

## SHORT COMMUNICATION

## Effect of gas cell pressure in FTIR analysis of fire effluents

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## SUMMARY

The analysis of fire effluents using Fourier Transform Infrared Spectroscopy (FTIR) is increasing in the field of fire science. This technique is very powerful and may be very selective and precise if the FTIR instrument is properly calibrated. However, results are sensitive to instrumental parameters, including especially pressure effects on the contents in the measurement cell. This communication presents experimental and numerical evaluation of pressure effects in FTIR analysis, and an evaluation of the feasibility and limitation of pressure corrections. The work performed concerns experimental measurements on pressure influence with four different gases, at different levels of concentration, and for one of the gases with different equipment from two laboratories. Some of these results are compared with theoretical models obtained from HITRAN database. Finally, this communication proposes limitations to the range of validity of correction if the actual pressure and the pressure for calibration differ, and suggests a tolerance of  $\pm 10$  Torr on pressure variation for application of the method. Copyright © 2014 John Wiley & Sons, Ltd.

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## 1. INTRODUCTION AND BACKGROUND

The analysis of fire effluents is a challenge, as smoke is composed of many compounds, and the analysis is generally very sensitive to sampling conditions. The thermodynamical properties of smoke may affect the gas composition in an important manner [1, 2]. Fourier Transform Infrared Spectroscopy (FTIR) was introduced in fire gas analysis after several studies in the nineties [3, 4]. The procedure is standardized nowadays as ISO 19702 [5], and this standard is currently under revision [6]. For FTIR technique, an infrared beam does excite the molecules of the sample gas into a gas cell. The gas cell is defined according to its path length, volume and thermodynamic conditions inside, including temperature and pressure. As the system very often uses an extractive sampling with a pump placed after the gas cell, the pressure inside the cell is normally below atmospheric pressure. This communication evaluates the effect on quantitative analysis performed by FTIR of the pressure conditions into the gas cell. Tolerance corrections for pressure regulation are then proposed for such applications.

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## 2. THEORETICAL APPROACH

The effluent from any fire test is typically extracted by a probe, pre-filtered, transported along sampling tubing and filtered again. The gas flows continuously through a FTIR gas cell. All these steps involved in gas transportation, from the sample taken in the test apparatus to the FTIR spectrometer, have a significant effect on the final analysis result.

The FTIR gas cell has a constant volume, typically between 200 and 2000 mL. A beam of Infra Red (IR) radiation of path length,  $L$ , is crossing the cell.

As with conventional gas phase IR analyzers, the FTIR analysis is based upon the selective absorption of IR radiation by different chemical compounds of a sample into the gas cell. A specific given gas will absorb particular ‘bands’ of wavelengths depending mainly on its molecular structure, giving the basis for compound identification. Quantification of compounds identified in this way is based on the degree of absorbance of IR radiation over one or several of these bands of wavelengths. The FTIR method differs from conventional IR spectroscopy in the way to resolve absorption bands for specific compounds. In practical terms, FTIR analyses can be achieved over a period of a few seconds for a lot of gas compounds simultaneously (unlike NDIR) and is also capable of providing a quasi-continuous analysis of fire effluent like NDIR.

For quantification of a compound, the spectral radiative intensity  $I_\lambda$  (rather than absorbance) of the wavelength band corresponding to the compound is assumed to be related to the background spectral radiative intensity (i.e. the spectral radiative intensity with no absorbing sample present)  $I_{0,\lambda}$ . The relation between absorption coefficient and transmittance is given by Beer–Lambert law, as stated in Eqn. 1, where  $\kappa_\lambda$  is the ‘absorption coefficient’ of the gas in the cell at the wavelength  $\lambda$ . This equation allows determining the concentration according to Eqn. 2.  $\sigma_{\lambda,S}$  is the cross section of the studied species at the given wavelength  $\lambda$ ,  $C_S$  is the molar concentration of the species and  $M_S$  is its molar mass.

$$\frac{I_\lambda}{I_{0,\lambda}} = e^{-\kappa_\lambda L} \quad (1)$$

$$\kappa_\lambda = \sigma_{\lambda,S} \cdot C_S \cdot M_S \quad (2)$$

In practice, due to interfering species through absorption over same wavelengths as the required species, Eqn. 2 can be stated more generally as proposed in Eqn. 3 to include these interfering species.

$$\kappa_\lambda = \sum_S \sigma_{\lambda,S} \cdot C_S \cdot M_S \quad (3)$$

The absorption coefficient  $\kappa_\lambda$  is measured and the specific absorption area of the species  $\sigma_{\lambda,S}$  is obtained indirectly by separate calibration. This calibration is achieved by integration over a complete region of the spectra. Different calibration methods may be used, such as *Classical Least Squares* (CLS) for example, to model the answer of a dataset of experimental spectrum covering a given range of concentration. The precision of the final analysis depends on the spectral resolution used. This parameter has to be fixed during calibration step and re-used at the same during tests. With conventional spectral analysis methods, the determination is easily achieved when no interferences are observed between absorbing bands produced by the gas mixture analyzed. Nevertheless, it turns very difficult to quantify concentrations when some overlapping of the bands does exist. With calibration techniques associated with FTIR, it is possible to resolve that issue, by knowing the concentration of one interfering component in another spectral region and making subtractions. These interference cross-corrections are done by a matrix calculation. Care has to be taken on the interpretation of results: if an unexpected species (not included into the calibration spectrum datasets) appears in the sample, cross-correction

assumed in the calibration phase (in number, nature, etc) will produce an error. The amount of gas present in the gas cell is linked with total pressure, volume and temperature within the cell. Eqn. 4 provides the relation assuming the gases to be 'perfect', with  $R$  as the perfect gases constant and  $x_s$  the molar fraction of each species present in the gas cell.

$$\frac{PV}{T} = R \sum x_s \quad (4)$$

Eqn. 4 allows interpreting the theoretical answer of the analytical system under various conditions of pressure and temperature, and these two parameters have to be known, in addition to the volume of the gas cell and path length to properly resolve each FTIR spectrum.

It is therefore essential to have identical conditions for all these parameters between calibration and measurement, especially because such analyzers are calibrated on a non-frequent period, often more than annually. Examples of calibration conditions are presented in references [7] and [8]. Path length is given by the construction of the gas cell and is constant. The temperature of the gas cell is supposed identical between calibration and experiment steps. Indeed it is regulated in most FTIR systems by heated elements (sampling line and gas cell). The temperature of the gas entering into the gas cell and the sampling flow rate are therefore supposed identical. In contrast, pressure may significantly change during experiment for various reasons: filter clogging, variation of pressure at the sampling point due to the fire itself, etc. Any drift from calibration conditions leads to erroneous concentration prediction given by the calibration step.

In detail, the number of molecules of interest along the optical path defines the transmitted signal. An absorption coefficient contains the effect of pressure, and in general, the absorption coefficients used in FTIR are based on a particular total pressure. For a constant molar concentration, an absolute pressure increase leads to an increase in the number of molecules along the IR path. The consequence is an increased absorption, and an overestimation of the concentration. Inversely, an absolute pressure reduction gives an underestimation of the predicted concentration. Changes in pressure cause both linear and non-linear effects in gas spectra. Linear effects may be adjusted with corrections as presented hereafter, but pressure changes also influence the shape of the absorbance bands; a lower pressure causes the bands to grow sharper, a higher pressure causes bands to grow broader. To minimize pressure effect, an absorption coefficient may be calculated. It should be noticed that the measurement of this coefficients is subject to some limitations, mostly linked to the detector type used. It includes the 'saturation' of the detector (i.e. signal too strong to be properly resolved) and of the difficulties of measurement of very low transmittances. It is therefore important for the analyst to ensure that the measurements are made only in a restricted range corresponding to the best compromise for the particular analytical system being used. Thus, different spectral regions may have to be used for different concentration ranges.

As the objective of this communication is to test pressure effects on quantitative analysis, different series of experiments have been defined:

- First, the pressure correction efficiency is tested for five different gases, at one level of concentration. As the concentration is fixed and known, pressure is modified in gas cell and influence is directly measured, then corrected. These results allow determining if the correction is efficient depending on the gas.
- Second, the same protocol is applied on two different spectrophotometers, in two different laboratories. These results allow determining if the pressure effect is independent from parameters such as equipment and gas cell size.
- Third, different levels of concentration are tested for the same gas, before and after correction. These results allow determining if the pressure effect is independent from concentration.
- Fourth, results are compared for one gas and one concentration level with spectra generated from theory, to consider if pressure broadening effects may explain the pressure effects.

### 3. EFFECT OF PRESSURE ON MEASUREMENT

#### 3.1. Experimental approach

**3.1.1. Experimental setup.** This set of experiments has been performed at LNE laboratories, in Paris, France. The FTIR analyzer used by LNE is a Nicolet MAGNA550 type, equipped with a MCT-A detector and a KBr beam splitter. Resolution is  $0.5\text{ cm}^{-1}$  between  $650\text{ cm}^{-1}$  and  $4000\text{ cm}^{-1}$  and apodization is Hepp–Gentzel. The FTIR analyzer is previously calibrated for each gas of interest using reference gas cylinders and CLS (Classical Least Squares) technique. At least 10 points of calibration have been used for all gases of interest and main interfering species such water and various hydrocarbons. For some gases, several spectral regions are used for quantitative analysis, or to check at non-calibrated interfering species. The bands used for the analysis are detailed in Table I. The conditions for calibration of the gas cell are a pressure of 650 Torr (86 660 Pa) and a temperature of  $180^\circ\text{C}$  (453.15 K). The gas cell is manufactured by Thermo-Nicolet. It has a volume of 2 L and a path length of 10 m. Mirrors are gold-coated and windows are in zinc selenium (ZnSe).

The temperature of the gas cell is calibrated as the average of 12 measurement points in the gas cell, using K-type thermocouples and similar flow conditions. The temperature in the gas cell is constant at better than 1.5 K.

Pressure is measured using a MKS Baratron 122B pressure transducer directly connected to the gas cell using a 20-cm filtered connector. This pressure transducer is annually calibrated against reference standard, with a calibration uncertainty of  $(0.11 + 1.9 \times 10^{-5} p)$  Torr,  $p$  designing the total pressure in Torr.

**3.1.2. Influence of the gas nature.** Various reference cylinders have been used to investigate pressure effects, and to cover a large part of the spectral domain, as stated in Table I. Uncertainty on pressure measurement in end-use conditions is estimated at  $\pm 3$  Torr. Uncertainty on gas analysis is considered as  $\pm 2.5\%$  for clean standard gases, including uncertainty on calibration function and uncertainty on standard concentration.

Each gas is introduced at a given flow rate of few liters per minute, in order to produce a selected total pressure in the gas cell in the range of 500–750 Torr. Measurement is taken when the system is stable in pressure since 2 min. For each gas, a first series of data points is determined by the measured concentration obtained without correction (Raw data). This series allow considering the effect of error from lack of regulation in cell pressure. A second series of data points is calculated by application of pressure correction algorithm included in ‘TQ analyst’ FTIR software package. This algorithm works in two steps: first, it considers the Standard Gas Law to correct the concentration from pressure effects, according to Eqn. 5. This is the linear part of the correction. Second, it uses the CLS calibration curve to correct from non-linearity. This algorithm allows determining if post-corrections are efficient when pressure in the cell is logged during a test. Pressure broadening effects are not considered in this correction.

Table I. Standard concentrations used to investigate pressure effects.

Gas	Short name	Reference concentration ( $\mu\text{L/L}$ )	Uncertainty on standard concentration ( $\mu\text{L/L}$ )	Bands used for quantification and to check interfering species ( $\text{cm}^{-1}$ )
Carbon monoxide	CO	1044.0	20.9	2033.09–2026.82
Carbon dioxide	CO <sub>2</sub>	5040.0	100.8	3664.57–3660.95 938.70–934.10
Methane	CH <sub>4</sub>	634.0	12.7	2870.52–2891.01
Sulfur dioxide	SO <sub>2</sub>	1001.4	2.0	2505.08–2497.58 1333.53–1335.95 1164.55–1162.14
Nitrogen monoxide	NO	105.0	2.1	1930.64–1928.23

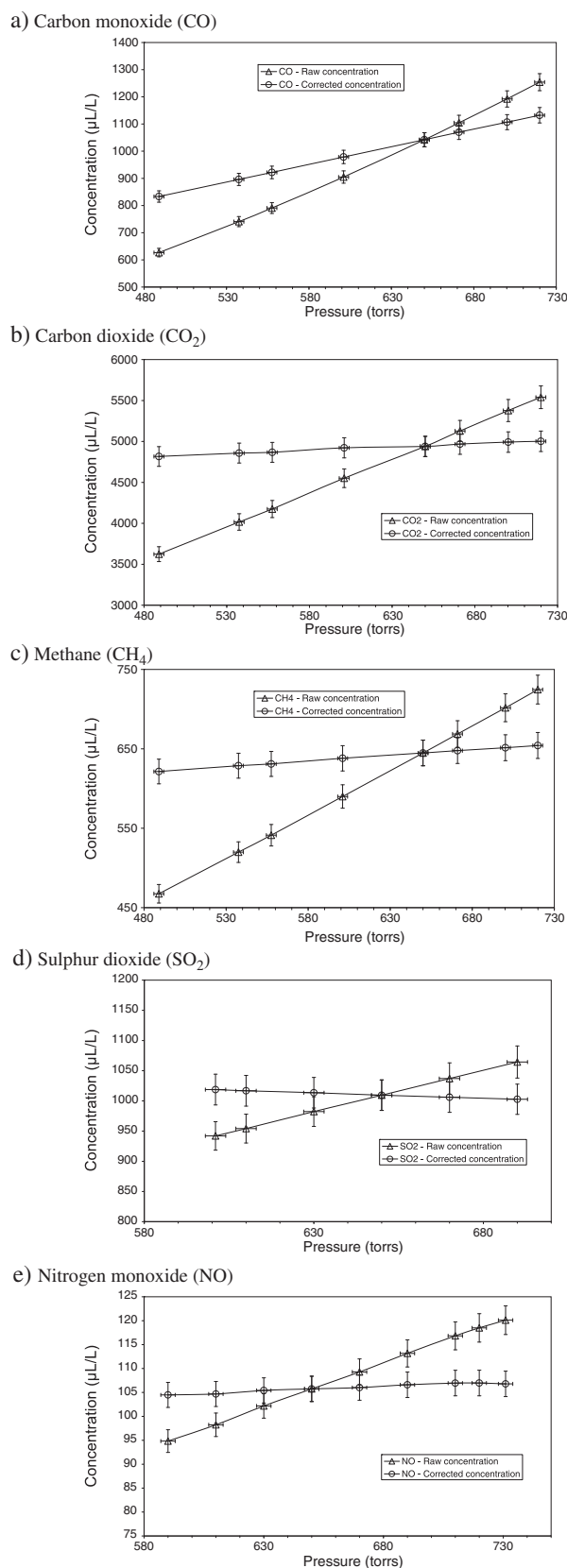


Figure 1. Experimental results—effect of pressure vs. gas nature; a) carbon monoxide (CO); b) carbon dioxide (CO<sub>2</sub>); c) methane (CH<sub>4</sub>); d) sulphur dioxide (SO<sub>2</sub>); e) nitrogen monoxide (NO).

Table II. Pressure effects—results before correction.

Gas	Ref, theory ( $\mu\text{L/L}$ )	Ref, measured ( $\mu\text{L/L}$ )	Pressure effect (before correction)		Effect of pressure variation ( $\mu\text{L/L}$ ) (before correction)			
			( $\mu\text{L/L}$ )/Torr	Relative%	For 10 Torr	For 20 Torr	For 50 Torr	For 100 Torr
CO	1044.0	1042.1	2.72	0.3%	27.2	54.3	135.8	271.7
CO <sub>2</sub>	5040.0	4939.2	8.30	0.2%	83.0	166.0	415.0	830.1
CH <sub>4</sub>	634.0	644.8	1.11	0.2%	11.1	22.3	55.7	111.3
SO <sub>2</sub>	1001.4	1009.4	1.38	0.1%	13.8	27.5	68.8	137.6
NO	105.0	105.7	0.18	0.2%	1.8	3.6	9.0	17.9

$$f_{\text{corr}} = f_{\text{measure}} \frac{P_{\text{calibration}}}{P_{\text{measure}}} \quad (5)$$

Results are presented graphically in Figure 1a) to e) for the different gases. All results show a quasi-linear behavior of the measurement results of the instrument in the narrow range of concentration/pressure analyzed. Table II presents results before correction. The effect from variation in the cell pressure is significant and depends on the chemical species. Results highlight the need to consider pressure effects and to continuously measure cell pressure during tests. A variation of  $\pm 10$  Torr in cell pressure induces a variation of  $\pm 2.6$  relative% on CO reading. Table III presents the effect of pressure correction according to standard gas law in a narrow range. The correction is efficient as the concentration effect induced by a pressure variation is generally well compensated for the range of pressure variation studied. The effect is decreased by more than a factor of 2 for CO and even more for other gases. Nevertheless, all effects are not compensated and the compensation is less effective the larger the difference between actual pressure and the pressure for calibration is. This is especially evident for CO, as the correction using the standard gas law seems not to solve all parameters of influence. SO<sub>2</sub> presents furthermore an unusual behavior, where the correction is negative after application of standard gas law. The calibration function, which is not linear for these gases, probably affects the correction.

**3.1.3. Influence of the gas concentration.** The same procedure as described above was applied to carbon monoxide, using two gas concentrations of respective concentrations 119  $\mu\text{L/L}$  and 1000  $\mu\text{L/L}$ . These experiments were performed at SP, Sweden, on a FTIR equipment very similar to that of LNE (see Table IV). A major difference was, however, that the volume of the gas cell was 0.2 L for the SP equipment. Further, different spectral bands were used for quantification. The nominal pump flow rate was 3.5 L.min<sup>-1</sup> at 650 Torr, and the inlet valve of the gas cell was restricted to modify the pressure conditions in gas cell which resulted in a reduced flow rate at lower cell pressures.

Table III. Pressure effects—results after correction according to Standard gas law.

Gas	Ref, theory ( $\mu\text{L/L}$ )	Ref, measured ( $\mu\text{L/L}$ )	Pressure effect (after correction)		Effect of pressure variation ( $\mu\text{L/L}$ ) (after correction)			
			( $\mu\text{L/L}$ )/Torr	Relative%	For 10 Torr	For 20 Torr	For 50 Torr	For 100 Torr
CO	1044.0	1042.1	1.30	0.1%	13.0	25.9	64.8	129.6
CO <sub>2</sub>	5040.0	4939.2	0.80	0.0%	8.0	16.1	40.2	80.4
CH <sub>4</sub>	634.0	644.8	0.14	0.0%	1.4	2.8	7.1	14.2
SO <sub>2</sub>	1001.4	1009.4	-0.18	-0.0%	1.8	3.6	9.0	18.0
NO	105.0	105.7	0.02	0.0%	0.2	0.3	0.8	1.6

Table IV. SP spectrophotometer parameters.

Instrumentation	Specification
Spectrometer parameters	Resolution: $0.5\text{ cm}^{-1}$ Spectral range: $4800\text{ cm}^{-1}$ – $650\text{ cm}^{-1}$ Scans/spectrum: 10 Time/spectrum: 12 s Detector: MCT Apodization: Happ-Genzell Calibration: CLS
Gas cell	Volume: 0.2 L Path length: 2.0 m Temperature: $180\text{ }^{\circ}\text{C}$ Calibration pressure: 650 Torr
Bands used for CO quantification and consideration of interferences ( $\text{cm}^{-1}$ )	2242.57–234.37 (high) 2133.62–2125.89 2113.12–2092.15 2184.47–2164.46
Pump	Sampling flow: 3.5 L/min

As preliminary analysis, results obtained by SP for  $1000\text{ }\mu\text{L/L}$  ( $\pm 2$  relative%) are compared to those obtained by LNE at the  $1044\text{ }\mu\text{L/L}$  level (Figure 1b). These results are presented in Figure 2. A comparison of slopes using ANOVA techniques proves that the results are statistically identical considering uncertainties, even with a 10 times size factor between both cell volumes.

Two series of measurements are then performed by SP at each concentration level, and measurements at an intermediate concentration level at  $500\text{ }\mu\text{L/L}$  are performed by LNE. Results are shown in Figure 3 a) to c). Slopes obtained for linear regression are plotted versus concentration of the standard as Figure 4. The results show that the quality of the correction is strongly influenced by the level of concentration. The pressure effect is reasonably well compensated for CO at  $100\text{ }\mu\text{L/L}$ , but the discrepancy is larger at  $500\text{ }\mu\text{L/L}$  and is increased at  $1000\text{ }\mu\text{L/L}$ . A perfect correction means a slope trend to zero. This is not observed, and the higher is the concentration, the worse is the correction. This may be due to the calibration function, which is not linear in FTIR for most species, including CO.

### 3.2. Numerical approach

To confirm the experimental results, an alternate theoretical method has been used. This method is based on calculation of reference spectra using HITRAN database [9]. HITRAN offers the parameters obtained by experiment and calculation to obtain line-by-line intensity with high

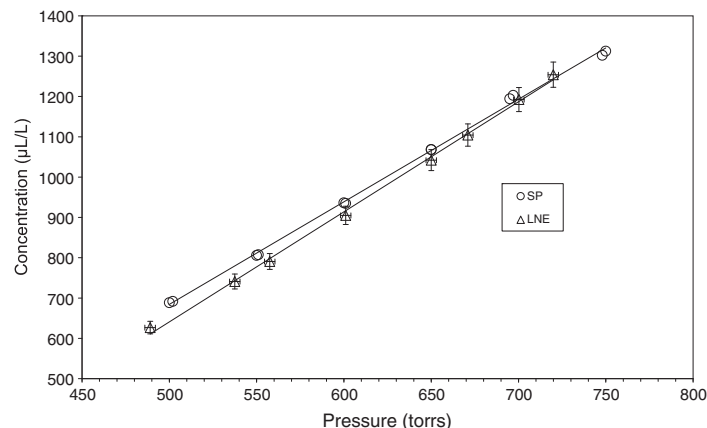


Figure 2. Comparison of pressure influence between laboratories.

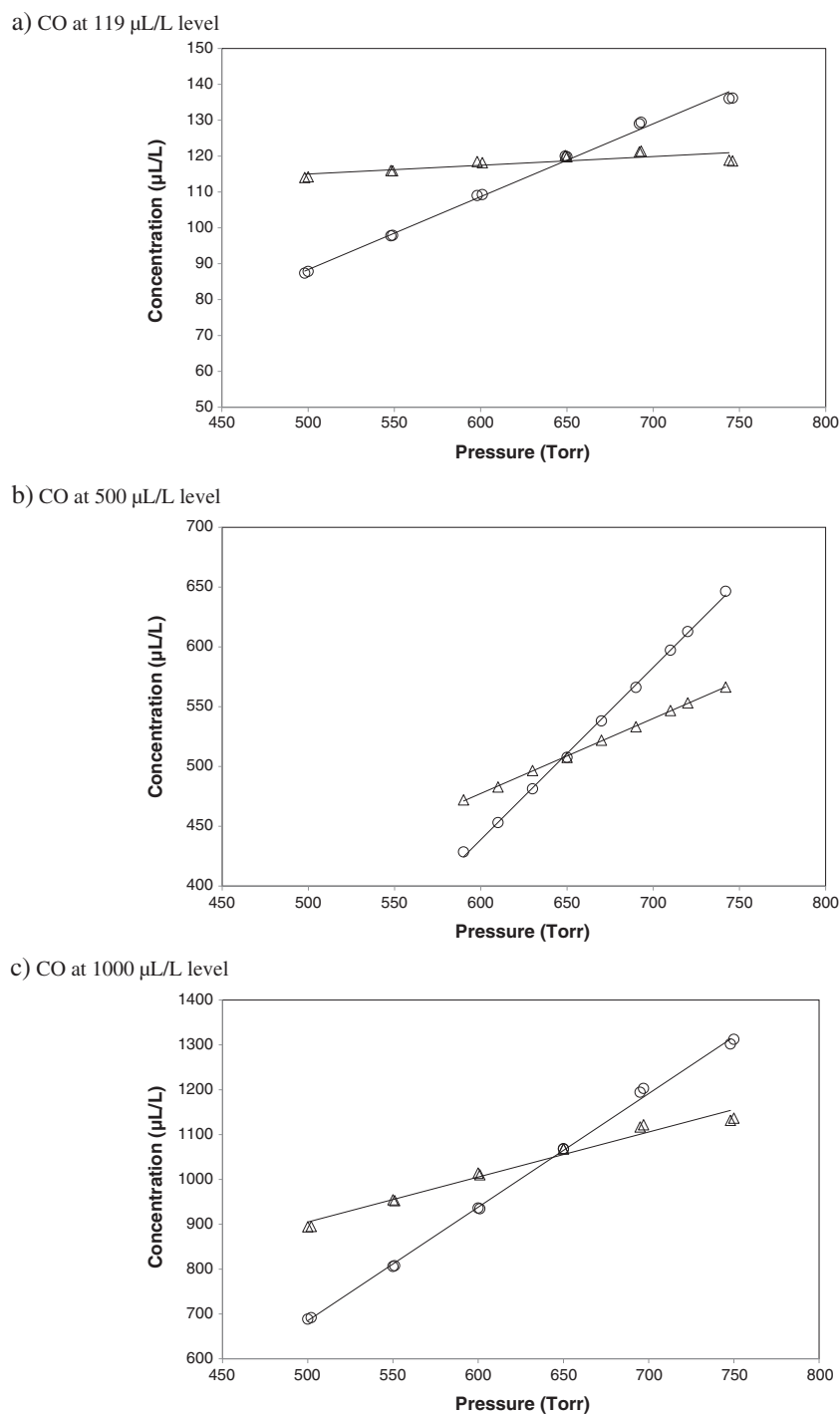


Figure 3. Experimental results—effect of pressure vs. gas concentration.

resolution and can calculate temperature dependent line intensity verified experimentally up to 600 K. Application of HITRAN for fire gases has been proposed by Wakatsuki *et al.* [10]. Pressure broadening effects are considered with this approach.

In this paper, software E-trans ver. 2.4 by SpectraSoft Technology (now Ontar Corporation, USA) program utilizing the HITRAN database was used to calculate spectral absorbance by input of concentration, temperature, resolution and pathlength to compare LNE absorbance data. This calculation has been performed at NRIFD, Japan. The calculation has been performed on methane at



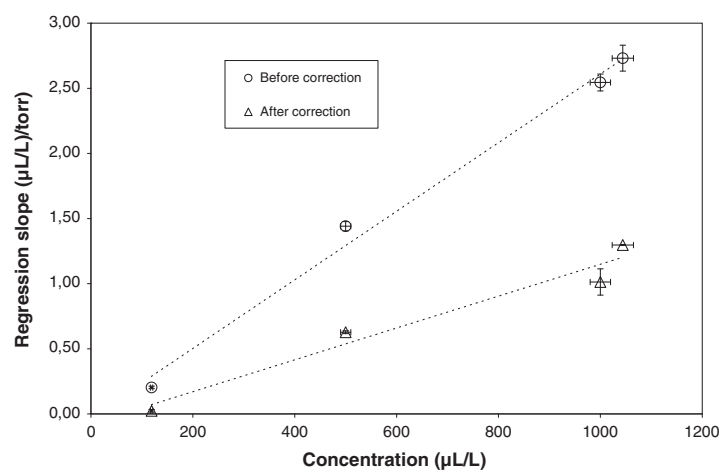


Figure 4. Quality of the correction vs. gas concentration.

Table V. Results of pressure effects—numerical approach.

Parameter	Wavenumber (cm <sup>-1</sup> )	Total pressure (Torr)				
		490	540	600	650	700
Absorbance	3007.447	0.259	0.285	0.317	0.344	0.371
	3014.919	1.04	1.14	1.28	1.38	1.49
	3017.330	1.06	1.18	1.31	1.43	1.55
Absorbance fraction = absorbance (each total pressure) / absorbance (650 Torr)	3007.447	0.752	0.829	0.922	1.00	1.08
	3014.919	0.749	0.827	0.922	1.00	1.08
	3017.330	0.741	0.821	0.917	1.00	1.09
Apparent concentration (μL/L)=(634 × absorbance fraction)	3007.447	478	527	585	634	683
	3014.919	4.77	526	585	634	684
	3017.330	475	524	584	634	683

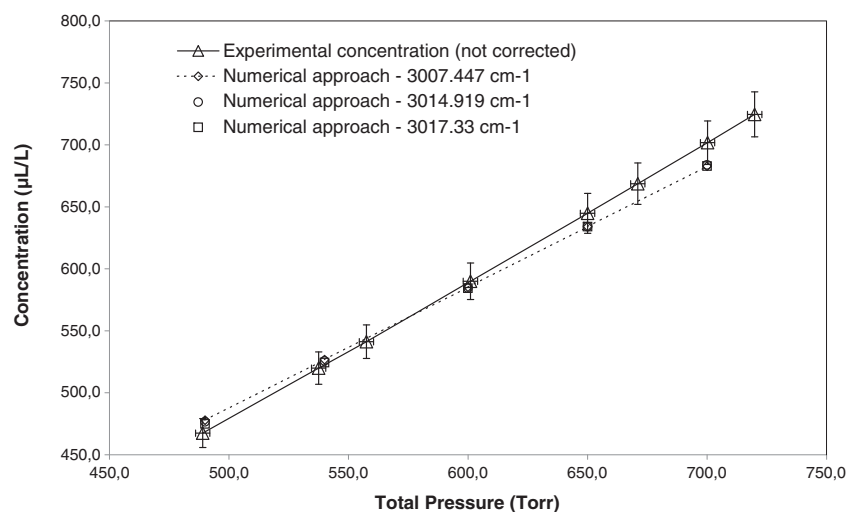


Figure 5. Numerical results and comparison with experimental approach, case of methane.

the same concentration as tested experimentally ( $634 \mu\text{L/L}$ , quantified in the region  $2870.52\text{--}2891.01 \text{ cm}^{-1}$ ) and the analysis was confirmed at several wavelengths outside this region. Results are presented in Table V. Results are plotted and compared with the experimental ones in Figure 5. They show the same trend. The small deviation observed may be due to pressure broadening effects, as they are not considered in the experimental approach.

#### 4. DISCUSSION AND PERSPECTIVES

The results obtained both experimentally, with two FTIR instruments with different gas cells, and numerically, highlight the importance of pressure monitoring, and if possible pressure regulation, in gas cell during FTIR analysis of fire effluents, independently from cell volume. However, a correction based on the Standard gas law and considering the non-linearity of calibration function as in CLS may be insufficient to correct the values in post-treatment, especially for high concentrations and wide ranges of pressure variation. Thus, the recommendation is to maintain a gas cell pressure that deviates not more than 10 Torr from the calibration pressure during the experiment. This corresponds to a maximum error of 2.6% on the concentration (without correction) in the example for CO at  $1044 \mu\text{L/L}$ .

These results will give a technical basis to the revision of ISO 19702 standard, in order to fix tolerances for pressure conditions in the gas cell during experiments.

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