# SPECTRA

Scientific Validation of the Measurement Method

# Publication in Applied Spectroscopy: Scientific Validation of SPECTRA Measurement Method

## SPECTRA in the spotlight in Applied Spectroscopy: innovation in odorant measurement thanks to entrepreneurial talent and scientific collaboration with the university.

**The detection of odorants in methane gas distribution networks is an absolute necessity**. The minimum quantity of odorant (a chemical compound generally unpleasant to smell) must guarantee certainty of olfactory detection but also minimum pollution of the atmosphere both in accidental leaks and during combustion. **AUTOMA srl** is a company located in the Marche region, Italy, that has been **dealing for years with problems relating to the distribution of methane gas**. **SPECTRA** solution is the result of **AUTOMA**'s desire to propose an **odorant measuring instrument as an alternative to the gascromatographs** traditionally used to measure odorant in natural gas.

Although gas chromatographic measurement is precise and accurate, it is expensive both in terms of purchase and maintenance: maintenance requires the involvement of specialised personnel and routine operation also requires the use of expensive materials. At the moment, gaschromatographs are measuring instruments that do not allow continuous monitoring of methane gas lines because they consist of *in situ* sampling to be analysed in remote laboratories. Discontinuous monitoring over time, besides being inconvenient, is not very effective in detecting malfunctions and unusual situations that need to be immediately corrected. To overcome these difficulties and innovate the system for measuring odorants in gas distribution lines, **AUTOMA** has designed **SPECTRA**.

**SPECTRA**, on the other hand, which is **based on UV-Visible absorption spectroscopy**, is designed for on-site installation and fully automatic operation without human supervision, allowing **continuous and timely monitoring of abnormal events** occurring in the distribution network. In short, **SPECTRA** provides constant routine analysis and real-time detection of any event that deviates from it. These objectives were achieved by basing the **SPECTRA** instrument not on the separation of the components of a gaseous mixture as happens in gas chromatography, but on the principle of the different interaction of gaseous components with UV-Visible light, called UV-Visible absorption spectroscopy.

Since 2014, **AUTOMA** has been testing **SPECTRA** on gas distribution lines with very positive results in terms of both detection and measurement. In parallel with experimentation in the field, **AUTOMA**, in collaboration with the University of Camerino and CNR-ICCOM in Florence, aimed at and obtained the publication of an article describing the measurement method behind the **SPECTRA** solution in the prestigious journal **Applied Spectroscopy**.

***Applied Spectroscopy: the scientific journal on spectroscopy***

**Applied Spectroscopy** is one of the world's leading scientific journals highly specialised in spectroscopy and its many applications**.** It has been chosen by **AUTOMA** because it is a niche journal that only publishes high quality articles through a peer-review procedure, that means that the article is reviewed by external, anonymous experts who initiate a scientific debate between the parties before giving a favourable opinion on publication. It is therefore a source of pride to say that the publication in **Applied Spectroscopy** confirms the scientific rigour of the study and the originality and innovation of **SPECTRA**'s measurements compared to those found in the scientific literature.

***The article: Odorant Monitoring in Natural Gas Pipelines Using Ultraviolet–Visible Spectroscopy***

The scientific article "*Odorant Monitoring in Natural Gas Pipelines Using Ultraviolet–Visible Spectroscopy*" was written thanks to the collaboration of **AUTOMA** with various experts in the sector: **Dr. Rossana Galassi** (University of Camerino), **Dr. Christian Contini** (Automa), **Engineer Matteo Pucci** (Automa), **Dr. Ennio Gambi** (Polytechnic University of the Marche) and **Dr. Gabriele Manca** (Institute of Chemistry of Organometallic Compounds, Florence) and is composed of four main sections:

- Introduction
- Spectroscopic analysis
- Computational analysis
- Experimental section

The introduction describes the **state of the art of odourant concentration measurement in natural gas**. An overview is given of the most common odorants and their importance in preventing explosions caused by gas leaks. A comparison of the main measurement techniques is also presented, with a focus on their desirable and undesirable characteristics. Finally, the theory behind spectroscopy is explained, with particular focus on UV and visible gas phase spectroscopy

In the section on spectroscopic analysis, **the spectra are presented**, meaning the signals logged by **SPECTRA** directly in the natural gas distribution lines; the UV-Visible spectra of the two most common odorants, THT and TBM (tetrahydrothiophene, THT, tetrabutylmercaptan, TBM) are shown for the first time in the scientific literature. It is also shown that light hydrocarbons (mainly methane and ethane) do not interfere with the measurement of odorants, irrespective of their concentration.

In the third part of the paper, concerning the computational analysis of the energy levels of the two odorants, **the correspondence between the experimentally detected signals and the signals obtained mathematically from the theory of molecular orbitals is demonstrated**. The simulation of the orbitals and energy levels of the two odorants has thus made it possible to assign each UV signal to a specific energy transition within the molecule, and this has made it possible to understand the nature of each absorption characteristic of the two substances.

Finally, in the experimental section it is shown that the two odorants - THT and TBM - respect the **Lambert-Beer law** - a fundamental law of spectroscopy - even within a complex matrix such as natural gas. In this section, the observable variations in the spectra of odorised natural gas over the long term are also presented, highlighting specific cases and occasional events. In the present study, the characteristic signals of specific substances that were unexpected in the gas matrix were also recognised and assigned, laying the foundations for their future quantitative measurement, such as dimethyl sulphide (a compound similar to the odorants examined in this study) and aromatic hydrocarbons (highly toxic and unexpected substances in gas mixtures such as benzene, toluene and xylene).

***Conclusions***

**SPECTRA** solution is based on a scientifically rigorous measurement method, and odorant concentration measurements are totally independent of the variability of the concentration of the hydrocarbons that make up almost all natural gas and that these absorptions are due to the specific molecular structure of the odorants. In addition, the method can also be effectively applied to the measurement of other sulphur compounds and aromatic hydrocarbons.

The article is available at the following permanent link: https://doi.org/10.1177/0003702820960737.

This result represents the first scientific acknowledgement of the validity of the **SPECTRA** measuring system in the field of natural gas odorant measurement and joins many other successes that over the years have rewarded the continuous research of **AUTOMA.**