

Publishable Summary for 22IEM04 MQB-Pascal Metrology for quantum-based traceability of the pascal

Overview

Accurate pressure measurements are essential for key applications in climate, medicine, manufacturing, energy, science, safety and quality control. Previous projects demonstrated that quantum-based methods enable faster calibration of pressure sensors and lead to improved uncertainties. However, further work is needed to establish an integrated metrological infrastructure for a SI-traceable quantum-based pascal between 1 Pa to 1 MPa, as no primary standard currently exists that covers the whole range. This project will develop instruments and quantum-based methods and it will evaluate these in terms of practical applications to meet stakeholder needs. The project will aim at disseminating the technology to stakeholders with a minimal loss of performance, to allow for future products and services which are internationally competitive.

Need

Accurate, reliable, and cost-efficient pressure measurements are key for a variety of applications within a broad spectrum of industrial, scientific and regulatory sectors. Examples are altitude determinations to prevent airplane collisions as well as frequent unnecessary flight manoeuvres, the operational safety of power plants, leak prevention in the storage of toxic or nuclear waste, and the assurance of medical sterility. The importance of these measurements was expressed by the Comité international des poids et mesures (CIPM) in the 2017-2027 strategic document of the Consultative Committee for Mass and related quantities (CCM), and by the EURAMET Technical Committees for Mass and related quantities (TC-M) in their guidelines (roadmap).

While current methods rely on realising the pascal, the unit for pressure, through conventional means such as force over area, the revision of the SI-system in May 2019 opened an alternative path to realise the pascal by measuring the refractivity and the temperature of a gas. Such a realisation of the pascal, and other similar quantum-based approaches, do not depend on weights or movable parts, but instead measure the gas properties directly, using density-based methods. This will decrease uncertainties and at the same time will improve the efficiency of calibration chains. While significant efforts within Europe and internationally have proven that quantum-based methods have the capability to supersede conventional methods in certain relevant pressure ranges, there is not yet any realisation that has successfully combined all the advantages of the techniques.

To make full use of the inherent potential of these methods, it is crucial to consolidate and integrate expertise and efforts in Europe, so that quantum-based high-performance instrumentation (i.e. based on Fabry-Perot (FP) refractometry) can be realised, and consequently utilised. This includes improved uncertainties with a pressure-independent term of 2 mPa and a pressure dependent term of 10 ppm (k=2) for the realisation of the Pascal in the 1 Pa to 30 kPa range. Without the existence of standards that can provide these low uncertainties for this pressure range, several independent realisations are needed for comparison and validation purposes. In addition to primary realisations, the density-based methods offer advantages of ease of use, time savings, potential cost savings, compactness, and robustness, making them an excellent choice as pressure sensors or transfer standards. Based on practical experience and the plans of industrial stakeholders, the 1 Pa to 1 MPa range must be covered soon, and this pressure range must be targeted with an expanded uncertainty of 5 mPa + 30 ppm. To ensure acceptance of the novel methods amongst metrology and industry, an inexpensive, safe, and well characterised measuring gas with a high measuring effect is required. Nitrogen is an ideal candidate, and it is already widely used for conventional pressure measurement. Despite its broad use, there is a surprising lack of knowledge particularly for the dielectric and optical properties, and more work is required on this for a broad temperature and frequency range. This way, nitrogen and the corresponding infrastructure can be maintained conveniently which is expected to increase the acceptance of the novel

Report Status: PU – Public, fully open	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.	European Partnership	Co-funded by
Publishable Summary	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.	METROLOGY PARTNERSHIP	EURAMET

Issued: June 2023



methods. However, to promote acceptance of this, all results must be validated, which can be done through ring-type comparisons as well as comparisons with the best available standards. Furthermore, an investigation of the long-term stability is needed to show the extent to which the new quantum-based methods potentially do not require recalibrations.

Objectives

The overall objective of the project is to establish a metrological infrastructure for a traceable quantum-based pascal in the 1 Pa to 1 MPa range via the realisation of instrumentation and dissemination of the technology with minimal loss of performance to stakeholders. The methods will also be evaluated in terms of practical applications.

The specific objectives of the project are:

- 1. To develop high-accuracy primary pressure instruments based on Fabry-Perot (FP) refractometry for traceability to the pascal and covering the 1 Pa to 30 kPa range. The target uncertainty is 2 mPa + 10 ppm (k=2).
- 2. To develop validated quantum-based methods (including FP-based techniques, Rayleigh scattering, and polarising gas thermometry methods) to enable traceability within the 1 Pa to 1 MPa range with a target uncertainty of 5 mPa + 30 ppm (k=2). Applications should include gauge mode measurement, measurement of dynamic pressure and measurements with nitrogen and dry air. The concepts of miniaturisation and transportability should also be investigated.
- 3. To improve the metrological reference data and estimate the relevant uncertainties for the thermodynamic and electrodynamic properties of primarily nitrogen, i.e., density and dielectric virial coefficients, temperature dependent static and dynamic polarisabilities. The target uncertainty of the molar polarisability is less than 10 ppm.
- 4. To verify that the developed instruments utilising the developed quantum-based methods are consistent with their combined uncertainties and with existing primary standards, as well as to assess their long-term stability.
- 5. To demonstrate the establishment of an integrated European metrology infrastructure and to facilitate the take up of the technology and measurement infrastructure developed in the project by the measurement supply chain (EMN Quantum, European initiatives like the quantum flagship), standards developing organisations (CCM WGPV, EURAMET TC-M, ISO TC112) and end users (key stakeholders from science and industry).

Progress beyond the state of the art and results

By developing quantum-based methods for pressure measurement, this project aims to establish not only one, but at least three, fully operational quantum-based primary FP-refractometers. The project will also investigate, and improve upon, quantum-methods in general and investigate their possibility for a multitude of applications e.g. for the measurement of dynamic pressure and gauge mode measurements. Furthermore, theoretical calculations of the relevant properties of nitrogen, as well as verification and comparison against conventional methods, will be carried out. This project builds on the results and conclusion from its predecessor, EMPIR project 18SIB04 QuantumPascal, which successfully demonstrated the potential of quantum-based methods.

Realisation of primary FP-refractometers (Objective 1)

This project aims to improve the performance of FP-cavity-based refractometers, by consolidating efforts and recent progress across Europe. The goal is to demonstrate a confirmed uncertainty of at least 2 mPa + 10 ppm (k=2) in the 1 Pa to 30 kPa range. Furthermore, in an integrated effort, where the participants will collaborate closely, at least three instruments in at least three different countries will be realised. This will effectively establish an infrastructure consisting of several primary FP-based refractometers across Europe. This would be a significant step beyond the current state-of-the-art, given that currently only two fully characterised systems exist in Europe.

Development of quantum-based methods for traceability and practical applications (Objective 2)

To fully utilise the advantage of quantum-based methods beyond their use as potential primary standards, efforts will be put into further investigation and improvement of systems based on Rayleigh scattering, polarised gas thermometry, and non-primary FP-based refractometers. These methods will be developed to



jointly provide traceability in the range from 1 Pa to 1 MPa with a target uncertainty of 5 mPa + 30 ppm (k=2). Furthermore, to bring the technology within reach of stakeholders and industry, these novel methods will be developed and investigated to address important practical applications, such as the measurement of atmospheric pressure (gauge mode), the measurement of gas with unknown refractivity, and dynamic measurements, and the feasibility of realising transportable and miniaturised devices.

Metrological reference data for nitrogen (Objective 3)

While the relevant properties of helium can be calculated with an uncertainty of less than 1 ppm, which was addressed within EMPIR project 18SIB04 QuantumPascal, nitrogen is by far the most used gas by national metrology institutes (NMIs), calibration laboratories and industry. Furthermore, since its refractivity is eight times higher, and it is much easier to work with, it offers significant advantages over helium. Despite this, there is a surprising lack of exact dielectric data for nitrogen. Due to its more complex structure, a combination of highest-level experiments and theoretical *ab-initio* calculations will be used in this project to determine the required values. By providing a complete and validated set of all of the required properties for nitrogen beyond the state-of-the-art, this project aims to enable the use of nitrogen for the targeted quantum-based methods.

Comparisons and stability assessments (Objective 4)

This project will carry out several comparisons between quantum-based methods and conventional transfer standards aimed at providing reliable data to assess the performance and stability of quantum-based systems, and therefore pave the way to the widespread use of these methods and systems. The quantum-based instrumentation will also be subject to an extensive circular comparison, which will be carried out with highly stable conventional standards. By utilising the stability of conventional standards, the goal is to be able to show that the newly developed instruments agree within their claimed uncertainties.

Outcomes and Impact

Outcomes for industrial and other user communities

The primary outcome of the project is to develop quantum-based pressure standards i.e. systems and methods. As the methods offer potential for improved calibrations in terms of performance, speed and cost, the outcomes of the project are expected to be taken up by a wide range of stakeholders that rely on accurate and precise pressure measurement, such as pressure sensor manufacturers. This project also aims to address relevant practical applications, such as measurements of air, measurements in gauge mode, and dynamic measurements (of non-constant pressures). It is expected that this will have a significant impact for industrial end-users.

To foster the uptake of the results, considerable engagement with a multitude of stakeholders will take place throughout the project. The training and hands-on demonstration of the novel methods which are planned within the project aim at promoting early uptake of the technology by stakeholders and end-users e.g. sensor and instrumentation manufacturers, to allow for future competitive products and services.

Outcomes for the metrology and scientific communities

The metrological and scientific communities will be the first to benefit from this project, which will integrate capacity and efforts within Europe to establish an infrastructure of quantum-based methods and realise at least three fully operational FP-based refractometers in at least three different countries. As these instruments have a target uncertainty of 2 mPa + 10 ppm (k=2) in the 1 Pa to 30 kPa range, it will represent a significant improvement in the important realisation of primary pressure standards, particularly at pressures below the typical working range for piston-cylinder systems. To provide traceability up to the 1 MPa range, this establishment will be complemented by the continued development of other quantum-based systems.

The project's outputs will be disseminated to CIPM, CCM, EURAMET TC-M and the EMN-Quantum, as they are the prime repositories of developments related to pressure metrology and quantum-metrology. The active engagement of these key stakeholders will ensure that the outcome will be disseminated worldwide to NMI laboratories and subsequently to any user who needs improved, traceable measurements of pressure in order to increase their commercial capacity or to address specific upcoming scientific or societal challenges.

The improved quantum-based methods in general, have the potential to be taken up by several other scientific and metrology areas, such as density, temperature, length and time.

To promote the uptake of the results of this project by these communities, the consortium will invite them to attend the project workshops.



Outcomes for relevant standards

Currently, no documentary standards exist on this subject, due to the novelty of the quantum-based realisation of the pascal. To maximise the outcomes of the project, the consortium will liaise closely with key metrological bodies, namely CCM Working Group on Pressure and Vacuum (CCM WGPV) and EURAMET TC-M Subcommittee Pressure to ensure that they are kept up to date. The developments and results obtained will be presented at the regular meetings and their feedback will be directly taken into account.

Furthermore, the consortium will inform ISO TC 112 "Vacuum Technology" about the results achieved and will provide reports to this committee, so that they can use these and consider the inclusion of quantum-based methods in a future revision of existing standards (e.g. ISO 3567: 2011 and ISO 27893: 2011). Furthermore, this will initiate the preparatory process for the development of new standards.

Longer-term economic, social, and environmental impacts

A more accurate realisation of the pascal in certain pressure ranges will have impact on a wide range of communities. In addition to improved uncertainties, it indirectly affects quality and safety controls in a multitude of processes and applications. There are a number of companies in Europe that manufacture pressure gauges, vacuum pumps, and process tools, with their products being among the best quality in the world. More accurate pressure standards will help the users to compare different instruments from different manufacturers and to select the most appropriate instrument for their application, which will have a positive economic impact for both manufacturers and end-users. The development of new technologies will also enable manufacturers to produce a completely new generation sensors that are more precise, less expensive and which can potentially self-calibrate. Therefore, the output of this project will lead to higher profit for European companies compared to their competitors.

Precise differential pressure assessments are important in many processes e.g., for climate control in critical environments. As an additional pressure difference of 1 Pa in a medium-sized cleanroom requires around 3000 kWh of additional energy per year, more accurate differential pressure measurements can lead to considerable energy-savings. The improved means to monitor operational conditions will contribute to safer and more efficient conditions at power plants and critical facilities that handle toxic substances. Furthermore, vacuum and pressure related processes are key to many industrial applications that require clean and well-controlled environments. Better control of vacuum and pressure processes will lead to both increased profit margins and to the reduction of chemical waste. Volume flow and gas composition (via partial pressures) can be determined more precisely, which is important for relevant quality control and billing. In medical applications, especially in early detection, even the smallest changes in the partial pressures of relevant marker molecules are of utmost importance. An example would be a non-invasive COVID test based on exhaled air at the airport.

Project start date and duration:		01 June 2023, 36 months	
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1.PTB, Germany	10. FBK, Italy	16. Iberoptics, Spain	
2.CEM, Spain	11. HSU, Germany	17. Toptica, Germany	
3. CMI, Czechia	12. UCM, Spain	18. WIKA, Germany	
4. CNAM, France	13. UM, Slovenia		
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