FINAL PUBLISHABLE REPORT

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Project short name: Real-K

Project full title: Realising the redefined Kelvin — Realising the redefined Kelvin

Project start date and duration:1 September 2019	44 months (originally 36)	
Coordinator: Professor Graham Machin Tel: +44 20 8943 6742 E-mail:graham.machin@npl.co.uk ▪ Project website address: https://real-k.aalto.fi		
Internal Funded Partners: 1. NPL, United Kingdom 2. CEM, Spain 3. CMI, Czech Republic 4. CNAM, France 5. INRiM, Italy 6. INTiBS, Poland 7. IPQ, Portugal 8. LNE. France 9. PTB, Germany 10. SMU, Slovak Republic 11. TUBITAK, Turkey 12. UL, Slovenia 13. VSL, The Netherlands (withdrew Autumn 2020) 14. VTT, Finland	External Funded Partners: 15. Aalto, Finland 16. FBK, Italy 17. HSU, Germany 18. UW, Poland	Unfunded Partners: 19. NIM, China 20. TIPC-CAS, China 21. VNIIOFI, Russia (suspended from the consortium, March 2022)
RMGs: RMG1: INRIM, Italy (Employing organisation); CNAM, France (Guestworking organisation) RMG2: SMU, Slovakia (Employing organisation); CNAM, France (Guestworking organisation) RMG3: INRIM, Italy (Employing organisation); CNAM, France (Guestworking organisation) RMG4: CMI, Czech Republic (Employing organisation); INRIM, Italy (Guestworking organisation)		

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1 Overview

On the 20th May 2019 the implementation phase of the redefinition of the international system of units (the SI) was completed and the new unit definitions came into force. This project has taken the kelvin redefinition, and its associated *mise-en-pratique* and began to turn it into a reality by: a) developing primary thermometry techniques at high and low temperatures which can be used to realise and disseminate the redefined kelvin b) perform research to ensure the on-going fitness of the current temperature scale the International Temperature Scale of 1990 (ITS-90), and c) undertake longer-term research for primary thermometry to be the basis of temperature traceability throughout the entire range.

2 Need

The kelvin redefinition and its associated *mise-en-pratique* (*MeP*-K-19) are essentially just a documentary framework that need significant work in the coming years if the experimental approaches to thermodynamic temperature realisation and dissemination given in that document are to become a reality. This was clearly recognised at the most recent Consultative Committee of Thermometry (CCT) meeting (CCT/28) in June 2017 where the explicit recommendation (recommendation T1) “that member state NMIs take full advantage of the opportunities for the realisation and dissemination of thermodynamic temperature afforded by the kelvin redefinition and the *mise en pratique* for the definition of the kelvin” was issued.

Currently nearly all temperature measurements performed around the world are traceable to one of the two defined scales (either the ITS-90 or the specialist low temperature scale, the Provisional Low Temperature Scale of 2000 (PLTS-2000)). With the impetus given by the redefinition there will be a rise in primary thermometry approaches for realising and disseminating temperature, *directly linked to the redefined kelvin*. Realising the redefined kelvin through primary thermometry will have a number of advantages compared to defined scales. Firstly, traceability will be directly linked to the redefined kelvin and not an intermediary defined scale. This over time will lead to practical primary thermometry being adopted by users with decreasing reliance on traceability to defined scales, improving the long-term reliability of measurements. Secondly, the low temperature part of the current scales could be replaced with simpler primary thermometry approaches, whilst the high temperature part will be replaced with more robust indirect primary radiometry. Thirdly in the long term practical primary thermometry could well be developed from the innovations under development in Real-K

This research supports the world metrology community in the realisation and dissemination of the redefined kelvin, with EURAMET continuing to lead in this important metrology field. Without this research the realisation and dissemination phase of the kelvin redefinition could falter.

3 Objectives

The overall goal of this project is to take the kelvin redefinition (and the *MeP*-K-19) and begin to turn it into a reality. It will do this through the following objectives:

1) To demonstrate and establish traceability directly to the redefined kelvin from ~1300 K to ~3000 K. Low uncertainty thermodynamic temperatures of four new High Temperature Fixed Points (HTFPs) will be determined. Then, through the *MeP*-K-19, HTFPs will be used to realise and disseminate thermodynamic temperature with uncertainties competitive with the defined scale (the ITS-90) (target Uncertainty [U]<0.05%).
2) To demonstrate practical primary thermometry for realisation and dissemination of thermodynamic temperature below 25 K and so demonstrate that primary thermometry can be used: to replace the currently complex ITS-90 scale realisation arrangement below 25 K and to ensure a smooth transition to the PLTS-2000 range below 1 K (target U = 0.2 mK at 25 K and <1% at 1 K).
3) To extend the life of the ITS-90 giving users continued access to low uncertainty realisations of the scale whilst allowing time for primary thermometry methods to mature. The troublesome issue of scale non-uniqueness will be investigated, with the objective of reducing its uncertainty by 30 %, and a suitable fixed-point replacement for the mercury triple point identified, constructed and tested. Integration of the new fixed point within the ITS-90 will be addressed.
4) To reduce the uncertainty in a number of different primary thermometry methods, approved for use in the *MeP*-K-19, and so begin to facilitate an extension of their applicability for temperature realisation

and dissemination into the temperature region 25 K and above. This long-term objective will be facilitated through reducing the uncertainties of the calculated thermophysical properties of gases (e.g. He, Ne, Ar) used as thermometric fluids in primary thermometers.

5) To work closely with the CCT to issue formal recommendations and definitive guidance on the realisation and dissemination of the redefined kelvin, to ensure rapid uptake of the results of this research. Engagement with the global thermometry community by regular briefings to Regional Metrology Organisation (RMO) Technical Committee for Thermometry (TC-Ts), papers and conference presentations. Wider user engagement will be through the stakeholder community and events.

4 Results

Objective 1: To demonstrate and establish traceability directly to the redefined kelvin from ~1300 K to ~3000 K. Low uncertainty thermodynamic temperatures of four new HTFPs will be established. Then, through the mechanism of the MeP-K-19, HTFPs will be used to realise and disseminate thermodynamic temperature with uncertainties competitive with the defined scale (the ITS-90) (target U<0.05 %).

This objective used primary thermometry (indirect primary radiometry) for temperature realisation and dissemination at temperatures >1300 K. Before this project was undertaken the state of the art for temperature realisation and dissemination >1300 K is through the defined scale the International Temperature Scale of 1990 (ITS-90). This was significantly advanced by constructing and assigning definitive low uncertainty thermodynamic temperatures to the High Temperature Fixed Points (HTFPs) of Fe-C (1426 K), Pd-C (1765 K), Ru-C (2226 K) and WC-C (3020 K). Trial dissemination of thermodynamic thermometry was performed and was the first practical demonstration of the *MeP*-K-19 by indirect primary radiometry (>1300 K). The way has now been opened for temperature dissemination at high temperatures to be realised directly to the redefined kelvin.

The following high temperature fixed points were constructed in line with the construction protocol; 5 WC-C cells (CNAM, NPL), 4 Ru-C cells (NPL, VNIIOFI), 5 Pd-C cells (CEM, NIM) and 4 Fe-C (PTB, CEM) cells. This was in excess of the minimum required for by the project but allowed for some redundancy in case of breakage of the fixed point cells. A section through a HTFP is shown in Figure 1.

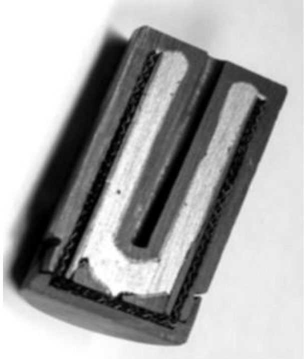


Figure 1: Section through a high temperature fixed point, the shiny metal-carbon ingot surrounds the blackbody tube and is encased within the graphite crucible. The outer diameter is 24 mm.

All the HTFP cells constructed were compared and ranked according to agreed selection criteria such as melting range, repeatability, plateau shape and value of the inflection point. INRIM compared the Fe-C cells, CEM compared the Pd-C cells, NPL compared the Ru-C cells and LNE-Cnam compared the cells of WC-C. The best two of each cell were selected for thermodynamic temperature assignment, the next best 2 cells were selected for dissemination trials.

Led by NPL, CEM, CNAM, PTB, NIM and VNIIOFI the effects of the furnace on the performance of the HTFP was evaluated, especially the temperature step used to initiate the melt/freeze and the temperature gradient around the HTFP cell, was characterised for all types of cells constructed. This is important to understand the magnitude of these effects on the resultant performance of the HTFP and overall uncertainty.

The protocol for assigning thermodynamic temperature to the selected HTFPs was drafted by CNAM and agreed by the partners. The measurements were broken into two loops. In loop A, PTB, CEM, LNE, Cnam and

NPL completed the measurements. In loop B, there was some disruption due to the exclusion of the Russian NMI (VNIIOFI), and laboratory issues in INRIM prevented assignment of thermodynamic temperature, however in loop B sufficient measurements for thermodynamic temperature assignment were undertaken by TUBITAK and NIM. All the measurements have been analysed and a paper presented at the ITS-10 conference reporting preliminary thermodynamic temperatures of the new HTFPs. These will be finalised, published (M.Sadli *et al*, Assigning thermodynamic temperatures to a set high-temperature fixed points in the range 1400 K to 3000 K, ITS-10 proceeding, *Submitted* 2023) and once having undergone peer review and published, incorporated within the *MeP*-K annex reporting HTFP values for use in realising and disseminating thermodynamic temperature by relative primary radiometry.

The quality of these results are illustrated by Figure 2 below. There the point-of-inflection of the melt of WC-C is reported by six participating institutes and the unified weighted mean given. This is the lowest uncertianty evaluation of these temperatures ever and it is excellent to see such good agreement between the participants showing that all are able to realise high temperature low uncertainty (radiance) thermdynamic temperature.

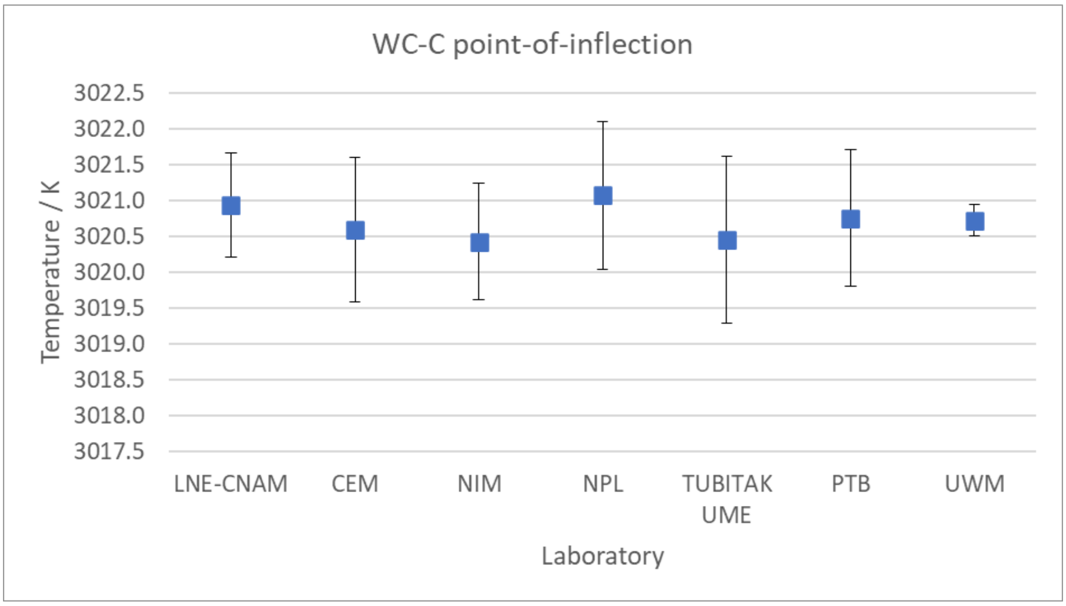


Figure 2: Results of the point of inflection of six independent evaluations (by six NMIs) of the melt of the WC-C metal carbide-carbon high temperature fixed point.

A step-wise guide of how to use the HTFPs for thermodynamic temperature realisation and dissemination was presented at the ITS-10 conference. A paper has bee nwritten and has been accepted for publication in the proceedings as an open access paper (D. Lowe and G. Machin, Low uncertainty thermodynamic temperature measurement using relative primary radiometry setting up n=2 scale using copper and rhenium-carbon with uncertainties, ITS-10 proceeding, *Accepted* 2023).

The trial dissemination trials of thermodynamic temperature was run by PTB. Traceability receiving partners (TUBITAK and CMI) received and measured the HTFP cells. In addition special large 6 mm aperture HTFP cell was constructed by CEM for a trial dissemination to an commercial accredited laboratory. The results of the dissemination trial have been analyses by PTB and will be summitted for publication, as well as forming a briefing document for CCT WG for non-contact thermometry.

The overall objective was achieved. A paper has been prepared for submission to the ITS-90 conference proceedings once accepted the thermodynamic temperatures will be added to the *MeP*-K-19 annex of accepted temperature values for HTFPs. The dissemination trial highlighted the effectiveness of using HTFPs for disseminating thermodynamic temperature at high temperatures and will feed into recommendations to use indirect radiometry as an approach to directly disseminate the kelvin at high temperatures.

Objective 2: To demonstrate practical primary thermometry for realisation and dissemination of thermodynamic temperature below 25 K and so demonstrate that primary thermometry can be used: to replace the currently complex ITS-90 scale realisation arrangement below 25 K and to ensure a smooth transition to the PLTS-2000 range below 1 K (target U = 0.2 mK at 25 K and <1 % at 1 K).

This objective used a number of low temperature primary thermometry approaches to provide a simplified approach to realising and disseminating temperature below 25 K which was at the same time thermodynamic (i.e. directly linked to the redefined kelvin) rather than using the defined temperature scales. The state of the art before the work in this project, for the temperature scale realisation <25 K, was complex. Traceable temperatures were referenced to one of the two defined scales the ITS-90 or the Provisional Low Temperature Scale of 2000 (PLTS-2000). Scale realisation required different sophisticated, time-consuming, experimental methods, which are only available in very few National Metrology Institutes (NMIs) or relied on historic thermometers calibrated many years ago at low temperatures. The work undertaken in this project fully achieved this objective with developing primary thermometers to covering the entire range from 1 K to 25 K for direct realisation and dissemination of temperature (target uncertainty <1%).

PTB constructed and improved the design of a variant of the Johnson Noise Thermometer known as a primary Magnetic Field Fluctuation Thermometer (pMFFT). A photograph of a pMFFT is shown in Figure 3. The redesign reduced the number of coil chips (to just one instead of two) and modified the arrangement of the thin-film calibration coilsSuch an arrangement reduced the overall uncertainty of the device by at least a factor 2. In addition, progress was made in the mathematical description of the thermal magnetic flux noise in conjunction with a new, extended model for an arbitrary number of layers of different electrical conductivities. These advances allowed better evaluation of the overall measurement uncertainty. Measurements using this variant of the pMFFT were performed at the well-known helium lambda point (2.1768 K), which is the temperature at which normal fluid helium transitions to superfluid helium. Agreement within 1.0 mK was found between the pMFFT result and another primary thermometry approach (Dielectric Constant Gas Thermometry) demonstrating that pMFFT could achieve the required measurement goal of <1%. In addition, and crucially for acceptance of this primary thermometry approach, the pMFFT demonstrated smooth overlap (better than the device uncertainty) between ITS-90 and PLTS-2000 between 0.6 K and above 1 K (that is in the overlap region between the two scales).

Figure 3: Photograph of a primary Magnetic Field Fluctuation Thermometer (pMFFT)

At VTT and Aalto the nanofabrication process for Al-and AlMn-based Coulomb Blockade Thermometers (CBTs) was significantly improved and arrays were manufactured with sub-100 nm tunnel junctions (see Figure 4 below). Al-based CBT devices were tested and shown to operate between 1.4 K and 25 K.

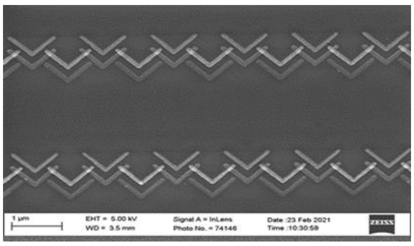


Figure 4: Photograph of a tunnel junction array for a Coulomb Blockade Thermometer (CBT)

PTB undertook performance evaluations between its pMFFT and the Aalto, VTT CBT (using ITS-90 and thermodynamic temperature using DCGT via calibrated rhodium-iron resistance thermometers). Good agreement was found between the PTB ITS-90 realisation between 2.5 K and 25 K, but for the CBT it found to deviate monotonically below 2.5 K (Figure 5). The pMFFT did not show this behaviour (Figure 6). Likely reasons for this deviation are either a partial disconnect of the CBT chip from its sample holder or the influence of random offset charges that modify the electrostatic environment of the device.

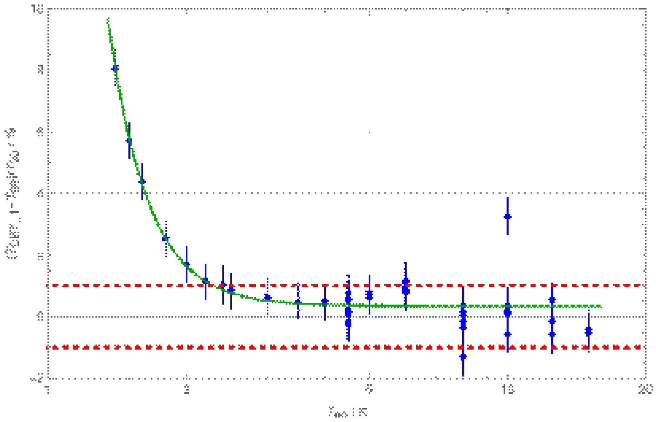


Figure 5: CBT thermodynamic temperature measurement compared to ITS-90. The CBT shows good performance above 2.5 K

However taken together these results demonstrate that CBT can perform as well as pMFFT over most of its operational range and within the target uncertainty of <1%.

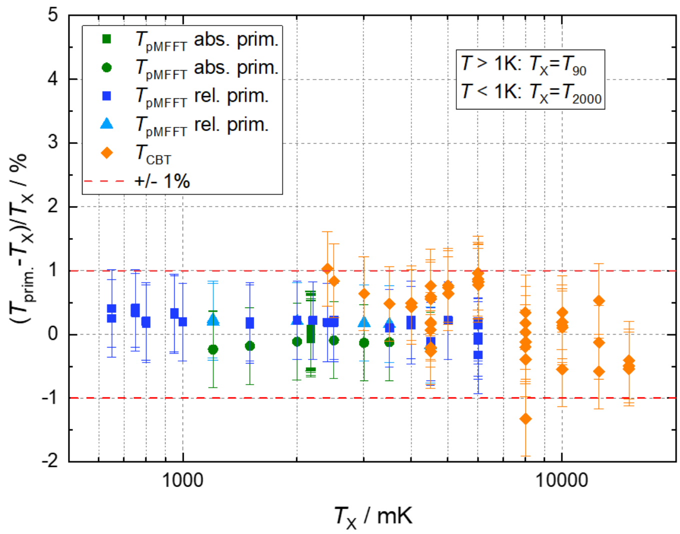


Figure 5: Comparison of pMFFT and CBT in the range of ITS-90 and crucially demonstrating smooth transition in the overlap region between ITS-90 and PLTS-2000 (0.65 K to 1 K)

With regards to the AGT activity between around 5 K and 25 K a pulse-tube cryostat with an Acoustic Gas Thermometer (AGT) has been used extensively (LNE-Cnam and TIPC-CAS) to perform thermodynamic temperature measurements at T = 24.5561 K (Ne triple point) – this was then used as an anchor temperature for fast-AGT. The results are published in C. Pan *et al,* 2021, *Metrologia* **58** 045006, https://doi.org/10.1088/1681-7575/ac0711. Classic AGT measurements between 4 K and 24 K were performed (LNE-CNAM) at several temperatures in parallel with fast-AGT tests. “Fast” measurement techniques have been developed at microwave frequencies on the single-pressure refractive-index thermometer (SPRIGT) installed at TIPC-CAS. The results are published in Bo Gao *et al*, 2020, *Metrologia* **57** 065006, https://doi.org/10.1088/1681-7575/ab84ca. A comparison of both thermometers gave very low temperature differences to ITS-90 values (Figure 6).

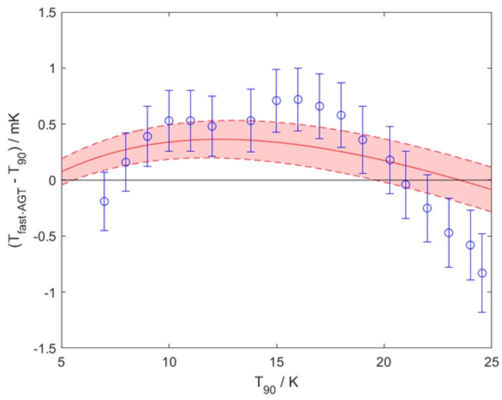


Figure 6: Measurements of T-T_{90} for fast-AGT. The shaded area is the current best estimate of T-T_{90}. This shows that for most of the temperature range fast-AGT is an excellent and rapid approach to establishing (and hence disseminating thermodynamic temperature)

The overall objective was achieved. Practical primary thermometry for realisation and dissemination of thermodynamic temperature below 25 K was demonstrated within the target uncertainty of <1 % at 1 K. Performance and validation reports, with uncertainties, have been submitted to CCT demonstrating the potential practicality of realising and disseminating thermodynamic temperature directly linked to the kelvin definition.

Objective 3: To extend the life of the current defined scale (ITS-90) giving users continued access to low uncertainty realisations of the scale whilst allowing time for primary thermometry methods to mature. The troublesome issue of scale non-uniqueness will be comprehensively investigated, with the objective of reducing its uncertainty by 30 %, and a suitable fixed-point replacement for the beleaguered mercury triple point identified, constructed and tested. The issue of integration of the new fixed point within the ITS-90 will be addressed.

This objective tackled two potential life limiting issues with the International Temperature Scale of 1990. The first was the issue of Type 1 and 3 non-uniqueness which are among the dominant uncertainties in ITS-90 calibrations. The work here performed extensive evaluations of both types of non-uniqueness. The second was the increasing restriction on the use of mercury that could potentially see a ban on the use (or at least the transport) of the mercury triple point, a key fixed point essential for a full realisation of the ITS-90. Here we work on two possible alternative fixed points to the mercury CO_2 or SF_6. We also examine the implications or replacing the mercury point and its impact on the ITS-90.

Results of non-uniqueness studies

The type 1 non-uniqueness or subrange inconsistency (SRI) of a large ensemble of long-stem standard platinum resistance thermometers (SPRTs) has been investigated for all pairs of overlapping subranges (NPL, IPQ, VSL (subsequently left the project). The contribution of the fixed-point uncertainty propagation to SRI was evaluated and was found to amount to a percentage between 60 and 130. Therefore, importantly, the currently calculated differences are probably a substantial overestimate of the true SRI. These results were published in Peruzzi *et al Metrologia* **58** (2021) 035009.

Robust evaluation of the type 3 non-uniqueness of SPRTs over a wide range of temperatures has been performed (NPL, INTiBS, CEM). Measurements of groups of SPRTs were carried out using the comparison method in stirred liquid baths over the temperature ranges from 178 K to 302 K at NPL and from 273 K to 353 K at CEM. Measurements were performed at the ITS-90 fixed points: triple point of Ar, Hg, H_2O and Ga, and close to secondary fixed points: triple point of SF_6, CO_2 and Xe. The measurements have been completed and the results showed that the interpolation non-uniqueness was ~0.1 mK from 178 K up to 302 K, rising to ~0.2 mK at 353 K. This is a significant improvement over previous comparisons using long-stem SPRTs, and they have been published. It was found that comparison measurements in a cryostat below 178 K (INTiBS) were too susceptible to temperature gradients, and hence not sufficiently repeatable to be included in this evaluation. A summary of the data is shown in Figure 7.

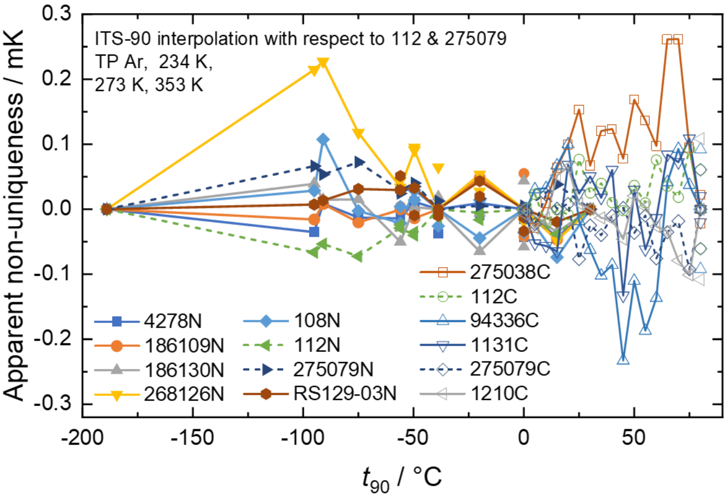


Figure 7: Summary of the type 3 non-uniqueness with the different SPRTs used uniquely identified

INRIM collected the required 6 High Temperature (HT)SPRTs (3 from SMU, 1 from INTiBS, 2 from NPL) for Type 3 non-uniqueness evaluation (NU3) at high temperatures – a very under-explored temperature region of the ITS-90. The sensors were calibrated at the fixed points of zinc, tin, silver, aluminium, and water prior to the Type 3 NU study in the sodium heat-pipe. Due to stability issues one of the HTSPRTs was excluded from the study. Measurements were performed with the 5 left HTSPRTs and results of the NU3 evaluation presented at the final meeting. The results are in very good agreement with previous determinations of the NU3 performed using completely different apparatus.

The preliminary results of the effectiveness of a least-squares approach to SPRT interpolation were presented at the 10th International Temperature Symposium in California in April ’23 by UL. The results were submitted to Measurement journal and currently under review. The SRI of two pairs of subranges of an ensemble of 30 SPRTs from UL database was investigated for three cases. In the first case, the calculations followed the standard procedure. In the second case, an SPRT was calibrated at all fixed points of the subrange and its deviation function was then determined using the least squares method. In the third case, the least squares method was weighted by the uncertainties at each of the fixed points. One significant benefit of the least squares approach over exact interpolation is the reduction in uncertainty propagated from the fixed points. The results also show that the mean and deviation of type 1 NU decreases if redundant fixed points are included. This is shown in Figure 8.

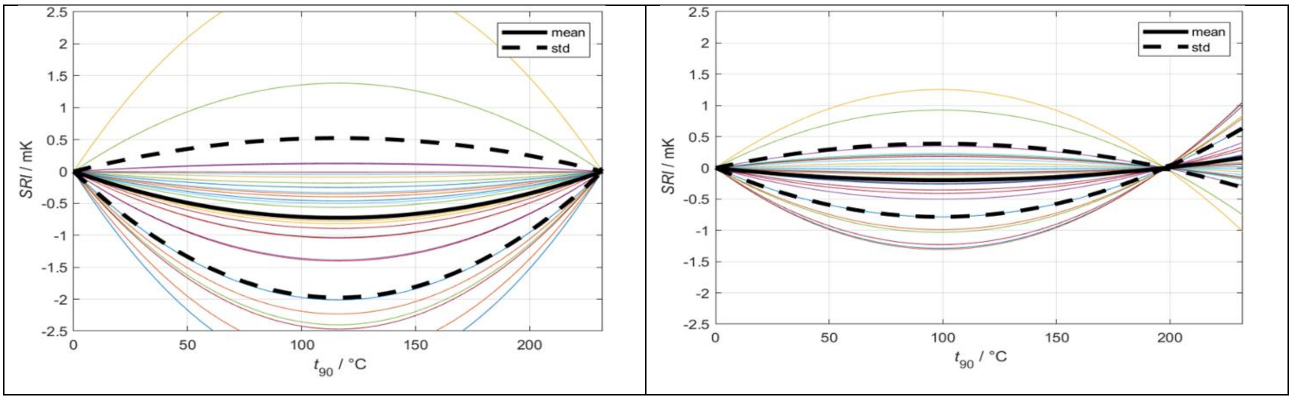


Figure 8. On the LHS the type 1 NU in the range Zn:Sn using the ITS-90 formalism and on the RHS the type 1 NU in the same range using the least squares approach

Results of alternative fixed-point studies

Extensive investigations have been performed on the triple points of SF_6 and CO_2 as possible alternative fixed points to the Hg triple point. Three SF_6 cells were constructed by LNE & Cnam and two CO_2 cells by TUBITAK.

CNAM and LNE completed the evaluation of the SF_6 cells, the results show excellent agreement with a previous LNE-Cnam SF_6 cell (223.555 K within 0.1 mK). Cnam and LNE have also completed the assembly of a dedicated SF_6 calorimeter and have installed a SF_6 triple point cell inside. A figure of the SF_6 calorimeter of LNE - CNAM is shown in Figure 9. Charaterisation of the SF_6 calorimeter was performed through realisng the SF_6 triple point. The results obtained with capsule-type SPRTs in the dedicated SF_6 calorimeter showed excellent agreement with previous data (within 0.2 mK). However, despite the use of the guard cell, long-stem SPRTs are influenced by heat conduction along the stem at the level of around 1 mK. However, despite that small issue the data shows very good consistency of the LNE-Cnam cells with the most recent results available in literature on SF_6. This work, along with that of others in teh thermometry community has shown that SF6 is a credible alternative fixed point to the Hg triple point, particularly for capsule type PRTs but also for long stem PRTs if one can accept a modest increase in uncertainty.

Two RMG researchers made additional contributions to this aspect of the work.

RMG2 (Peter Pavlasek, from SMU to Cnam, 4 months): from 1st June to 30th September 2022. The RMG designed and developed a CO_2 triple point cell for simultaneous CSPRT and SPRT calibrations. The tested CO_2 cell showed a consistent level of repeatability at the level of 0.30 mK. The realized plateaus also showed a high level of stability, corresponding to a temperature increase of 1.03 mK after a period of 22 hours. Results were presented at the 10th International Temperature Symposium ITS-10 and at the Real-K workshop.

RMG3 (Dario Imbraguglio, from INRIM to Cnam, 4 months): from 15th June to 14th October 2022. The RMG designed and implemented an environmental enclosure holding the pressure standards associated to the fast-AGT of LNE-Cnam, as well as an active pressure control system, to reduce pressure oscillations in the fast-AGT system due to ambient temperature variations. A full campaign of temperature measurements was realized with the fast-AGT in the cryogenic range from 54 K down to 7 K, to assess the quality of the developed enclosure. Results were presented at the 10th International Temperature Symposium ITS-10.

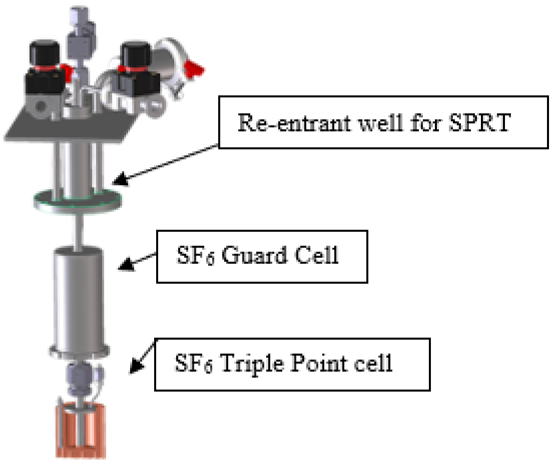


Figure 9: Cross Section of SF_6 calorimeter of LNE CNAM. The whole arrangement is established in a vacuum can and then immersed in an ethanol bath at around -50 ºC for realisng the SF_6 triple point

TUBITAK completed the construction and metrological characterisation of two CO_2 cells. A photgraph of one of the CO_2 cells is shown in Figure 10 below.

Figure 10: A photograph of a TUBITAK CO_2 triple point cell

To ensure the CO_2 filling gas was as pure as possible a gas getter (purifier) was introduced into the cell filling system and to confirm the fixed-point material purity the chemical analysis was performed by the Gas Metrology Division of TUBITAK using GC-DID. The analysis showed that the filter was effective in reducing residual oxygen inside the CO_2 gas samples to about 2% of its inital value. Metrological characterization was performed by measuring the plateau duration, plateau reproducibility and phase transition width. Measurements were performed over several months indicated very consistent triple point temperature values lying within 0.1 mK and plateaux lasting more than 10 hours with a plateau width of 0.3 mK. A comparison was performed between the cells containing 6N purity CO_2 sample and 6N-P (purified 6N purity) CO_2 sample. Both cells were immersed in the same stirred liquid bath and two SPRTs were employed for the measurements which were taken through high accuracy resistance bridge. These measurements showed that removing the oxygen did not influence the CO_2 triple point, the cells agreeing with each other to 0.03 mK. The triple point plateaus were obtained through melting after a fast freeze and pre-heating at the beginning of the melting plateau. The cells were then emptied and filled once again with the same gas samples after several weeks from the first comparison to check the reproducibility of results. A second comparison was then carried out using the same experimental apparatus and indicated very similar results to the first one. A final evaluation was performed by comparing CO_2 cells containing 6N purity and 5N purity CO_2. This enabled an evaluation of the uncertainty linked to the chemical impurities in the gas. The results yielded a temperature difference of only 0.15 mK between these two cells. These studies with CO_2 cells show very consistent results and crucially have successfully been used to calibrate long stem SPRTs with an uncertainty better than 0.5 mK. This work shows that the triple point of CO_2 (216.591 K) is a credible alternative to the mercury point.

An investigation was performed by SMU to evaluate the effect of replacing the triple point of Hg in the cryogenic sub-range of ITS-90 from the triple point of water to the triple point of argon. The fixed points that were introduced as replacements for Hg were the two investigated in this project (SF_6, CO_2) and the other possible alternative Xe. The effects for these fixed points were expressed in the form of uncertainty propagation as compared to the conventional realisation. It is clear that Xe yields superior performance to SF_6 and CO_2, but the TP Xe (~160 K) is too low to be used with long-stem SPRTs. This means that if one is only using capsule SPRTs then Xe would be the preferred fixed point to replace the mercury triple point. However, it is worth pointing out, that in most cases long stem SPRTs are the interpolation thermometer of choice and then CO_2 or SF_6 would have to be used.

Meanwhile NPL performed an analysis of alternative interpolations for long-stem SPRTs in which the ITS-90 is extended below the triple point of water to the argon point, without including the Hg point. An important conclusion is that these interpolations can be used with uncertainties of 0.3 mK to 0.5 mK, similar to current uncertainties for long-stem SPRTs. Figure 11 shows the effect of replacing the Hg triple point with an already established ITS-90 fixed point of Ga. Although the type 3 non uniqueness increases, it is only a small amount and not appreciably significant.This work was presented at the International Temperature Symposium in April 2023.

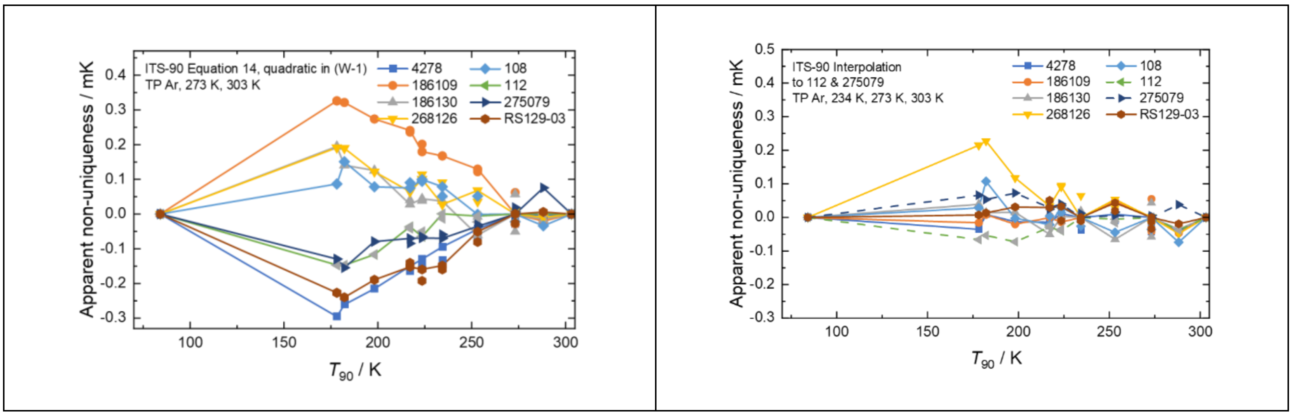


Figure 11: Type 3 non-uniqueness uncertainty without (LHS) and with (RHS) the mercury triple point included in the interpolation. Although the type 3 NU increases a little without the use of the Hg triple point the increase is still small

The overall objective was acheived with the useful life of the current defined scale (ITS-90) extended until at least the end of the decade. Both types of scale non-uniqueness were comprehensively investigated and quantified. Two alternative fixed-points (CO_2 and SF_6) were investigated and found to be suitable replacements for the Hg triple point. The issue of integration of the new fixed point within the ITS-90 was also addressed. Recommendation documents on both these aspects of the work have been prepared and sent to the CCT WG for Contact Thermometry.

Objective 4: To reduce the uncertainty in a number of different primary thermometry methods, approved for use in the MeP-K-19, and so begin to facilitate an extension of their applicability for temperature realisation and dissemination into the temperature region 25 K and above. This long-term objective will be facilitated through reducing the uncertainties of the calculated thermophysical properties of gases (e.g. He, Ne, Ar) used as thermometric fluids in primary thermometers.

This objective had the very ambitious goal of establishing the foundations for practical gas-based primary thermometry so as to deliver temperature traceabilty directly to the kelvin. At the start of the project traceable temperatures above 25 K were really only achieveable through calibration to the defined scale, that is calibration to the ITS-90. For gas-based primary thermometry methods, i.e. AGT, Dielectric Constant Gas Thermometry (DCGT) and Refractive Index Gas Thermometry (RIGT), to compete with the ITS-90 for kelvin dissemination the approaches needed to be substantially simplified. The crux of how to achieve this was to reduce the uncertainty in the *ab initio* calculations of the non-ideality of monatomic gases He, Ar and Ne *and* ensuring those calculations were valid by comparison with selected low-uncertainty measurements over the temperature range of (10 K to 350 K) and pressures (<100 MPa). If achieved this would allow for gas-based thermometry to be simplified *and* crucially speeded up (traditional gas-based thermometry required taking isotherms at different pressures meaning one temperature could take a week or more to measure. By knowing the non-ideality of the thermometric gases through *ab initio* calculations a measurement at one pressure then applying corrections one could much more rapidly arrive at a temperature value). Thanks to the significant advances in these calculations this goal has been achieved.

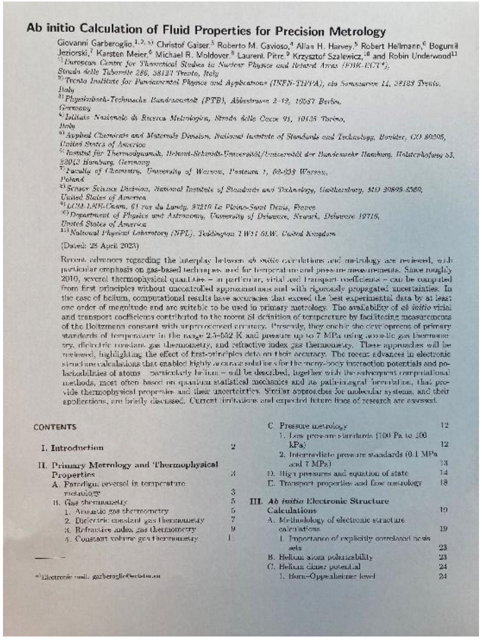
Calculation of interaction potentials and thermophysical properties of thermometric gases

Excellent progress has been made in the calculation of thermophysical properties of thermometric gases (UW, FBK). This was achieved through calculating improved pair and three-body potential calculations (UW) for He, Ne and Ar. These values were then used to develop improved values of the 2nd, 3rd and 4th density and acoustic virial coefficents for He, Ne and Ar. Highlights include:

- for He, six-fold improvement in the 2nd density and 2nd acoustic virial coefficients and a factor of 3 to 5 improvement in the estimates of the 3rd density and acoustic virial coefficients, in addition an estimate of the 4th virial coefficient was made
- for Ne, 5-10 level of improvement in the calculation of the 2nd density and acoustic virial coefficients and improved estimates of the 3rd and 4th density and acoustic virials

- for Ar, the calculation of an improved 2-body potential leading to significantly more accurate calculated estimates of the thermophysical properties.

This work has been submitted for publication: G. Garberoglio *et al*, *Ab initio* Calculation of Fluid Properties for Precision Metrology to the Journal of Physical and Chemical Reference Data (2023), the first page of which is shown in Figure 12. Note the results reported in this paper will also have signficant beneficial impact in pressure standards work.



Ab initio Calculation of Fluid Properties for Precision Metrology

Giovanni Garberoglio,[1,2,a)] Christof Gaiser,[3] Roberto M. Gavioso,[4] Allan H. Harvey,[5] Robert Hellmann,[6] Bogumił Jeziorski,[7] Karsten Meier,[6] Michael R. Moldover,[8] Laurent Pitre,[9] Krzysztof Szalewicz,[10] and Robin Underwood[11]

[1)] European Centre for Theoretical Studies in Nuclear Physics and Related Areas (FBK-ECT*), Strada delle Tabarelle 286, 38123 Trento, Italy
[2)] Trento Institute for Fundamental Physics and Applications (INFN-TIFPA), via Sommarive 14, 38123 Trento, Italy
[3)] Physikalisch-Technische Bundesanstalt (PTB), Abbestrasse 2–12, 10587 Berlin, Germany
[4)] Istituto Nazionale di Ricerca Metrologica, Strada delle Cacce 91, 10135 Torino, Italy
[5)] Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO 80305, United States of America
[6)] Institut für Thermodynamik, Helmut-Schmidt-Universität/Universität der Bundeswehr Hamburg, Holstenhofweg 85, 22043 Hamburg, Germany
[7)] Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland
[8)] Sensor Science Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8360, United States of America
[9)] LCM-LNE-Cnam, 61 rue du Landy, 93210 La Plaine-Saint Denis, France
[10)] Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, United States of America
[11)] National Physical Laboratory (NPL), Teddington TW11 0LW, United Kingdom

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Recent advances regarding the interplay between *ab initio* calculations and metrology are reviewed, with particular emphasis on gas-based techniques used for temperature and pressure measurements. Since roughly 2010, several thermophysical quantities – in particular, virial and transport coefficients – can be computed from first principles without uncontrolled approximations and with rigorously propagated uncertainties. In the case of helium, computational results have accuracies that exceed the best experimental data by at least one order of magnitude and are suitable to be used in primary metrology. The availability of *ab initio* virial and transport coefficients contributed to the recent SI definition of temperature by facilitating measurements of the Boltzmann constant with unprecedented accuracy. Presently, they enable the development of primary standards of temperature in the range 2.5–552 K and pressure up to 7 MPa using acoustic gas thermometry, dielectric constant gas thermometry, and refractive index gas thermometry. These approaches will be reviewed, highlighting the effect of first-principles data on their accuracy. The recent advances in electronic structure calculations that enabled highly accurate solutions for the many-body interaction potentials and polarizabilities of atoms – particularly helium – will be described, together with the subsequent computational methods, most often based on quantum statistical mechanics and its path-integral formulation, that provide thermophysical properties and their uncertainties. Similar approaches for molecular systems, and their applications, are briefly discussed. Current limitations and expected future lines of research are assessed.

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a) Electronic mail: garberoglio@ectstar.eu

Figure 12: First page of G. Garberoglio *et al*, *Ab initio* Calculation of Fluid Properties for Precision Metrology the results of which will transform practical gas-based thermometry

Measurement of selected thermophysical properties of gases

Whilst it is not possible to measure all the required thermophysical properties of gases for primary thermometry selected values have been determined to confirm that the theoretical calculations described above are realistic. Excellent experimental confirmation was found of the calculated values showing how impressive the theoretical calulations have been.

These include:

- For He: The 2nd and 3rd density virial coefficients of helium were determined by PTB through coupled DCGT and Burnett expansion experiments at 273 K and 296 K. A comprehensive uncertainty budget was established for the method. The measured density virials of He were found to agree well with the most accurate theoretical values currently available, within their standard uncertainty (< 1%). A cryogenic apparatus for AGT was used by INRIM to measure the speed of sound in helium at several temperatures between 10 K and 273.16 K. From these measurements accurate estimates of the 2nd and 3rd acoustic virial coefficients of He were obtained at 13.8 K which favourably compare to the best theoretical estimates of these quantities obtained during this project.

- For Ne: In an AGT based on a spherical resonator INRIM determined an accurate estimate of the 2nd acoustic virial coefficient of Ne was obtained at 273.16 K. In addition, HSU performed speed-of-sound measurements in supercritical neon gas were carried out between 80 K and 420 K in steps of 20 K at pressures between 20 MPa and 100 MPa. The combined expanded uncertainty of the speed of sound amounts to 0.007%, From this data the 4th-order acoustic virial expansion in pressure along with the 2nd acoustic virial coefficient were determined.

- For Ne and Ar: PTB used DCGT + Burnett apparatus to perform measurements of the thermal properties of Ne and Ar at 253 K, 273 K, 296 K and 303 K. The data evaluation yielded a reduced uncertainty for the second density virial coefficient ur(B) = 0.5 % and for the third density virial coefficient ur(C) = 1.5 % to 3 % (k = 1). The measured density virials agree very well with the best calculations from first principles, with the deviations are typically less than the combined standard uncertainty (See Figure 13 for sample comparison of the second density virial coefficient of Ne calculation compared to experiment.

- For Ar: Analysis of speed of sound by NPL measured using a quasi-spherical resonator yielded low uncertainty values of the second acoustic virial coefficient of argon in the range 120 K to 330 K. These results were found in remarkable agreement with the most accurate *ab-initio* calculations of the same properties obtained within the project.

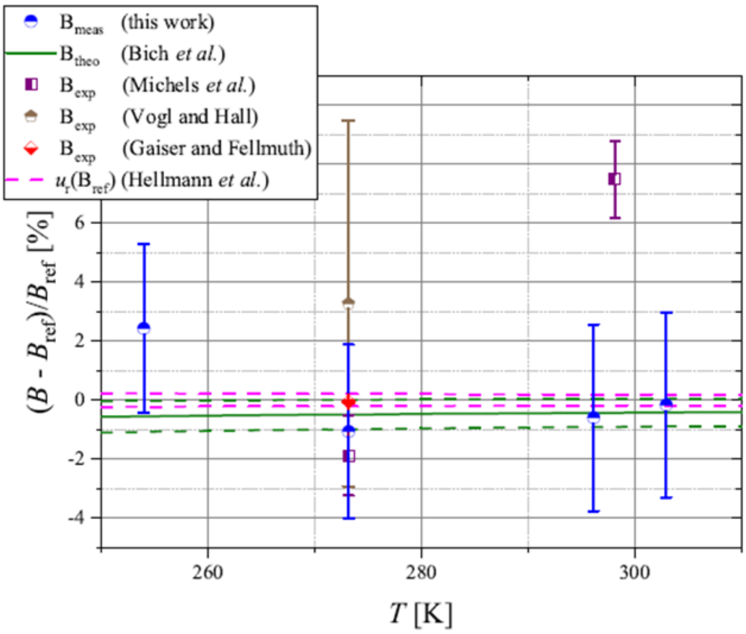

Figure 13: Comparison of experimental data (from PTB) with the measured values of the second density virial coefficent of Ne. Experimental data confirms the calculated values, the latter having the lower uncertainty.

Easy access for the community to all these results has been provided by the work of RMG1 (Alberto Albo, from INRIM to Cnam, 4 months): started the 1st May 2022, Alberto was at Cnam from 1st May to 30th June 2022 and 1st October to 30th November 2022. The RMG developed a software implementing state-of-the-art physical models for helium and realized software libraries for supporting online analysis of measurements in acoustic thermometry. They are freely available on Zenodo and Real-K websites with an open-source license. Results were presented at the Real-K closing meeting.

Preparing for improved primary thermometry

Given the extensive new theoretical values for thermophysical gas properties, validated by key experimental evaluations, the path is now open for improved primary thermometry for dissemination of temperature linked directly to the kelvin defintion. Here we perform some proof-of-concept studies to serve as a preliminary demonstration of the validity of the approach. This will be extensively demonstrated in the follow-on funded Disseminating the Redefined Kelvin (DireK-T) project.

Two different approaches have been trialed in Real-K, simplified DCGT and RIGT

- Automated experiments with argon around room temperature were performed with DCGT by PTB. A comprehensive uncertainty budget for this primary thermometry method was developed that had standard uncertainties of about 7 mK. This very simplified approach will be developed, and the uncertainties significantly improved, in the follow-on project DireK-T.

- RIGT measurements at 273.16 K in He, Ne and Ar were completed by INRIM using a quasi-spherical resonator (see Figure 14). In this simplified experimental arrangement, the RIGT thermometer was found to deviate by as much as 3 mK, with standard uncertainties in the order of 2 mK. This shows promise but requires more work, which will be performed in DireK-T to reduce the uncertainties to be comparable with the best ITS-90 realisations.

Finally it is pleasing to report the work of RMG4 (Michal Voldán from CMI to INRIM 3 months1 June 2021 to 30 August 2021). Extending the Working Range of Acoustic Gas Thermometry. The RMG researcher contributed to the development and test of a protoype primary Acoustic Gas Thermometry experiment suitable for operation in the temperature range above ambient up to 1000 K. Particularly, the RMG researcher tested the acustic and microwave waveguide transmission system of the apparatus and conducted preliminary tests of its performance up to 500 K.

Figure 14: A photograph of the quasi-spherical acoustic resonator used by INRIM for the proof-of-concept implementation of improved primary thermometry using Refractive Index Gas Thermoemtry (RIGT)

It is pleasing to report that the goals of the objective fully met. Theoretical evaluations of relevant gaseous thermophysical properties have been calculated, and confirmed with selected measurements, with sufficiently low uncertainty so as to expand the temperature range of gas-based primary thermometry to higher temperatures. This work has laid the essential foundation for the follow-on project Disseminating the redefined kelvin (DireK-T) which would not have been possible if this objective had not been successfully completed.

5 Impact

General outreach: This has been through the project website and circulation of five newsletters to stakeholders. An introductory article was published in the British Cryogenics Council newsletter. Written progress reports have been circulated to the CCT and all the RMO TC-Ts.

Seminars/talks/conferences: The coordinator gave invited seminars about Real-K at 7 European universities. The coordinator gave eight invited plenary/papers on Real-K during the project. Of particular note were; an invited keynote in Jan 2022, NPL India 75th anniversary celebration, “The kelvin redefinition and its implications” (based on Real-K results) and in April 2023 the James Schooley Plenary Lecture at the prestigious tenth International Temperature Symposium (ITS-10) “Progress with the redefined kelvin”. Oral presentations on Real-K were given at the virtual Euramet TC-T meeting in 2020 and in Apr 2022. On 19th April 2023 an international workshop on “Realising the redefined kelvin: Turning the *MeP*-K into reality”, was hosted by SMU.

Papers: There are currently 19 refereed articles published with at least 18 more awaiting publication.

Stakeholder community: The project stakeholder committee is comprised of 39 members. A wide spectrum of organisations is represented from industry bodies such as the British Cryogenics Council, Accreditation Bodies, Universities, RMOs and NMIs outside Europe, as well as 12 companies.

Impact on industrial and other user communities

Temperature is one of the most measured parameters in both industry and science. As such these developments will have significant impact in bott areas of human activity. ***At low temperatures*** (<25 K) cryogenic equipment manufacturers will welcome the possibility of direct traceability to the redefined kelvin through a simplified calibration route. Contact has been made with companies in Finland and Germany that specialise in the manufacture of cryogenic equipment. ***At high temperatures***, (>1300 K) these developments impact wide spectrum of industries, e.g. materials processing and aerospace. More reliable traceability directly to thermodynamic temperature will be established through known temperature HTFPs, with NMI-like uncertainties available closer to the point of measurement. *In the mid-temperature range*, one early impact would potentially be the commercial exploitation of the mercury (Hg) fixed triple point replacement. End users will, for the first time, have reliable estimates for Type 1 and Type 3 non-uniqueness uncertainties.

Impact on the metrology and scientific communities

Significant impact on the global temperature metrology community is envisaged through step changes in the SI system in approaches to realisation of the kelvin in the NMI/Designated Institute (DI) community, examples are:

- The processes and equipment in place for temperature realisation and dissemination through the *MeP*-K-19, at temperatures >1300 K and <25 K, and mature enough for wide adoption
    - For *T*>1300 K: By the mid-2020s, the current ITS-90 could be supplanted, in several leading NMIs, by direct traceability to thermodynamic temperature through HTFPs.
    - For *T*<25 K: By the mid-2020s replacement of ITS-90 <25 K underway through the primary thermometry methods developed here, leading to more robust traceability and dissemination.
- The life extension research for the ITS-90 will impact the NMI thermometry community worldwide by:
    - The reduction in uncertainties due to scale non-uniqueness effects, enabling all NMIs to improve their realisation of the ITS-90.
    - The identification of a viable replacement for the mercury triple point, ensuring the ITS-90 will be able to continue well into the 2020s.

The NMI thermometry and wider scientific community will benefit from the “facilitating full range primary thermometry” activity. A reliable and comprehensive set of *ab initio* values of key thermophysical properties for thermometric gases (e.g. Ar, Ne, He) are now available. These values will facilitate the use of primary thermometry for traceability, demonstration of which to 300 K is one of the key objectives of the follow-on project Dissemination of the Redefined Kelvin (DireK-T).

Impact on relevant standards

This project will have a profound impact on the whole thermometry community. This will be affected chiefly through the CCT, the global authority on temperature, and the relevant standards body for this research.

Key inputs to the CCT, which will influence its guides and recommendations are:

- Definitive thermodynamic temperatures of new HTFPs, namely Co-C, Pd-C, Ru-C and WC-C
- Recommendations on the realisation and dissemination of thermodynamic temperature >1300 K
- Report on the realisation and dissemination of thermodynamic temperature from ~1 K to 25 K
- Synthesis report on characterisation and reduction of uncertainties due to scale non-uniqueness
- Recommendation report on the replacement the mercury triple point
- Recommendation report of uncertainties for primary thermometry methods, for the next version of the *MeP*-K
- Summary report to CCT-WG-SP (Strategic Planning) of the findings of Real-K

Longer-term economic, social, *and environmental impacts*

Thermometry is the most widely measured physical parameter so any change will have far reaching impacts in all areas of human endeavour. This project will begin a paradigm shift in the practice of thermometry. *From an economic perspective*. This change will first occur at the NMI level, but over time will be established in accredited laboratories. The effect of this will be to reduce the dependency on NMIs, providing traceability at reduced cost to the user. *From a social perspective*. These developments will stimulate new industries, protecting high-value manufacturing employment. *From an environmental perspective.* As practical primary thermometry becomes a reality then *any* industrial process requiring reliable temperature measurement will, through the deployment of such sensing techniques, always be able to run optimally minimising energy use and harmful emissions. Any user requiring long-term reliable thermometry will benefit from the availability of *in-situ* practical primary thermometry having significant *social and environmental impact*.

6 List of publications

A. Peruzzi, *et al*, Survey of Subrange Inconsistency of Long-Stem Standard Platinum Resistance Thermometers *Metrologia* https://doi.org/10.1088/1681-7575/abe8c1

C Gaiser, B Fellmuth, Primary thermometry at 4 K, 14 K, and 25 K applying dielectric-constant gas thermometry *Metrologia* https://doi.org/10.1088/1681-7575/ac0d4a

Bo Gao, *et al* Measurement of thermodynamic temperature between 5 K and 24.5 K with single-pressure refractive-index gas thermometry *Metrologia* https://doi.org/10.1088/1681-7575/ab84ca

D. Madonna Ripa *et al* Refractive index gas thermometry between 13.8 K and 161.4 K *Metrologia* https://doi.org/10.1088/1681-7575/abe249

Changzhao Pan *et al* Acoustic measurement of the triple point of neon T_{Ne} and thermodynamic calibration of a transfer standard for accurate cryogenic thermometry *Metrologia* https://doi.org/10.1088/1681-7575/ac0711

O.M. Hahtela *et al* Coulomb Blockade Thermometry on a Wide Temperature Range *CPEM 2020 Proceedings* https://doi.org/10.1109/CPEM49742.2020.9191726

C. Pan *et al*, Direct comparison of ITS-90 and PLTS-2000 from 0.65 K to 1 K at LNE-CNAM, *Metrologia*, **58** (2021), 025005, https://doi.org/10.1088/1681-7575/abd845

G. Machin *et al* Progress in realising the Redefined Kelvin, SMSI 2021 Conference Proceedings, AMA Service GmbH, ISBN 978-3-9819376-4-0, 2021, p. 29-30 (2021) https://doi.org/10.5162/SMSI2021/PT4

Giovanni Garberoglio *et al* Path-integral calculation of the fourth virial coefficient of helium isotopes *The Journal of Chemical Physics* https://doi.org/10.1063/5.0043446

D. Imbraguglio *et al* Comparison of ITS-90 realizations from 13 K to 273 K between LNE-CNAM and INRIM *Measurement* https://doi.org/10.1016/j.measurement.2020.108225

M. J. Martín *et al* Construction, Characterization and Measurement of Fe–C and Pd–C HTFPs at CEM *International Journal of Thermophysics* https://doi.org/10.1007/s10765-022-02978-2

D. Madonna Ripa *et al* Corrigendum: Refractive index gas thermometry between 13.8 K and 161.4 K *Metrologia* https://doi.org/10.1088/1681-7575/ac2d9e

P. Czachorowski *et al* Second virial coefficients for 4He and 3He from an accurate relativistic interaction potential *Physical Review A* https://arxiv.org/abs/2007.09767

G Machin, The Kelvin Redefinition and Practical Primary Thermometry: Implications for temperature traceability and sensing, Johnson Matthey Technology Review, https://doi.org/10.1595/205651323X16620342873795

J. P. Pekola, Influence of device non-uniformities on the accuracy of Coulomb blockade thermometry, Metrologia, https://doi.org/10.1088/1681-7575/ac79e8

G. Machin *et al* Towards realising the redefined kelvin Measurement https://doi.org/10.1016/j.measurement.2022.111725

A. Kirste *et al*, Comparison of Different Johnson Noise Thermometers From Millikelvin Down to Microkelvin Temperatures, JPS Conference Proceedings, https://doi.org/10.7566/JPSCP.38.011198

R. Veltcheva *et al*, Investigations of Type 3 non-uniqueness in Standard Platinum Resistance Thermometers between 83 K and 353 K, Measurement, https://doi.org/10.1016/j.measurement.2023.112863

C.Gaiser *et al*, 2022 Update for the Differences Between Thermodynamic Temperature and ITS-90 Below 335 K, Journal of Physical and Chemical Reference Data, https://doi.org/10.1063/5.0131026

This list is also available here: Research Publications Repository Link - EURAMET

7 Contact details

Prof. Graham Machin, *FREng, BSc (Hons), DPhil, DSc, CPhys, CEng, FIPEM, FInstMC, FInstP*

NPL Senior Fellow; Head, Temperature Standards

NPL science lead for nuclear decommissioning metrology

Chair of CCT Working Group on non-contact thermometry

Honorary Professor (Physics and Astronomy) University of Birmingham

Visiting Professor (Physics) Universities of Surrey and Strathclyde

Colaborador Honorífico, University of Valladolid, Spain

Thermal and Radiometric Metrology Department

National Physical Laboratory

Hampton Rd | Teddington | Middlesex | UK | TW11 0LW

Tel: +44 20 8943 6742 Mobile: 07718 193 725

Email: graham.machin@npl.co.uk