

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

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

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Software Support for Metrology

Interim Status Report on the Mass Area

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Abstract

This report describes the status of the mathematics and software used to support the Mass area of metrology, particularly as used within the NMS Mass 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 Mass programme projects applying SSfM outputs to specific problems in the Mass area.

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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 **Mass** area, concentrating on what is used within the NMS **Mass Metrology 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 Mass Metrology 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 in contrast has relatively little direct impact upon industry, although there is some 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.

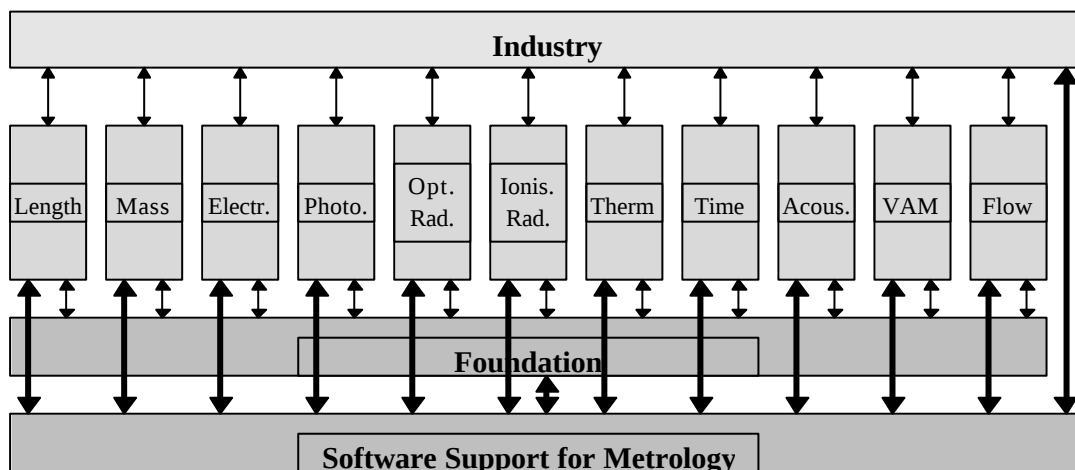


Figure 1. Relationship of SSfM to other NMS programmes and industry

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 Mass 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 November 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 [7]. A summary of the differences from the initial Mass status report is provided at the end of this report.

2. Scope of the Area Covered

The central aim of the Mass programme is to provide a minimum national measurement infrastructure for mass and related mechanical quantities in support of trade, quality assurance in

industry, innovation and a range of important social activities. The first requirement for this is provision of a UK standard for the unit of mass, the kilogram, which is a base unit of the International System (SI) of Units.

The metrology of mass and derived mechanical quantities is a broad and challenging field which extends from routine, but essential, measurement of small masses with balances to a spectrum of innovative activity involving basic science and advanced engineering. It calls for an understanding of surface adsorption on primary mass standards, of molecular dynamics at very low pressures in vacuum standards where gases no longer behave as fluids, and of properties of materials to be used in force transfer standards for heavy engineering applications up to 30 MN (3000 tonnes weight) and in pressure balances used for standardising extreme pressures. Mechanical standards also provide essential support to the standardisation of other quantities including some of those found in dimensional, electrical, thermal, acoustical, optical and ionising radiation metrology.

The programme includes three technical themes that are outlined below.

Standards for mass and density

This theme underpins the whole programme in that it provides the UK's primary standard of mass, copy No 18 of the International Prototype Kilogram in terms of which the SI unit is defined internationally. Provision is made for occasional intercomparisons with the International Prototype held at the BIPM at Sevres near Paris and for realising a consistent mass scale from 0.5 mg to 2.7 tonnes. In support of this fundamental work, special attention is given to the correction for air buoyancy in weighing for which a capability in density measurement also needs to be maintained, to surface contamination of weights and the use of weights in vacuum.

Standards for force, torque, hardness and extensometry

The customer base for force calibrations and consultancy is one of the largest with numerous UKAS laboratories and over 300 companies drawn from the mechanical and civil engineering, aerospace, defence, nuclear power, iron and steel, shipping, off-shore and motor vehicle industries. The core of the theme is the provision and maintenance of a suite of dead-weight and hydraulic force machines used to calibrate force transfer standards. The theme also addresses the need for traceable measurement of dynamical forces based on static force calibrations, for the calibration of extensometers used for tensile testing of materials and for the measurement of torque. In addition, the theme aims to re-establish hardness standards in the UK on which there is wide industrial dependence.

Pressure and vacuum standards

Pressure measurement standards are provided in support of UKAS laboratories and a wide range of industries, including the instrumentation, aerospace, defence, nuclear, power, gas, petrochemical, biological, pharmaceutical, meteorological, environmental, semi-conductor, optical, ventilation, filtration and process industries in general. The standards provided cover absolute, gauge or differential pressures over nearly 15 orders of magnitude, from high vacua at approximately 10^{-6} Pa to ultra-high pressures at approximately 10^{+9} Pa.

3. Modelling Techniques

3.1 Methods for Modelling Measurement Data

3.1.1 Types of data

There are three categories of measurement data sets:

1. discrete measurement data, which means:
 - a) data obtained by sampling a discrete variable: e.g., a variable that may take only integer values such as in counting processes, and
 - b) data obtained by sampling a continuous variable.
2. continuous measurement signal, which means an analogue signal prior to any analogue to digital conversion, which would result in data of type 1 b).
3. hybrid measurement data composed of both discrete and continuous data sets.

Most quantitative data in the Mass area relates to essentially continuous variables. Examples include air temperature, pressure and humidity. However, such data is often collected and recorded as discrete data by digital sampling, so that the measurement data that is subsequently processed consists of sets of discrete values.

It is noted that pressure presents some particular problems. Pressures cannot be added, subtracted, multiplied or divided in the way that lengths and masses can. Consequently, it is necessary to independently realise pressure over its entire range which amounts to of the order of fifteen decades. This contrasts with length and mass for which it is possible to start with a well defined reference standard and generate multiples and sub-multiples.

3.1.2 Modelling

Types of model

There are three categories of model:

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

It is appropriate to distinguish 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).

Given infinite precision arithmetic, the set of equations derived from a discrete model can 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.

Models used in the Mass Programme

Both *empirical* and *physical* models are used to describe the measurement systems and data arising in the Mass area. Furthermore, there is considerable variation in the complexity of these models. For example:

- The swing of the beam of the NPL primary mass balance is described using a combination of a physical model representing the damped oscillation of the beam about its rest-point, and a polynomial function that models (empirically) drift of the rest-point position.
- A single weighing appearing in a weighing scheme for calibrating a collection of masses uses a linear model to relate the corrections for the masses involved in the weighing to the recorded balance reading [1]. This is a physical model.
- The pressure generated by a pressure balance [2] is expressed in terms of

- (a) applied forces from various sources, including the applied load, the mass of the piston of the balance, applied and calculated trim weights, and corrections accounting for surface tension and the fluid head, and
- (b) the effective area of the piston-cylinder assembly depending on temperature and pressure.

When expressed in terms of “basic” uncorrelated quantities, the resulting model is considerably complex.

- In the calibration of force-measuring instruments for verifying the force indication of testing machines [3], the relationship between the applied force and the deflection of an elastic force-measuring instrument is expressed in terms of a polynomial function. This is an empirical model.

Discrete modelling is undertaken and includes:

- the calculation of summary sample statistics (sample mean and standard deviation) in the analysis of measurement repeatability, and
- regression in which a (continuous) function is fitted to discrete data in a least-squares sense through the solution of a system of algebraic equations.

Linear regression, as in the fitting of linear, polynomial and spline models to data with error in the response variable only, is widely used. There is awareness in the Mass area that there exists a number of numerical schemes for solving these regression problems, but general guidance concerning the choice of an appropriate scheme is lacking.

In both the Mass and Density, and Pressure and Vacuum, areas there is on-going debate with other National Measurement Institutes (NMIs) concerning the precise form of some of the modelling undertaken.

In Mass and Density, there are differences in the way that *a priori* information about calibration standards is incorporated into the analysis of data from weighing schemes, and the way this information affects uncertainty estimation (Section 3.2). However, because the differences in the results obtained from the various approaches are not significant, this is not regarded as presenting a problem, but instead serves to provide some form of validation of the methods used (Section 4.2).

In Pressure and Vacuum, there are fundamental differences in the approaches taken by NMIs to processing the data arising from the calibration of pressure balances using the cross-floating method. Work has been undertaken to understand the consequences of these differences, and to show the greater robustness of the NPL approach. Recently, new approaches have been investigated that attempt to account properly for the errors in the measured quantities, and to feed this information into the estimation of uncertainties (Section 3.2). However, these approaches lead to difficult optimisation problems, and the requirement for considerable quantities of numerical software. It is anticipated that detailed validation of the methods will be required before these approaches are generally accepted (Section 4.2).

In Force, the models used and the calculations undertaken tend to be simple, and so problems associated with modelling measurement data and uncertainty estimation (Section 3.2) generally do not arise.

Continuous modelling is also undertaken in which finite difference and finite element techniques are applied to the solution of systems of differential equations. This is undertaken in

- the Pressure and Vacuum area to understand the deformation of the piston-cylinder assembly of a pressure balance when under pressure, and

- in the Force area in the optimal design of load cells.

Some further detail relating to the modelling techniques undertaken in the Mass area are provided in Appendix 3.

3.2 Uncertainties and Statistical Modelling

The estimation of measurement uncertainties in the Mass area follows the principles of the ISO Guide to the Expression of Uncertainty in Measurement [4] and UKAS document M3003 [5]. Nevertheless, some deficiencies in these documents have been identified, and include:

- dealing correctly with numbers of degrees of freedom,
- calibration problems where there are errors in more than one variable, and
- applying the approach described in these documents in cases where the measurement system model is complex. For example, where it is not possible to express the output(s) of the measurement system as an explicit function of its inputs.

In Pressure and Vacuum, the calculation of an uncertainty for the estimate of the distortion coefficient for a pressure balance in the high pressure range is seen to lack robustness. There may be scope here for work to build an uncertainty budget around the finite element analysis used to model the deformation of the piston-cylinder assembly for such balances (Section 3.1).

Finally, there is seen to be a general lack of guidance concerning the statistical analysis of data arising from interlaboratory comparisons.

3.3 Visual Modelling and Data Visualisation

Visual modelling and data visualisation are generally not used in the Mass area, although in Pressure and Vacuum the visualisation of measurement data is used to inform the operator undertaking a range of measurement operations. There is potential for applying both visual modelling and data visualisation to the problem of understanding the deformation of the piston-cylinder assembly of a high pressure balance (Section 3.1).

3.4 Data Fusion

Data fusion is generally not used in the Mass area. The following possible applications have been identified:

- In Mass and Density, to remove any “mismatch” between the measurement data arising from the use of different mass balances.
- In Pressure and Vacuum, in the maintenance of the high pressure scale. The scale is established using data from a wide variety of sources, including calibration of gas operated pressure balances against a mercury barometer, piston-cylinder dimensioning, and, at the opposite end of the pressure scale, finite element analysis to determine distortion. There is also considerable extrapolation using non-linear devices in between. There is a requirement to develop a mathematical framework for the high pressure scale into which experimental and theoretical data from these various sources could be inserted, and of being able to investigate the affect on its associated uncertainties of changing the relative accuracies of the information provided.

4. Validation and Testing

4.1 *Spreadsheets and Other Mathematical Software Packages*

Commercial spreadsheets, such as Excel, as well as other mathematical software packages, including Matlab and Visual Basic, are used throughout the Mass area for processing, and presentation of, measurement data.

The processing undertaken includes:

- the use of basic arithmetic operations, as in the calculation of uncertainty budgets,
- the calculation of basic summary statistics (including mean and standard deviation), and
- solving linear and polynomial regression problems.

Where the spreadsheet application developed produces results as part of a calibration service or for the purposes of research, the application is registered within NPL's Quality System, and software quality procedures are followed in the development. Pre-processing of raw measurement data, including scaling and normalisation of the data, is sometimes used prior to the application of in-built spreadsheet functions for regression, and this helps to ensure the integrity of the results returned by these functions.

It is not common for a user of a commercial package to seek assurances from software suppliers that mathematical functions included in the package employ algorithms that are valid, accurate and stable over the likely range of values of the user's input data. It tends to be assumed that the developer of the commercial package will ensure that this is so.

4.2 *Model Validation*

Where possible, the models used in the Mass area are validated. This is done, for example, by comparing quantities predicted by a computed model with results that can be measured independently or calculated from theoretical considerations. Where physical models are used, these are underpinned by theoretical analysis, and are generally accepted on this basis. In addition, validation of empirical models by applying statistical tests to the computed models taken from within a *family* of functions is sometimes undertaken: for example, in the Force area, the ASTM standard [3] presents a procedure for determining the degree of the best fitting polynomial to measured deflection-force data.

4.3 *Measurement System Validation*

In Mass and Density, the software embedded in instruments such as mass balances is generally simple, and consequently extensive validation is not required. Where there is the need to extend the functionality of the software controlling these instruments, this is undertaken "in-house", and separate from the instrument, and can be validated in isolation from the instrument.

In Pressure and Vacuum, some problems with the software embedded in instruments are known about. For example:

- for a particular vacuum gauge, the software embedded in the gauge introduces a "kink" into the measured characteristic, and
- some instruments include procedures for calibration where the calibration points are fixed by the manufacturer, even though there is evidence for non-linear behaviour between these points. (In this case, the calibration of the instrument is driven by the manufacturer's procedure rather than good metrology.)

In Force, the software embedded within instruments is limited. However, hardness machines used in the area include software developed by a TickIT approved supplier for obtaining dimensional information from images. Here, testing of the software on its own is undertaken as well as testing of the instrument as a whole.

5. Metrology Software Development Techniques

5.1 Software development methods

Software development within the Mass area is undertaken according to NPL's software quality procedures. NPL is certified to ISO 9000 plus TickIT. However, a number of different approaches to software development are used within the Mass area. These are described below.

5.1.1 Mass and Density

In Mass and Density, software is developed using a variety of software packages including Excel, Visual-Basic, Quick-Basic, Pascal, FORTRAN and Matlab. Software is developed both for

- instrument control, and
- data processing.

Software development is undertaken "in-house" as well as with the assistance of software engineers and numerical analysts from NPL's Centre for Information Systems Engineering (CISE). The role here of CISE has predominantly been concerned with the conversion of existing software to run within a PC environment. There is concern expressed that extant software is difficult and costly to update within the confines of the Quality System (Section 5.2).

5.1.2 Pressure and Vacuum

In Pressure and Vacuum, a great deal of software has been developed "in-house" as part of the test and measurement work undertaken in this area. The software is predominantly written in HP-Basic, and links with certificate generation software (written in WordPerfect for DOS) that resides on a dedicated PC. The software is

- well-established,
- generates repeatable results (and in a precisely repeatable document format), and
- flexible: for example, certificates are built from component parts in order to meet the general requirements of customers (Section 5.2).

There is again concern that it is difficult to upgrade, in a cost effective manner, the software (for example, to include a more sophisticated data analysis capability) and satisfy the requirements of the Quality System. Work has begun concerned with converting this HP-Basic software to Visual-Basic, which will help to resolve some of these legacy software problems (Section 5.2). However, the decision to move to Visual-Basic (instead of, for example, LabVIEW) is regarded as a difficult one, and there is seen to be a shortage of good advice to support such decisions.

5.1.3 Force

The instruments and machines used in the Force area are generally operated manually, and the requirement for instrument control software is therefore limited. However, software has been implemented as part of the DC ratio meter calibration service and to assist with the testing of strain gauges, and it is planned to develop software for the computer control of force machines. Software development, where it is necessary, is undertaken "in-house", usually using Visual Basic, to ensure the software is

- reliable,
- controlled.

The experience reported in this area is that software bought-in from other sources is invariably unreliable and/or not delivered to schedule. Where this has applied to software delivered by CISE, measures are now in place to rectify the problems.

5.2 Software reuse

As described in Section 5.1, software re-use is seen as an important means of reducing software maintenance costs. In some instances, software *re-use* takes the form of software *re-engineering* where existing software is modified for use in a similar context or to solve a similar problem.

There is generally a trend to migrate applications to modern systems, both hardware and software. As noted in Section 5.1, some legacy software suffers from hardware incompatibilities and will not operate on modern systems. In these cases, it can be difficult to re-use or re-engineer software, and consequently there can be significant overheads and costs involved in upgrading these systems, particularly within the context of Quality Systems. Mixed language programming is generally not used in the Mass area.

The Year 2000 (Y2K) problem has been recognised for some time. NPL has a task group working on this issue and is responsible for testing every piece of appropriate equipment for Y2K compliance. It has been concluded that the Y2K problem will have no impact on the delivery of NMS milestones within the Mass area.

5.3 Virtual Instruments

Virtual instruments and LabVIEW are generally not used in the Mass area.

6. Support for Measurement and Calibration Processes

6.1 Automation of Measurement and Calibration Processes

The extent to which measurement and calibration processes are automated within the Mass area is varied. The various approaches are described below.

In Mass and Density, a paper-based system with manual transfer of data between systems is currently used. This is recognised as being time-consuming and expensive to operate, but the costs associated with installing a Laboratory Information Management System (LIMS) and configuring the system to the particular calibration services offered are regarded as considerable. Nevertheless, it is anticipated that more efficient electronic data gathering and transfer between the various software packages and systems used will form an important part of the activity in this area in the future.

In Force, there is very little software used in the calibration services offered and, in this sense, this area of the programme lags well behind the others. At present, much of the process from data measurement to calibration certificate involves the manual completion of forms. Work is currently underway to introduce a LIMS to help with data management aspects and eliminate much of this paperwork. However, it is anticipated that there will be deficiencies in the system: for example, the inability to automatically prompt customers for calibrations, and to manage scheduling. In the interim, a system called SCIRT (Small Contracts Information Recording Tool), based on an Excel spreadsheet, has been implemented and is used for booking-in and scheduling

test work. Guidance (provided by someone experienced in the provision of comparable services in other metrological areas) is seen to be paramount.

6.2 Format Standards for Measurement Data

There is generally little requirement within the Mass area for format standards for measurement data. Where there is a requirement for transmitting or sharing measurement data and results with other organisations, the data is usually stored in the form of ASCII files or as spreadsheet files. Hard copy certificates are regarded as providing definitive calibration information in the Mass area.

7. Suggestions for Future Activities

7.1 Expected Benefits of the SSfM Programme

Benefits for the Mass area arising from the SSfM programme are looked for in the following areas:

- Modelling: for example, the development of robust and reliable estimators for analysing measurement data.

The example of a pressure balance, and the comparison of methods for calibrating pressure balances, has been used as the basis of a case study within the SSfM Modelling project. This work led to the presentation of a paper [6] at the 3^d CCM International Conference on Pressure Metrology from Ultra-High Vacuum to Very High Pressures.

- Uncertainty estimation: particularly covering correlation, and the analysis of data from interlaboratory comparisons.

The pressure balance, as an example of a measurement system described by a model that is not directly dealt with by the documents [4, 5], has been used within the SSfM Uncertainties and Statistical Modelling project.

A new milestone in the SSfM Uncertainties and Statistical Modelling project concerned with uncertainty aspects of interlaboratory comparisons will satisfy part of the requirement identified here.

- Data fusion: for example, in the analysis of data coming from a variety of instruments.
- Support to software development by way of guidance and tools to help the development process.

The Mass area, specifically the Mass and Density theme, is providing a case study for the SSfM Guidance on Developing Software for Metrology project.

- Support to system development for the automation of measurement and calibration processes, particularly with regard to the integration of different software systems.

7.2 Case Studies and Feasibility Studies

Possible case studies and feasibility studies in the following areas have been identified:

- The application of robust methods for the statistical analysis of measurement data including that obtained from interlaboratory comparisons.
- The application of data fusion techniques to the maintenance of a unified high pressure scale.

- The application of the guide on developing software for metrology in the Mass and Density area.
- The application of LIMS technology to the calibration services provided in the Force area.

7.3 Future SSfM Topics

There is scope for further work in the next SSfM programme on modelling techniques (discrete and continuous), uncertainty estimation, data fusion, and support to software development.

7.4 Future Mass Programme Topics

There are a number of SSfM topics that are expected to benefit the Mass programme: these are detailed in Sections 7.1, 7.2 and 7.3. The topics could be progressed either in the Mass programme, in the current or future SSfM programmes, or perhaps more usefully as combined activity between the Mass and SSfM Programmes.

8. Summary of Changes

The principal changes from the initial restricted status report on the Mass area are as follows:

- the description, under the Data Fusion project, of the maintenance of the high pressure scale in Pressure and Vacuum updated,
- the application of visual modelling and/or data visualisation to understand piston-cylinder deformation in pressure balances removed as a case study for the current SSfM programme,
- the application of the guide on developing software for metrology in the Mass and Density area added as a case study for the current SSfM programme, and
- the addition of future SSfM and Mass programme topics.

9. Acknowledgements

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Appendix 1: Glossary of Abbreviations

Abbreviation	Expansion
ASCII	American Standard Character for Information Interchange
ASTM	American Society for testing and Materials
BIPM	Bureau International des Poids et Mesures
ISO	International Organization for Standardization
LIMS	Laboratory Information Management System
NAG	Numerical Algorithms Group (Ltd.)
NMI	National Measurement Institute
NMS	National Measurement System
NPL	National Physical Laboratory
PC	Personal Computer
SI	International System (of units)
SSfM	Software Support for Metrology
UKAS	United Kingdom Accreditation Service
Y2K	Year 2000

Appendix 2: Bibliography

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6. A.B. Forbes and P.M. Harris. Estimation algorithms in the calculation of effective area of pressure balances. Presented at the 3rd CCM International Conference on Pressure Metrology from Ultra-High Vacuum to Very High Pressures, Turin, Italy, 1999. Submitted to *Metrologia*.
7. Rayner, D., *Initial Report on the Status of Software and Mathematics in each Metrology Area*, NPL Report CISE 18/99, February 1999.

Appendix 3: Modelling Techniques

In this appendix we give some further detail relating to the modelling techniques (Section 3) undertaken in the Mass 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.

1. Are the models used in the given area of metrology typically **simple or complicated**?

Simple	Score	Complicated
Simple relationship between input and output.	3	Pages of equations to describe the system.
Small number of parameters.	3	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.	2	Non-Gaussian behaviour, outliers likely.
Input quantities well controlled, understood.	2	Inputs estimated, not all influence factors have been identified.

2. Are the models used in the given area of metrology typically **accepted or speculative**?

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

3. Are **uncertainties** in the input quantities typically **incorporated adequately**? (This question really relates to Section 3.2 but is included here for completeness.)

	Score	
All main sources of measurement uncertainty modelled.	4	Only some measurement errors modelled. Other quantities taken as exact.
Variances and correlation amongst inputs taken into account.	3	

4. Are the methods of model solution typically **approximate or comprehensive**?

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 the sources of measurement error, variances and correlation amongst the input quantities.	4	Easiest method of finding a solution employed. Data weighted inappropriately.

5. Do the methods of model solution used in the given area of metrology **perform as expected**?

Expected	Score	Exceptional
Solutions consistent with those predicted by theory, established by other methods.	2	Solutions at variance with other results.
Method always returns a solution.	2	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.	2	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.

6. Are there **adequate ways to validate the model**? (This question really relates to Section 4.2 but is included here for completeness.)

Good validation	Score	Poorly validation
Fit of model to the measurement data consistent with the expected measurement error.	2	Residual error much larger than expected, have a systematic pattern.
Results agree with other methods of calculation.	2	
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).	2	Behaviour at variance with prediction.

Document History

Issue	Date	Author	Description of change	Approved
0.1	16/06/99	PMH	Document created.	
0.1	23/06/99	PMH	Last amended. To Dr, MG for review.	
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