of research investigations and consultancy.

In a sense, Humidity straddles both Mass and Thermal programmes, since it requires mass and pressure measurement of gases. The Humidity work relates to continued development of instruments such as the primary gravimetric hygrometer and offering measurement services. Often, this is achieved by building on existing systems, though a recent EC project is to develop hardware and software for humidity measurement using wavelength measurement, which is a relatively new principle in humidity measurement.

As with other metrology areas, mathematics and software are important, but the impact of SSfM themes depends on the relative maturity of that branch of metrology. The calibration services part has concerns which relate to

a) uncertainty estimation and data visualisation (in SSfM Theme 1)

b) numerical software testing and measurement system validation (in SSfM Theme 2)

c) metrology software development techniques (SSfM Theme 3)

d) support for measurement and calibration processes (SSfM Theme 4)

whereas the other themes in Thermal metrology are less mature and hence have greater need for the design (modelling) and validation projects in SSfM themes 1 and 2.

In the Thermal programme, as elsewhere in metrology, software has to satisfy many requirements. Indeed, it is instructive to categorise software by requirement. It is precisely the presence of seemingly incompatible requirements that leads to software proliferation and difficulties of choice amongst scientists. The categories of requirement include:

- Physical modelling falling within the scope of a commercial package such as Fluent, Zemax, Opticad etc. Nobody would want to write software to duplicate these, although it is often difficult to find exactly what is on the market and how good it is.

- Raw number crunching for physical modelling when no dedicated package is available. As an example, Gordon Edwards had to write code for calculating the energy transmission through an optical system to an accuracy of 1 in 10^6, requiring approximately10^9 calculations / data point. Largely for reasons of familiarity, he used compiled HT-Basic, which is flexible and fast. He believes MatLab would have been a good alternative, possibly Pascal too; he could not comment on C++. LabVIEW would be unsuitable, as would Mathematica etc.
- Symbolic manipulation supporting “pen and paper” studies of concepts and designs, as addressed by commercial symbolic mathematical packages, e.g., Mathematica and Maple. These are fine if what you want to do fits into the limits of the package, e.g. integrate a complicated function. If the task requires a number of software modules to be written, C, FORTRAN or MatLab are often better.
- Data acquisition and control. LabVIEW is good for PC-based systems and other data buses. HT-Basic is good for IEEE interfaces but is otherwise limited; this will improve when the Windows version is released. MatLab seems limited in this area.. For much instrumentation, particularly from National Instruments who make good PC-based A/D cards, drivers are provided in only LabVIEW and Visual Basic.
- Good interfacing and display (e.g. graphing and tables) facilities. MatLab and LabVIEW are good; HT-Basic is poor (the Windows version should greatly improve this)

When faced with the purchase of a new data acquisition and analysis system (as, for example, Gordon Edwards was recently) the problem is how to get a package that is good *simultaneously* at
1) instrument control,
2) real-time data analysis (number crunching, not just statistical functions) and
data display.

LabVIEW provides 1) and, to some extent, 3), but not 2). MatLab and HT-Basic provide the 2) and 3) but not 1). As a result a combination of packages is employed. In principle, DLLs and OLE can be used to link modules in different packages, but the perception among metrologists is that, despite software suppliers’ claims, this is a time-consuming business which should really be handled by staff who understand the intricacies of the process. Furthermore, it is believed that much software development effort at the NPL is spent on debugging the interfacing of different software packages.

3. Modelling Techniques

3.1 Methods for Modelling Measurement Data

We classify both the nature of the *measurement data* as well as the model of the *measurement process*.

3.1.1 Measurement Data

There are three categories of measurement data:

1. a discrete set of measurement data by which we mean:
   a) data obtained by sampling a discrete variable: e.g., a variable that may take only integer values such as in counting processes ($x \in Z$), and
   b) data obtained by sampling a continuous variable ($x \in R$). In reality, we sample from a finite representation of R.

2. a continuous set of measurement data by which we mean an analogue signal prior to any analogue to digital conversion.
3. a hybrid set of measurement data composed of both discrete and continuous sets of data.

Both heat and temperature (and derived properties) are continuous quantities, since they are usually functions of space and time. The design of novel measurement systems, whether generic (e.g., to measure the temperature of hot gases) or specific (e.g., to measure a given thermophysical property of an artefact, material or system) requires continuous modelling. Typically, the metrologist is faced with time-dependent differential equations, e.g., those governing heat flow and/or electromagnetism (for laser systems) and/or fluid mechanics (for liquids and gases). In practice, the data obtained will be discrete (sampled at fixed intervals in time or space) and approximation problems need to be solved (discrete modelling). Discrete modelling is often required at the design stage to take account of the effects of sampling (discretisation), and to assist in the estimation of the uncertainties of output quantities. There is scope for hybrid modelling if data fusion techniques are used to combine discrete (measured) data and continuous (simulated) data.

3.1.2 Measurement Process Model

There are three categories of model:

1. a discrete model in which the outputs of the measurement system are related to measurements of its inputs by a system of algebraic equations.
2. a continuous model in which the outputs of the measurement system are related to measurements of its inputs by a system of differential equations.
3. a hybrid model in which the outputs of the measurement system are related to measurements of its inputs by a system composed of both algebraic and differential equations.

Note the distinction here between the nature of the model and the approach to solving the model (which for a continuous model typically also involves solving algebraic equations). Also, given infinite precision arithmetic, a discrete model can generally be solved exactly. This is not the case for a continuous model which typically requires approximations to be made, for example, in terms of domain discretisation.

The techniques used in continuous modelling include

a) Finite Element Analysis, using third-party products such as Ansys and Pafec

b) Finite Difference methods for steady-state heat flow (a home-grown Pascal program)

Particular problems include design of apparatus, where the metrologist is required to model the steady-state response (typically governed by partial differential equation, e.g., in the case of the steady-state guarded hot-plate Laplace’s equation) and transient responses (often with nonlinear boundary conditions) in problems involving diffusion and hot wires (typically governed by a (non-)linear diffusion equation). The steady states of the guarded hot-plate apparatus are currently being modelled by a finite element analysis (jointly with NPL’s Centre for Information Systems Engineering (CISE)) to help optimise the design.

The techniques used in discrete modelling include

a) Monte Carlo techniques for emissivity calculations, largely implemented as FORTRAN programs
b) data approximation, using spreadsheets and third-party software

Recently, there has been considerable growth of interest in multi-property measurement. However, this is characterised by augmenting continuous modelling of the governing differential

equations (e.g., heat conduction) with filtering (discrete modelling) of measurement data, with optimisation (effectively a discrete process). The drivers for this development of interest include:
a) multi-property measurement offers attractive cost savings;
b) improved uncertainty estimation, since it may be possible to take greater account of correlated input quantities.

Multi-property measurement's success will depend on
a) building, solving and validating comprehensive models of the "signal";
b) building, solving and validating comprehensive statistical models of the "noise", if the uncertainty estimates are to be reliable and sharp;
c) visual modelling, to support a) and b);
d) data fusion techniques to combine all the data obtained (discrete and continuous) into a coherent whole.

Modelling has had considerable success, to the extent that many temperature and thermophysical property measurements (partly those which are steady-state and have simple geometries) are relatively routine, and the issues relate to effective implementation of the software solutions.

For more difficult problems, considerable modelling effort is needed, and deficiencies of "package" solutions become more apparent:
a) compromise between ease-of-use but inflexible, versus complicated but configurable;
b) investment: cost of purchase and training.

In Humidity work, the basic model is often quite simple, e.g., humidity is modelled as a function of temperature, when other factors are held constant. The relationship is often laid down in the relevant standard. Hence calibration curve fitting is rarely required and there is little need to develop models; they are generally used to evaluate results from given measured inputs. Some error correction is implemented in software, e.g., relating to the dew-point temperature.

Thermal Modelling is important throughout metrology. For example, in work on measurement standards for thermal properties of liquids (such as metals and polymers), the transient heat flow in liquids is important. In the NMS Ionising Radiation programme, work is in progress in conjunction with those involved in SSfM on modelling the heat flow in an irradiated calorimeter.

Tables characterising the modelling typically used in the Thermal area are given in Appendix 1.

3.2 Uncertainties and Statistical Modelling

Uncertainty estimation associated with discrete models arises most commonly in the measurement services area of Thermal metrology. As such, UKAS guide M 3003 [2], which is an interpretation of the *Guide to the Expression of Uncertainty in Metrology* (GUM) [1], is used. Concern was expressed that metrologists still need to think carefully about contributions to uncertainty, and that slavish adherence to M 3003 and similar procedures can hide important issues.

In the area of signal processing, the Type A and B classification of uncertainty is unhelpful, but it can be reinterpreted as Type A = stationary noise and Type B = nonstationary noise. Noise in laser-based measurement requires careful modelling, e.g., whether the assumption of Gaussian noise is always appropriate, and whether there is a dependence on frequency.

Two-channel radiometers are correlated across channels, hence the more general GUM model (which includes correlation terms) is required.

Often the 95% confidence level was used (particularly for calibration), but in more theoretical work it is more common to use standard uncertainty, which is less influenced by the assumption of a distribution. For some Humidity work for the UK MoD, 99% confidence is required, but this is rare.

Some staff, particularly those involved in measurement services, have attended the UKAS uncertainties course, which was judged to be very helpful. However, it was agreed that uncertainty estimation is sometimes difficult and more guidance would be welcomed. It was agreed that uncertainty estimation is generally better and more consistent since the UKAS M3003 Guide was made mandatory in UKAS laboratories. In measurement services work, many of the contributions are Type B, because the measurements are obtained from calibrated instruments.

With regard to continuous modelling, the GUM model is not easily applied. The *perception* is that this is not always appreciated by metrologists who have attended measurement uncertainty courses such as that provided by UKAS, where the emphasis is on “how to” complete an uncertainty budget, rather than on how to interpret it. Also, the examples are often too simple, such that the dominant errors are Type A, which can be reduced by further measurement, which is often difficult in the Thermophysical Properties area, for example.

It was suggested that a follow-up training scheme would help to relate to how uncertainty estimation works in practice for a given metrological task.

Continuous modelling, in particular, is perceived to have significant *model uncertainty* in addition to the uncertainty of measured inputs. The former is not easily quantified, except indirectly by means of model validation. Recording full traceability details for each component in a measurement system is a chore, but the benefits are clear. Lumping of uncertainty estimates tends to lessen the burden, at the cost of less discrimination if problems arise. Correlation errors are present in instruments such as the Gustafsson probe.

3.3 Visual Modelling and Data Visualisation

Visual modelling is seen as very valuable in this metrology area. Most of the continuous modelling packages, e.g., Fluent, offer visualisation of the results to aid interpretation and analysis. However the graphics are not truly interactive. Hence, it is generally not easy to use them for design of the measurement system.

Visual modelling is one of the leading items on a “wish list” provided by Dr J Redgrove, the head of Thermophysical Properties work within the NMS Thermal programme. It is seen as an enabling technology to assist metrologists in modelling more difficult materials (composites, etc.).

The main concern is that visual modelling should be implemented in such a way as to exploit the mathematical strengths of the application packages. There was also concern about validating a visual model.

The SSfM competitively tendered contract for visual modelling and data visualisation was won by SIRA and they have decided to use a case study from the Thermal area. In conjunction with CISE (providing modelling support using finite elements) the heat flux through a guarded hot-plate design will be visualised. It is at present too early in the project to comment on the success or otherwise of the study.

Humidity data is generally univariate, hence simple graphs are adequate. However, the primary gravimetric hygrometer requires knowledge of flow rate, pressure, mass of moisture and mass of dry gas in addition to temperature. If these were varying, e.g., to test the apparatus, more sophisticated data visualisation would be desirable.

3.4 Data Fusion

Data fusion, in a conceptually simple form, is already used in the ITS-90 scale, which employs a composite discrete model, the individual models applying over finite regions of the temperature scale. Other forms of data fusion employed in thermal metrology include

1) processing and reconciling measurements from an array of sensors
2) fault and error detection/diagnosis by inter-comparison between measurements

Other forms of data fusion which might be considered at a later stage, particularly in the context of multi-property measurement, include

1) combining results from several very different measurement processes, because the target measurement was infeasible
2) dealing with predictive data from models, or historical or archive data, in tandem with current measurement data (e.g., by Kalman filtering)
3) handling numerical, image, and/or qualitative data within a single framework

Data fusion is one of the three themes in the INTErSECT Faraday partnership; Thermal programme staff are involved in the LUMITHERM Sensors Theme Flagship project. There are fewer links with the Data Fusion theme.

4. Validation and Testing

4.1 Spreadsheets and Other Mathematical Software Packages

The main off-the-shelf software packages used in Thermal metrology are:

1) HT-Basic (for instrument control and data acquisition); there is a heavy investment in legacy software; a Windows version is due;
2) LabVIEW, which is beginning to replace HT-Basic, particularly in Thermophysical Properties Section;
3) FEA packages such as Ansys;
4) Opticad and Zemax for ray tracing and optical modelling in the advanced measurement techniques area;
5) thermal modelling packages (often research/non-commercial code)
6) Excel and calculators for basic data processing, particularly in the calibration services area;
7) Fluent, for CFD modelling of high temperature gases and combustion;
8) Mathematica (limited);
9) NPLFIT (a package designed at NPL for calibration curve fitting in accordance with the GUM);
10) Sigmaplot (for measurement services data analysis);
11) Software from hygrometer manufacturers which relate dew-point to vapour pressure.
12) Matlab has recently been acquired. Matlab is being used to perform post-processing on data (such as for data fitting) and is also being used for some numerical modelling. An early application is a one-dimensional steady state heat problem. The ease of programming, matrix handling and graphical output from Matlab makes it particularly attractive.

In addition, there are several in-house FORTRAN and Pascal programs (generally for production software) for

1) FDM solution of the steady-state heat transfer problem;
2) blackbody cavity design;
3) Monte Carlo simulation for estimating the emissivity of cavities;
4) Estimating the coefficients in ITS-90, and for generating data in RTF format to go into WordPerfect calibration certificates (to be converted eventually to Word);

Home grown software is tested, since it needs to satisfy NPL's Quality System requirements for production software, by regression testing, etc. Records of past data are kept for this purpose.

Some testing of bought-in packages is carried out, though this is often difficult, owing to incomplete specification of their functionality.

Generally, the spreadsheets used are not particularly complicated, but they do rely on in-built functions such as standard deviations. In Humidity, determination of saturated vapour pressure requires a polynomial with a minimum of 4 terms, implemented in Excel. Graph plotting within spreadsheets also contribute to their use.

There is a high level of awareness of the limitations of the packages with regard to useful parameter ranges, etc.

There was no evidence that metrologists in this area *demand* assurances from software suppliers that their software is fit for purpose.

Software is clearly a key part of the measurement chain in the calibration services area, however in the more research-based activities, the link is more tenuous, with the consequences not being immediately obvious.

4.2 Model Validation

There is a very high awareness of model validation, and an acceptance that it is vital to the success of modelling in the Thermal metrology programme. In particular, it is an issue as new models and methods of modelling are considered. It is closely linked, in practical terms, to visual modelling. Validation of continuous models is a concern, particularly if there are few test cases.

As an example of model validation in practice, eddy currents can provide information on temperature profiles inside material artefacts. Numerical models can be validated against (semi)analytical techniques, symmetries tested, etc.

4.3 Measurement System Validation

Software is endemic in measurement systems used in Thermal metrology. Usually, measurement systems are validated as complete systems, e.g., by comparing the results of a measurement of a *known* (i.e., fully characterised) black body with what would be expected.

Thus, in a sense, reference data is used, but generally software is not formally tested with third-party reference data in that way. Consequently, Thermal metrologists tend to avoid instruments with embedded software for critical applications, e.g., the spectrum analyser.

There is a concern that instrument vendors may run “obvious” tests which are insufficiently rigorous to catch all the errors and hence such instruments must be viewed as unpredictable. Therefore, because of the difficulty and expense of doing such testing, Thermal metrologists do not always do much further testing. They are sceptical of the manufacturer’s claims and rely on validating with simple cases to give some confidence in the operation of the measurement system. Generic guidelines were not seen as a priority, since each instrument is subject to bespoke testing during commissioning, and further checks thereafter.

4.4 Validation of Simulated Instruments

Continuous modelling is often used to simulate the operation of an instrument or measurement technique. However, there is no evidence that this includes statistical modelling of the errors, and the ability to configure such models to simulate actual instruments, which is the case with the Virtual Co-ordinate Measuring Machine (CMM) concept.

5. Metrology Software Development Techniques

5.1 Software development methods

Software that has been developed by NPL within the Thermal programme was generally produced before the introduction of a formal quality system, but validated in practice over several years of operation. New software is developed according to NPL's quality system.

A structured V-model ("specify, design, code, test") development procedure is followed. The nature of testing depends on the application: data logging software is tested by inspection, certificate production by using standard data files, etc.

There are no smart instruments at present, but newer instruments have increasingly sophisticated software control (such as the new radiometer).

There is a lot of legacy software in place, some of it due for replacement, e.g., the thermocouple calibration data processing software, which is being rewritten and re-engineered for a PC.

The biggest software problem facing the Thermal programme is that of converting more than 70 programs to LabVIEW. The reasons for this conversion include

1) the old programs are becoming increasingly difficult to maintain;
2) new staff and students have experience in LabVIEW, hence new software is being developed in such languages/environments;
3) NPL's IT Services Unit (ITSU) favours LabVIEW/VB and will support those packages.

The argument could also be supported on cost grounds. Humidity has different legacy requirements, reflecting its separate history; software has been upgraded in line with the hardware: from Commodore Pet, to BBC micro, to Archimedes, to Windows NT (Visual Basic). The conversion would be performed by software engineers in CISE. It should also be noted that Humidity is affected by changes elsewhere, e.g., converting from the IPTS-68 to ITS-90 temperature scales necessitated change in humidity software.

Thermal staff have avoided mixed-language programming where possible.

The Thermal programme also uses home-grown IT systems such as an equipment database implemented in Access 2 and utilities such as a data logger which reads the system clock.

Generally, software errors could have a major impact on Thermal business, so the hazard probabilities are minimised by use of the review/test procedures mandated by the NPL quality system.

There was no explicit mention of NPL Guide No. 5, but it would appear that many of the software development practices are consistent with that document.

5.2 Software reuse

Generally, externally-supplied HT-Basic and LabVIEW instrument drivers are used where possible. There has been a move away from software on the NPL mainframe, e.g., the NAG library, as software is ported to PCs.

Subroutines are re-used as much as possible, e.g., for acquiring data from DVMs. Problems have arisen managing disk file directories.

Sometimes the software is drawn from non-traditional sources, e.g., from specialist magazines and user clubs. Such software is carefully tested before use, but is often very flexible in use.

Because of the limitations on mixed-language programming and the desire to update much of the software, software re-use is limited, and a programme of planned obsolescence of legacy software is under way.

The most common form of module reuse remains “copy and edit” of source code. Greater re-use of object code would be possible if there was a more formalised way of organising software libraries.

There is little concern about the Year 2000 problem, because the software is generally not critically dependent on dates. Some auxiliary software such as the data logger might require modification, and Access 2 is known not to be millennium-compliant.

5.3 Virtual Instruments

LabVIEW is increasingly used, particularly for instrument control, as might be expected. An example was given of the case of a lock-in amplifier, which has progressed from being analogue, to digital, to being offered as a 24-channel card to be inserted in a PC, under LabVIEW control.

However, instruments such as lock-in amplifiers present special difficulties for testing and it is not clear whether these are made any easier using the virtual instruments model.

Being relatively new to LabVIEW, Thermal staff were becoming aware of the issues and would welcome some guidance. It was unclear at this stage whether developing virtual instruments was more or less efficient than developing conventional software modules, e.g., there was concern that some efficiency would be lost, since HT-Basic was ideal for system control using the IEEE bus. Matlab is now being considered for data acquisition tasks.

A lack of continuity of LabVIEW support offered from an external contractor is noted as giving serious cause for concern. The lack of control over such contractors and their methodology for working is seen as an issue. It was felt that increased level of support internally at NPL would be welcome.

6. Support for Measurement and Calibration Processes

6.1 Automation of Measurement and Calibration Processes

At present, LIMS (Laboratory Information Management Systems) are not used in the Thermal calibration services are, though this is under review, especially with corporate NPL’s study of LIMS. At present, there are concerns about flexibility, in particular, how the system would handle exceptions. There is already some automation of the production of calibration certificates.

The perception is that existing LIMS systems are geared towards high-volume test work. The existing system is manual and based on documented procedures and forms. Needless to say, any system which improved efficiency would be welcome, but there were concerns about cost and training.

Although a manual forms-based system is in place to track measurement service work, the actual measurement is as automatic as possible, e.g., in Humidity, cameras can be used to record digital displays.

6.2 Format Standards for Measurement Data

Format standards were not identified as an issue. To some extent, the ITS-90 standard imposes standard processing on the data, which tends to make the data transferable. Other format standards are tied to the software packages which operate on the data.

Common calibration records (sharing process data, not just raw data) would be welcomed. This might also be linked to intercomparisons.

7. Suggestions for Future Activities

7.1 Expected Benefits of the SSfM Programme

The key benefits that the Thermal Programme might be expected to gain from the SSfM programme include

a) support for mathematical modelling and guidance on modelling and validation with seminars, particularly of continuous/hybrid models;

b) uncertainty estimation for continuous/hybrid models;

c) testing and acquisition of third-party packages, e.g., spreadsheets, unit conversion, Matlab and LabVIEW and FEA packages;

d) visual modelling.

7.2 Case Studies and Feasibility Studies

There is a possibility of a major case study, including aspects of modelling of measurement data, uncertainties and statistical modelling, visual modelling, model validation, validation of numerical software packages.

Laser Flash: Multi-property Measurements:

Heat is instantaneously applied (by laser flash) uniformly to one side of a plane specimen disc at time t=0. For time t>0 it is radiating in vacuum, and conducting, though a negligible amount since it is mounted on pin-tips. The change in surface temperature on one plane surface is monitored and from that and the absorbed laser energy the specimen's thermal diffusivity and specific heat capacity are derived. The present model is one-dimensional and adiabatic (no heat loss from the specimen) and corrections for heat conduction and radiation losses are estimated as part of the model. Some preliminary work has been carried out through the Bristol University Industrial Mathematics MSc and a two volume summary document presented which points the way forward in modelling the proposed new multi-property measurement standard.

The aim of the case study would be to reduce the present relative uncertainty of several percent by an order of magnitude. This would be achieved by improved

a) modelling: 2-dimensional (axisymmetric) geometry and including additional physical effects, as indicated by model validation;

b) design of the apparatus (supported by visual modelling to provide near real-time exploration of the available parameter space);

c) uncertainty modelling, taking better account of uncertainties in input quantities, such as laser power, dimensions, etc.

In addition, the apparatus would need to be applied to more exotic materials, e.g., those that are thermally anisotropic (have directional thermal properties), or are composite (typically, fibre reinforced), have thin film coverings or are fibrous. Such materials pose greater modelling challenges, e.g., fibrous materials have more complicated geometry and convection properties.

The instrument can be designed to be more flexible, such that it can be used for multi-property measurement. This has potential cost benefits, which need to be weighed against traditional approaches.

The modelling would form part of Thermophysical Properties Section's proposed enhancement of an apparatus that is used world-wide for thermal diffusivity measurement, so it would be worthwhile for both metrological and industrial applications. Other possible areas for case studies include:

1) *Validation of spreadsheets used in measurement services work*

Spreadsheets used in measurement services require validation and configuration control.

2) *Procurement of metrology software*

This would examine the technical and cost implications of combining "best of breed" software versus choosing a single acceptable package which is not optimal for all requirements.

3) Gustafasson Probe:

In these measurements an electric heater that also acts as a thermometer is embedded in the sample. Time versus temperature data is collected and this can be used to obtain thermo-physical properties. Primary interest is to devise a robust method for extracting the relevant parameters from the data and determine the range of useful data. However the Gustafsson probe also offers interesting continuous modelling problems in dealing with contact and possible non-uniform heating. This combination suggests this as a possible hybrid modelling case study.

4) Modelling of linear heat probes: these forms of probes are widely used in industry.

5) Laser Flash Technique: measurement standards for molten metals and liquids. In this application determining the on-set of convection in liquids would be a useful modelling case study.

6) In Fundamental Gas Thermometry, modelling of the heat distribution in different geometries would be useful as part of establishing an optimal design.

7) In addition, other NMS programmes have interests in the modelling of heat flow and dissipation, particularly in Ionising Radiation, where a project is under way to model heat flow from an irradiated graphite plate, such that thermistor measurements can be corrected for indirect heating by surrounding parts of the graphite block.

7.3 Future SSfM Topics

Thermophysical Properties activity uses advanced mathematical and software techniques, principally in design and modelling. Possible future SSfM topics include:

1) multi-objective design, e.g., multiple property measurement;
2) numerical performance of large numerical simulations, e.g., of laser-based gas thermometry and combustion;
3) numerical analysis of linear and non-linear heat flow equations in various geometries - for design purposes this is related to 1. Such heat flow problems occur across the NMS Programmes not only directly for measurements but also for controlled environments.

7.4 Future Thermal Programme Topics

The Thermal Programme has a number of projects (detailed above in 7.2) that will benefit from continuous, discrete and hybrid modelling, a few examples of which are illustrated as potential case studies. These could be progressed either in the Thermal Programme alone or perhaps more usefully in combined activity between the Thermal and SSfM Programmes.

8. Summary

Principal changes from the restricted initial status report on the Thermal Metrology area are as follows:

- the report reflects the change in structure now that humidity has joined the Thermal programme;
- recently Gordon Edwards has acquired Matlab and this is being used both for discrete and continuous modelling;
- the text now reflects that modelling has started on a guarded hot-plate design and this has been chosen as one of the data visualisation case studies by SIRA;
- the view that additional support for LabVIEW and Matlab would be welcome has been added;
- further possible case studies have been added.

Thermal metrology offers a number of possibilities for future activities, in particular in the forthcoming SSfM programme (2001-2004). Thermal metrologists are keen to increase the mathematical modelling in this area, in particular to gauge the effectiveness and optimise the design of future equipment (such as the flash laser apparatus) for determining thermal properties. A number of case studies have been proposed, each of which has aspects which may be generalised to other modelling situations: for example optimisation of design by finite elements, error estimation and control in the numerical solution of differential equations.

In addition, the Thermal metrology area offers a good area for future work since control over the thermal environment is often vital for other NMS programmes. Thus, the determination of heat flows can effect experiments where the thermal properties are not the main area of interest.

9. Acknowledgements

The author gratefully acknowledges the help provided by Bernard Butler, Robin Barker, Brian Chu, Gordon Edwards, Dave Rayner, John Redgrove, David Robinson, Richard Rusby and Mark Stevens in providing input to this report and reviewing drafts.

Appendix 1: Summary of modelling issues

In this appendix we give some further detail relating to the modelling techniques (Section 3) undertaken in the Thermal area. In the following tables, a score of 1 is used to imply that the statement to the left is true (nearly) all the time, whereas a score of 5 implies the statement on the right is true (nearly) all the time. It is recognised that for certain of the questions, there can be considerable variation in the way that a score is assigned. In these cases, the score is intended to indicate an "averaged" answer across the area.

Table 1. Complexity of models used in the Thermal programme

Simple	Score	Complicated
Simple relationship between input and output.	4	Pages of equations to describe the system.
Small number of parameters.	4	Large number of parameters, with complicated inter-relationships.
Measurement errors limited to one measured quantity.	4	Many variables subject to significant measurement error.
Measurement errors consistent with Gaussian distribution.	3	Non-Gaussian behaviour, outliers likely under a Gaussian assumption.
Input quantities well controlled, understood.	2	Inputs estimated, not all influence factors have been identified.

Table 2. Maturity of models used in the Thermal programme

Mature or Accepted	Score	Developing or Speculative
Well understood and accepted physical theory.	2	A number of competing models or model incomplete.
Comprehensive theory adequately taking into account all main features.	3	Approximations employed, terms omitted to simplify model. Some components modelled by empirical functions, e.g., polynomials, splines. Behaviour of some components not understood and/or ignored.

Table 3. Incorporation of uncertainties in the Thermal programme

Thorough treatment	Score	Simplistic treatment
Measurement uncertainty modelled for all input quantities.	3	Measurement uncertainty modelled for only one or two input quantities. Other quantities either assumed to be exact or uncertainty contributions are assigned arbitrarily.
Variances and correlation amongst input quantities fully taken into account.	3	Possible variances and correlation among input quantities ignored.

Table 4. Comprehensiveness of solution methods for models used in the Thermal programme

Comprehensive	Score	Approximate
Solution method solves the computational problem posed by the model.	3	Approximations are employed. Some terms simplified/linearised/ignored.
Solution method takes into account all the sources of measurement error, variances and correlation amongst the input quantities.	3	Easiest method of finding a solution employed. All data treated as exact, independent and uncorrelated.

Table 5. Effectiveness of models in the Thermal programme

Effective	Score	Ineffective
Solutions consistent with those predicted by theory, established by other methods.	2	Solutions at variance with other results.
Method always returns a solution.	3	Method produces unrealistic solutions, fails to provide a solution, crashes.
Rerunning the method on perturbed data/ input quantities/ produces a nearby solution.	3	Small changes in the input data/quantities produces large changes in the output.
Iterative method converges quickly.	4	Method can make slow progress, fail to converge.
Estimate of statistical uncertainties consistent with the expected measurement error, noise in the data.	3	Unrealistic uncertainties calculated.

Table 6. Adequacy of model validation in the Thermal programme

Good validation	Score	Poor validation
Fit of model to the measurement data consistent with the expected measurement error.	3	Residual errors much larger than expected, have a systematic pattern.
Results agree with other methods of calculation.	2	Results inconsistent with other methods of calculation.
Results agree in situations for which an analytic/reference solution exists.	2	Solutions at variance with other results.
Numerical results in accordance with predicted behaviour of the algorithm (rate of convergence).	4	Behaviour at variance with prediction.

Appendix 2: Glossary of Abbreviations

Abbreviation	Expansion
A/D	Analogue to Digital conversion (of a signal)
ASCII	American Standard Code for Information Interchange
CBTM	Centre for Basic and Thermal Metrology
CFD	Computational Fluid Dynamics
CISE	Centre for Information Systems Engineering
DLL	Dynamically-Linked Library
DVM	Digital Volt Meter
EC	European Commission
FEA	Finite Element Analysis
FDM	Finite Difference Method
FFT	Fast Fourier Transform
GUI	Graphical User Interface
GUM	Guide to the expression of Uncertainty in Measurement [1]
INTErSECT	Intelligent Sensors and Control Technology (Faraday partnership)
IPTS-68	International Practical Temperature Scale, 1968
ISO	International Organization for Standardization
ITS-90	International Temperature Scale, 1990
LIMS	Laboratory Information Management System
NAG	Numerical Algorithms Group
NMS	National Measurement System
NMSPU	National Measurement System Policy Unit
OLE	Object Linking and Embedding
PC	Personal Computer
QMS	Quality Management System
RTF	Rich Text format
SSfM	Software Support for Metrology
UKAS	United Kingdom Accreditation Service
VB	Microsoft Visual Basic
Y2K	Year 2000 (millennium bug)

Appendix 3: Bibliography

1. *Guide to the Expression of Uncertainty in Measurement*, International Organisation for Standardisation, 1993, ISBN 92-67-10188-9.
2. *M3003: The Expression of Uncertainty and Confidence in Measurement*, United Kingdom Accreditation Service, 1997.
3. M Stevens and S A Bell. *The NPL standard humidity generator: an analysis of uncertainty by validation of individual component performance*. Meas. Sci. Technol. **3** (1992), pp 943-952.
4. *Modelling Survey*. Newsletter of the Food Refrigeration and Process Engineering Research Centre, University of Bristol. **15** (Sept 1996), p6.
5. M Raynaud. *Inverse modelling in thermal measurements*. TPAC News, Issue 6, Autumn 1997, pp14-16.
6. S Bell. *Validation of the NPL Primary Gravimetric Hygrometer.* (CD-ROM) Proceedings of the Third International Symposium on Humidity and Moisture, NPL, 6-8 April 1998.
7. ISO 9001: Quality systems - Model for quality assurance in design, development, production, installation and servicing, 1994, Geneva, Switzerland.
8. Rayner, D., *Initial Report on Status of Software and Mathematics in each Metrology Area*, NPL Report CISE 18/99, February 1999.

Document History

Issue	Date	Author	Description of change	Approved
0.1	29/06/98	G Lord	First Draft	
0.2	20/07/98	G Lord	Edited after comments from John Redgrove and Gordon Edwards	
0.3	4/08/99	D Rayner	Changes resulting from thorough review for consistency of style throughout the document, with companion status reports and with the current position within the SSfM programme. Yellow highlights are used to indicate things that the author should check.	
0.4	3/09/99	G Lord	Changes made from reviews by John Redgrove, Gordon Edwards and Dave Rayner	
0.5	3/09/99	G Lord	Revisions fully incorporated into the text	
1.0	30/09/99	D Rayner	Delivered version, approved by D Robinson	DR

Theme name:	Status Reports for Thermal Metrology Field
Path and filename:	f:\ssfm\5-status\interim\thermal\thermal-deliver.doc

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