

Report from the Mise en Pratique Task Group: the next international temperature scale and the mise en pratique for the definition of the kelvin

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1. Review of the terms of reference

The terms of reference for Working Group 1 of the Consultative Committee for Thermometry¹ (CCT WG1), as established at the 23rd meeting of the CCT, state in part [1]:

Working Group 1 is tasked ... to coordinate a task group (including a representative from Working Groups 3, 4, and 5) formulating an assessment and possible work plan for the next International Temperature Scale and to prepare and maintain the mise en pratique for the definition of the kelvin.

In response to this charge, the Mise-en-Pratique Task Group has produced the present document.

We begin in Section 2 by reviewing the status of the mise en pratique for the definition of the kelvin (MePK), including a discussion of possible extensions of the MePK. Over the next few years, we anticipate adding sections on supplementary information for the Provisional Low Temperature Scale of 2000 (PLTS-2000), low-temperature gas thermometry, absolute radiation thermometry, and the known differences between thermodynamic temperature T and temperature on the International Temperature Scale of 1990 (ITS-90), T_{90} .

In Section 3, we then consider the relationship of the MePK with both the International Temperature Scales and the thermodynamic temperature scale. By acknowledging that the International Temperature Scales are approximations to true realizations of the kelvin, the MePK indirectly encourages the greater dissemination of primary realizations of the kelvin or approximations to such realizations. We anticipate a period of time during which temperatures are disseminated on the thermodynamic temperature scale as well as the ITS-90 and the PLTS-2000.

Section 4 discusses the prospects for a new international temperature scale. A new scale should not be implemented until all technical issues are fully addressed, a new scale is proposed, and the proposed scale is fully tested. Many of the most pressing technical issues related to improved thermometry may be addressed directly in the MePK, rather than through an update of the ITS-90 or PLTS-2000. Section 4 also presents research opportunities that support a possible next temperature scale or expanded MePK.

Finally, in Section 5 we raise issues requiring CCT guidance.

¹ Working Group (WG) titles and numbers used in this document are: WG1: defining fixed points and interpolating instruments; WG2: secondary reference points and techniques for approximating the ITS-90; WG3: uncertainties; WG4: thermodynamic temperature, WG5: radiation thermometry; WG7: key comparisons; and WG8: calibration and measurement capabilities.

2. Overview of implementation of the mise en pratique

In 2006, the first version of the MePK was posted on the website of the Bureau International des Poids et Mesures (BIPM) [2]. Included are the brief text of the MePK itself and links to the ITS-90, the PLTS-2000, and the Technical Annex for the ITS-90, as well as supplementary information for the ITS-90 and approximations to the ITS-90.

2.1 Technical Annex for the ITS-90

The Technical Annex gives clear guidance on the isotopic abundances specified for both hydrogen and water fixed points on the ITS-90. In the paragraphs below, we assess the implementation of the Technical Annex in the three years following its approval.

2.1.1 Summary of recent activity on the TPW realization

In October of 2005, the International Committee for Weights and Measures (CIPM) approved a recommendation from the CCT to clarify the definition of the triple point of water (TPW) by specifying the isotopic composition of the water to be that of V-SMOW [3]. Accompanying the clarification, the CCT also approved, for inclusion in the MePK, an algorithm for correcting for departures of isotopic composition from V-SMOW. These changes were prompted by a study demonstrating the possible magnitudes of isotopic effects [4], and of larger than expected variations observed in the CCT-K7 TPW comparison, of about 170 μK p-p [5]. The results from a small group of laboratories that made isotope corrections showed that some of the variations in CCT-K7 were clearly attributable to variations in isotopic composition. However, a second and equally significant factor was the age of some cells and contamination of the water due to slow dissolution of the glass with time [6, 7].

In the three years following the CIPM recommendation, most national metrology institutes (NMIs) have been renewing their TPW cell ensembles to include cells of known isotopic composition, and in many cases, including cells manufactured from fused-silica glass rather than borosilicate glass. These changes prompted an unusually large number of papers (15) on triple point of water presented to the TEMPMEKO 2007 conference. These included papers from the major TPW-cell manufacturers demonstrating the improved reproducibility arising from the control of isotopic composition and the reduction in drift rates with the use of fused-silica glass [8-10]. Several NMIs presented papers that showed the improvements in their ensembles with the use of cells of known isotopic composition and related their latest measurements to their results in CCT-K7 [e.g., 11-13]. Some of these changes exceeded 100 μK and all generally correlated well with the differences observed in CCT-K7. All of the papers demonstrated a reduction in uncertainty in the realization of the TPW accompanying the clarification of the isotopic composition. Perhaps the best of the results was from NMIA [11], who demonstrated that the TPW can now be realized with expanded uncertainties (95 % confidence) of about 30 μK . They also compared a set of five new cells from three different manufacturers and found differences typically less than $\pm 20 \mu\text{K}$ (standard deviation = 6 μK). We conclude that the isotopic clarification accompanied by improvements in cell manufacture have led to a factor of four improvement in the reproducibility of the triple point of water.

2.1.2 Summary of recent activity on hydrogen fixed points

Isotopic variability of hydrogen can cause significant shifts in the triple-point and vapor-pressure temperatures of equilibrium hydrogen [14]. The CIPM approved in 2005 a recommendation from the CCT to specify the isotopic composition of hydrogen, and appropriate correction equations, for the ITS-90 defined hydrogen fixed points [3]. Less research has been published subsequently for hydrogen isotopic corrections than for the triple point of water. Several

laboratories have published descriptions of the isotopic corrections for their cells [15,16], but the number of published results is too small to conclude whether the isotopic correction has improved the reproducibility of the hydrogen fixed points. Definitive conclusions require a new intercomparison of fixed-point realizations, but such an activity is not planned for the next few years.

2.1.3 Recommended extensions for the Technical Annex

No changes are recommended for the Technical Annex at this time. Isotopic corrections for neon are desirable, but recent research results are somewhat puzzling [17, 18, 19]. In addition to problems with isotopic analysis, isotopic segregation during a melt, and chemical impurities, the melting plateaus in neon cells apparently are affected by the method used to form the solid phase, leading to difficulty in interpreting differences between cells [20]. Further investigation is needed before the neon isotopic correction factors can be determined with certainty.

2.2 Recommended extensions for the mise en pratique

Bearing in mind that the MePK should describe the definition of the kelvin (not just the water triple point or the ITS-90), the MePK should be reorganized as we insert additional material. The natural hierarchy is for material to be presented relating to T first. After a brief outline of thermodynamic methods, the first priority would be to list the best estimates of values of thermodynamic temperature for notable points up and down the scale, with uncertainties. (This is our equivalent to the list of laser frequencies in the MeP for the meter.)

The BIPM has published supplementary information for the PLTS-2000 [21] but a link to this material is not yet incorporated into the MePK. An appropriate link should be added as soon as possible.

We anticipate that the next version of the MePK will include new sections on primary and interpolating thermometry at low temperatures. A subsection on low-temperature gas thermometry (in particular, interpolating gas thermometry) needs to be completed prior to initiation of the next round of CCT key comparisons at low temperature.

CCT WG5 will prepare a new section on primary radiation thermometry, discussing both primary thermometry by absolute radiometry, and approximations to primary thermometry by use of high-temperature eutectic fixed points in conjunction with appropriate interpolation equations. For this section particularly, the appropriate level of technical detail for the MePK is not established (see section 5.1). Guidance from the CCT on this point would assist WG5 in its task. The MePK should contain the recommended eutectic fixed points, the thermodynamic temperature of these points, and the related uncertainty. The temperatures of the eutectic fixed points could be given in the “Approximating the ITS-90” document maintained by CCT WG2, although it would be important to categorize these points as secondary fixed points with no defined status on the ITS-90.

CCT WG4 has analyzed published literature on the difference $T - T_{90}$ and its associated uncertainty and has determined recommended values for these quantities. Subject to the approval of these values by the CCT, the MePK should include functional forms of $T - T_{90}$ and associated uncertainty $u(T - T_{90})$, and tabulated recommendations for the thermodynamic temperatures of the scale-defined fixed points.

CCT WG8 has already addressed the issue of primary temperature realizations in its harmonized list of service categories. Refinement of this list may be necessary as the scope of primary thermometry broadens.

2.3 Recommendations for international comparisons

Future temperature comparisons should identify the temperature scale (thermodynamic, PLTS-2000, or ITS-90) to be used. CCT WG7 and the BIPM should also consider the proper presentation of this material in the BIPM database.

In section 4.3 we discuss the increasing use of primary thermometry or approximations to primary thermometry for the dissemination of the kelvin. We recommend that WG1, WG4, and WG8 give guidance to the CCT on appropriate comparisons to validate the equivalence of primary realizations of the kelvin.

Comparisons and associated research are ongoing, as outlined in the WG5 “next steps” document [22], in the development of high-temperature eutectics and assignment of thermodynamic temperatures to the transition temperatures.

Recently, a new ^3He vapor pressure relation has been proposed that would give an improved approximation to thermodynamic temperature in the range 0.65 K to 3.2 K [23]. An international comparison over this range would provide confidence in the reproducibility of this method.

3. Relation of the ITS-XX and the MePK

3.1 Overview

The workshop “Towards the ITS-XX”, held in 2000 in Chicago [24], identified several weaknesses in the ITS-90 and anticipated a future temperature scale, labeled the ITS-XX. Perhaps the greatest weakness of the ITS-90 is its reliance on the calibration of radiation thermometers at a single fixed point. Other weaknesses identified were the absence of isotopic specifications of the fixed points, less than optimal thermodynamic accuracy of the assigned fixed-point temperatures, the limitations of SPRTs and existing fixed points, and possibly less than optimum interpolation equations.

Since that workshop was held, a broader view of possible solutions to these difficulties has emerged. Many of the identified limitations can be addressed by means other than adoption of a new scale:

- The Technical Annex for the ITS-90 addresses isotopic purities of the fixed points, while maintaining the ITS-90.
- The adoption of the MePK provides a route for dissemination of the kelvin through primary thermometry, or approximations to primary thermometry. We anticipate that the high-temperature eutectic fixed points will be assigned thermodynamic temperatures through absolute radiometry and will become a useful means of approximating thermodynamic temperature.
- The MePK can incorporate recommended values for $T - T_{90}$, enabling accurate thermodynamic temperature determination from measurements of T_{90} .

3.2 Adoption of a new temperature scale is not urgent

As a result of these alternative paths, the motivation for a new temperature scale is less compelling now than in 2000. As a task group, we weighed two opposing concerns. On one hand, coexistence of the ITS-90 with primary thermometry realizations creates the potential for two separate and possibly confusing realizations of the kelvin. On the other hand, creation of a new scale would require great effort by industry to convert software, firmware, and hardware to the new scale, on a magnitude not undertaken for previous scale conversions. For nearly all applications, this effort would not result in significant benefit.

There remain advantages for a new scale:

- The new scale would be more closely thermodynamically correct.
- There would be no ambiguity on whether temperature referred to T_{90} , T_{2000} , or T .
- The new scale could incorporate updated methods for fixed-points, interpolating instruments, and interpolating equations.
- The temperature scale conversion would provide a good opportunity to remove some flaws in the reference functions for industrial thermometers.

On consideration of these issues, the task group agreed that:

- The ITS-90 presently serves its industrial customer base well.
- Abolishing the ITS-90 and moving to a new scale would result in very high costs to industry, and the benefits for the large majority of users would be small.
- The MePK should be incrementally expanded to include thermodynamic methods, where these methods are practical and of appropriately low uncertainties. The conditions for expansion should be agreed upon by the CCT (see Section 5.2).
- The known limitations of the ITS-90 can be addressed in large part through the Technical Annex, documentation of $T - T_{90}$, and inclusion of thermodynamic methods in the MePK.

4. Looking ahead to the next temperature scale

4.1 Recommended research supporting the next temperature scale

To provide a firmer foundation for future temperature scales or for approximations to thermodynamic temperature, research is needed on the following topics.

1. The use of high-temperature SPRTs is difficult in practice, and consequently limited in scope. Few calibrations of high-temperature SPRTs are performed, and high-temperature SPRTs in industrial use often incur large drifts. The task group encourages further research on gold versus platinum (Au/Pt) thermocouples as potential candidates for an interpolating thermometer between the aluminum and silver fixed points. Further comparisons between Au/Pt thermocouples and high-temperature SPRTs or primary thermometers should be undertaken. Temperature amplifiers may prove beneficial in this temperature range as well. Potential research topics include a) comparing the results of calibrating Au/Pt thermocouples or high-temperature SPRTs in different temperature amplifiers, and b) using temperature amplifiers to examine the non-uniqueness of thermocouples.
2. The task group endorses the work of WG4 in assessing published values for $T - T_{90}$. The values of $T - T_{90}$ should be established by multiple research groups, over the full temperature range of the ITS-90, in order to form a firm thermodynamic basis for a future international temperature scale.

3. Over the past two decades, new mathematical methods have been developed for the construction of interpolation functions and the optimal use of calibration data. The application of these methods to interpolating thermometers should be explored.
4. Further research is required to address unresolved issues surrounding existing fixed points defined on the ITS-90 (e.g., isotope effect of neon), and to explore possible new fixed points or secondary reference points (e.g., xenon). Consideration also needs to be given to the impact of potential restrictions on the use of mercury.
5. Continued developments are required to improve the practice of high temperature thermometry including research into improved high-temperature thermocouples (e.g., improving the Pt/Pd type for temperatures up to 1500 °C and others above 1500 °C) and high temperature fixed points (e.g., M(C)-C eutectics) for non-contact and contact thermometry scale realization and dissemination.

4.2 Criteria for adoption of the next temperature scale

In the spirit of minimizing disruption to industry, we recommend that the ITS-90 remain in place at least until all key technical issues are solved and the recommended revisions are fully tested. Adoption of the ITS-90 was driven by significant technical limitations of the IPTS-68. Adoption of the PLTS-2000 was driven by the impending cut-back of research in that area and the lack of an international scale below 0.65 K. In contrast, the problems with the ITS-90 are significantly less serious. The task group recommends that all of the following criteria be satisfied, to the extent feasible, prior to adoption of the next temperature scale:

1. WG4 states that the thermodynamic bias of the existing scales (ITS-90 and PLTS-2000) has been adequately established over the full range of scale temperature, at an appropriate uncertainty.
2. WG5 states that methods have been established and fully tested for accurate calibrations of radiation thermometers by both absolute radiometry and high-temperature eutectics.
3. WG1 states that an acceptable interpolating instrument is available in the range from aluminum to silver fixed points, and that mathematical interpolating equations have been derived and tested for the whole scale range.
4. WG2 states that reference functions for common industrial thermometers have been derived and tested over the appropriate temperature range.
5. WG7 states that comparisons made on a primary temperature scale or by using any of the proposed methods for the next temperature scale show an acceptable degree of equivalence.

Note that satisfaction of these criteria does not imply that we should necessarily adopt a new temperature scale at that time. The CCT could recommend to the CIPM that we no longer refer to a temperature scale and associated temperature, but simply measure temperature, according to a set of practices recommended by the MePK. We discuss this option, and outlook, in the next section.

4.3 Transition towards thermodynamic temperature

An International Temperature Scale exists largely because the scale reproducibility is better than our ability to measure temperature by primary methods. As we improve our ability to measure thermodynamic temperature, there will be less need for a defined scale in some parts of the present range of ITS-90, notably at very high and very low temperatures, but in the medium SPRT range we see no prospect of dispensing with a defined practical scale.

The text of the MePK explicitly acknowledges that the ITS-90 and PLTS-2000 serve as good approximations to the ideal realization of the SI kelvin. Historically, the International Temperature Scales have always been meant to be the best practical realization of the kelvin, but this point has been lost at times in establishing international equivalence between NMIs. The proposed change to the definition of the kelvin in terms of the Boltzmann constant provides an excellent opportunity to explicitly affirm that T_{90} approximates T with a well defined reproducibility. This statement should be reflected in the way the MePK is written, discussed in other publications, and the way we educate users. We should continue the present practice of clearly distinguishing between T_{90} or T_{2000} and T .

Our increasing ability to measure thermodynamic temperature, coupled with the view of T_{90} or T_{2000} as an approximation to the kelvin, leads naturally to greater dissemination of either primary thermometry or approximations to primary thermometry.

5. Open questions for the CCT

5.1 Supplementary information for primary thermometry

Guides exist for the Supplementary Information for the ITS-90, colloquially termed the “Red Book”, and for Techniques for Approximating the ITS-90, colloquially termed the “Blue Book.” On its next revision, the MePK will explicitly endorse the realization of the kelvin through primary thermometry or approximations of primary thermometry. A parallel structure to the ITS-90 and the PLTS-2000 suggests that the MePK could contain a brief description of recommended methods, and a separate document could give expanded, supplementary information on both primary thermometry and approximations to primary thermometry.

On one hand, supplementary documents would provide a useful guide to conducting primary temperature realizations and could promote uniform practice according to proven methods. On the other hand, creation of such a document could stifle the advancement of new methods for realizing the kelvin or impose uniformity of practice when no uniformity is needed. We do not have consensus within the task group on whether the MePK should be supplemented by a comprehensive guide to practice. We encourage discussion of this point by the CCT.

5.2 Requirements for inclusion of a method in the MePK

The task group requests guidance on an additional issue, on which we did not reach consensus: What degree of validation is required for a primary thermometry method to be included in the MePK? In particular, should a minimum number of laboratories practice a particular method successfully prior to inclusion of that method in the MePK? What level of uncertainty should be achieved by a primary thermometry method, relative to the reproducibility of the International Temperature Scales, to merit inclusion in the MePK?

5.3 Managing the transition to primary thermometry

We foresee a transition period in which NMIs increasingly disseminate thermodynamic temperature alongside T_{90} and T_{2000} . At some point, when the thermometry community satisfies all of the criteria of section 4.2 to the extent feasible, the CCT can consider forming a new temperature scale or incorporating our knowledge into an extended MePK. The task group invites the CCT to consider any implications of disseminating multiple scales, and how best to educate our users on the transition.

6. References

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