Publishable Summary 22IEM03 PriSpecTemp
Primary spectrometric thermometry for gases

Overview

Accurate air temperature measurements are critical for climate change monitoring and evidence-based policymaking for early mitigation/adaptation planning. Spectrometric thermometry overcomes several practical challenges posed by contact thermometry in air and industrial processes. However high uncertainties in molecular spectral parameters and adoption to elevated temperatures hinders its use. The project will integrate knowledge and infrastructure across the EU to improve, standardise and implement novel, non-contact methods including primary ro-vibrational spectroscopic thermometry. This will be cross-validated against other non-contact and the ITS-90 standard methods. Ultimately, a new hybrid calibration service with minimal long-term drift will support SI-traceable calibration of classical contact thermometers in gas and air.

Need

The effect of climate change is paramount, exemplified by record drought and flooding on several continents. The latest IPCC report suggests that the EU is the most affected region in the World with almost doubled warming effects. Mitigation and adaption plans have received increased priority on WMO's agenda and by ministers and policymakers. Therefore, informed decision making tailored by clear uncertainty assessment is essential not only for optimising resources but also to understand climate change predictions better. Accurate gas/air temperature measurements are crucial for underpinning these issues.

The limitations of contact thermometers for gas/air measurements are investigated in the EURAMET project Air Temperature Metrology. Low heat transfer of gas/air leads to amplification of self-heating and radiation effects, causing biases up to 200 mK. Spectrometric methods directly measure the thermodynamic temperature of molecules/gases and have been advanced in recent years with respect to both methodology and optical technology, demonstrating accuracy at a few tens of mK level. Currently, the method is mainly limited by the accuracy of spectral line intensities of probing gases (e.g., CO, CO_2, O_2), the lack of SI-traceability and validations against existing primary standards and ITS-90.

Furthermore, gas/air temperature is a critical parameter in many international ISO/DIN/CEN standards and a strategic target quantity of the CIPM CCT committee. It is also needed to optimise industrial production processes where contact thermometry suffers from well-known limitations in real conditions. Knowledge of accurate temperature at 10 mK and below is vital for fundamental metrology fields e.g. pressure and length.

Combining the state-of-the-art *ab initio* calculations, broadband ro-vibrational spectroscopy and recent advances in optical techniques forms a strong basis for an accurate primary gas/air temperature method to provide high accuracy calibration of contact thermometers.

Objectives

The overall objective of the project is to define and develop a new primary traceable spectroscopic gas temperature measurement approach over a temperature range of 200 – 400 K with a target uncertainty of 10 mK.

The specific objectives of the project are:

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or EURAMET. Neither the European Union nor the granting authority can be held responsible for them.

The project has received funding from the European Partnership on Metrology, co-financed from the European Union's Horizon Europe Research and Innovation Programme and by the Participating States.

European Partnership Co-funded by the European Union

METROLOGY PARTNERSHIP EURAMET

1. To perform high accuracy quantum mechanical calculations on essential line parameters (line intensities and their rotational and vibrational dependence) of selected ro-vibrational bands of candidate "sensor" molecules (e.g., CO, CO_2, O_2) for temperatures in the range of 200 K to 400 K.
2. To perform high accuracy measurements of optimal selected molecular transitions (e.g., CO, CO_2, O_2) using high-resolution Fourier-transform spectroscopy (FTS) infrastructure, comb-assisted cavity ring-down spectroscopy (CA-CRDS) such as Doppler Broadening Thermometry (DBT), Cavity Mode Dispersion Spectroscopy (CMDS) and comb-based broadband techniques. To retrieve essential line parameters with high accuracy using refined line shape models (e.g. IUPAC recommended Hartmann-Tran profile). To compare and validate the *ab initio* results from objective 1 using the best experimental values.
3. To develop the methodology of multi-line ro-vibrational spectrometric gas thermometry (RVSGT) and to evaluate its performance under metrologically controlled laboratory conditions in the range of 200 K to 400 K, adopting spectral parameters from objectives 1 and 2. To develop the infrastructure for primary gas temperature measurements by updating existing NMI FTS infrastructure with a target uncertainty of 25 mK, to correspond to 0.1 % accuracy in relative line intensities of the probed molecular absorption lines.
4. To cross-validate spectrometric gas thermometry from objective 3 against other methods for the determination of thermodynamic temperatures (e.g., DBT, refractive index gas thermometry (RIGT), or via ITS-90 referenced SPRTs and $T-T_{90}$) maintained at NMIs. To adapt the NMIs' optimum experimental capacities and proven test scenarios to identify further opportunities to improve the uncertainty to 10 mK.
5. To demonstrate the establishment of an integrated European metrology infrastructure for primary spectrometric thermometry for gases and to facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain, European and international technical committees on thermometry (CCT, EURAMET and other RMOs TCs) and end users (remote sensing, automobile industry and aerospace industry).

Progress beyond the state of the art and results

Development of the primary RVSGT with targeted accuracy of 25 mK ($k = 1$)

Critical evaluation of the methodologies used for broadband spectroscopic thermometry will be made, identifying advantages of each method, and providing full GUM uncertainty estimations. HT line shape models will be adapted to take full advantage of the high SNR ($>10^5$) obtained, to meet the uncertainty target of 25 mK.

Accurate spectral line intensities of CO and CO_2 with 0.1 % uncertainty

Calculations of CO and CO_2 absolute and relative line intensities with accuracies better than 0.1 % and 0.03 %, respectively, will be performed; these go beyond the state-of-the-art accuracy of 0.5 %. This will be achieved by implementing a multi-reference method (MRCI-SD), which includes high order corrections.

Line intensities of CO and CO_2 spectra will be measured in multiple temperature steps with accuracies better than 0.1 % using complementary techniques: FTS, CRDS, CMDS and TDLAS. Spectral line parameters will be retrieved using IUPAC-recommended HT profiles and cross validated among the techniques and with ab initio calculations. The potential of the cutting-edge CMDS technique, demonstrated for the CO molecule, will be applied to CO_2.

Improved accuracy of ambient air spectrometric thermometry based on improved O_2 spectroscopy

Studies of the oxygen (O_2) A-band will be performed to develop the oxygen spectroscopy-based air thermometer researched by VTT into an accurate and traceable technique for ambient air thermometry.

First primary hybrid (thermo-spectroscopic) calibration service bridging spectroscopic and contact thermometry

A facility for hybrid air temperature calibration of classical contact thermometer will be constructed and validated. This facility will allow the calibration of secondary thermometers directly against a RVSGT facility. This will provide an alternative calibration method compared with traditional methods, and give insight about the various influence parameters, potentially leading to lower uncertainties.

First primary RIGT

Based on Refractory Index Gas (RIG) system from the EMPIR project 18SIB04 QuantumPascal, the project will build the first RIG thermometer.

Outcomes and impact

Outcomes for industrial and other user communities

The results from the project will have a wide impact on industry including food industry, steel industry, power plants, aerospace industry, pharmaceutical industry and biotechnology. In these sectors, gas/air temperature measurement is vital to improve production efficiency, reducing energy consumption and product quality control. In the food industry, temperature is regulated under European directives, such as 89/108/EEC, dealing with consumer well-being. In relation to the pharmaceutical industry, there are WHO recommendations regarding the temperature conditions in connection with transport and storage of medicines.

The project's hybrid facility for calibrating secondary thermometers against a primary thermometer will contribute to a reduction of the calibration uncertainty compared with traditional calibrations, thus having a strong impact on many users of secondary thermometers for air/gas temperature measurements.

Outcomes for the metrology and scientific communities

The number of primary techniques for gas temperature measurement are currently very limited, the provided uncertainties are not optimal, and the involved economical and personal investments are huge. The project will provide a novel non-contact primary method in a broad temperature range of 200 K – 400 K with an uncertainty of 25 mK (k=1). Furthermore, this project aims to increase the understanding of the gas temperature concept and improve the quality of calibration procedures. Thus, the outcomes will be influential in all the related metrological and scientific communities including those with air temperature interests.

The multidisciplinary concept of the project will secure the impact on several scientific communities, including academia, research institutes and NMIs. Research outputs will be disseminated via trade journals, peer-reviewed papers, and international conferences.

The impact on NMIs ties in with the reduction of calibration uncertainties of thermometers used for air/gas temperature measurements. The new calibration facility will have significant impact on primary laboratories for other quantities, where the air temperature knowledge is vital for the understanding of the overall uncertainty of their ser-vices, e.g. mass and length calibrations.

The project will develop a new primary method for gas temperature measurements. This is extremely important since, the number of primary techniques for gas temperature are currently very limited, the uncertainties provided are not optimal, and the economical and personal investments involved are huge. Furthermore, the project will increase the understanding of the gas temperature concept and improve the quality of calibrations.

Outcomes for relevant standards

Due to the fundamental nature of this project, outcomes for ISO/EN standards is not expected within the first three years. However, on a longer time scale the outputs of this project will have strong repercussions in ISO/EN standards, because traceable air/gas temperature measurements, is a key quantity in many industry applications and in a lot of societal fields.

Several participants are members of the three most important technical committees for thermal metrology (CIPM CCT, EURAMET TC-T and IMEKO TC12) and chairman or member of relevant working groups of standardisation bodies (DIN, ISO, IEC). The participants will endeavour to ensure that the reference documentation or guidelines of these committees in the future incorporate the most relevant achievements. This includes joint presentations at the working group meetings and, where appropriate, written reports to the committees and working groups.

The EURAMET Project No. 1459 (Air Temperature Metrology) is a research project aiming to write EURAMET guidelines for calibration of thermometers in air. The project will provide beneficial input to these guidelines linking the results from the ATM to spectroscopic measurements.

The consortium is active in several technical expert teams of WMO/CIMO and will make sure that relevant outputs of this project are submitted to the most appropriate working groups of WMO/INCOM/SC-MINT for use as reference documentation and include them as WMO reference guides.

The consortium are active members of the European Metrology Network (EMN) for Climate and Ocean Observations, Energy Gases and Pollution monitoring and will keep these EMNs informed on respective EMN-relevant output from the project e.g., accurate spectral data for remote sensing, improved calibration of gas/air temperature sensors, and new possibilities for gas temperature measurement.

Longer-term economic, social and environmental impacts

Air temperature measurements are the key quantity for determining the effect of Greenhouse gases on the climate. Accurate spectral line parameters for O_2 and CO_2, which considerably improve spectrometric thermometry in air, together with the development of a robust hybrid facility for contact thermometer calibration using spectroscopic techniques will directly affect the meteorology applied to detect climate change. For instance, the calibration services of the National Hydrological and Meteorological Agencies (NHMA) will considerably benefit from the new calibration facility.

The project will result in the improvement of multiple industrial processes due to improved gas temperature measurements. It will contribute to improved industrial competitiveness as a consequence of optimised production processes in industries such as automotive, pharmaceutical and aerospace. In addition, it will contribute to more efficient energy production through optimisation of temperature. The project will have a societal impact by providing information to support in addressing the rising temperature and the impact on environment and climate.

List of publications

-

This list is also available here: https://www.euramet.org/repository/research-publications-repository-link/

Project start date and duration:	01 September 2023, 36 months	
Coordinator: Gang Li, PTB Project website address: not yet available	Tel: 00495315923235	E-mail: gang.li@ptb.de
Internal Beneficiaries: 1. PTB, Germany 2. CEM, Spain 3. DFM, Denmark 4. JV, Norway 5. TUBITAK, Türkiye 6. VTT, Finland	External Beneficiaries: 7. DLR, Germany 8. Iberoptics, Spain 9. RUG, Netherlands 10. SUN, Italy 11. UCM, Spain 12. UH, Finland 13. UMK, Poland	Unfunded Beneficiaries: n/a
Associated Partners: 14. UCL, United Kingdom		