

A LOCAL MODEL AND CALIBRATION SET ENSEMBLE STRATEGY FOR OPEN-PATH FTIR GAS MEASUREMENT WITH VARYING TEMPERATURE

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Abstract

Open-Path Fourier Transform Infrared OP-FTIR spectrometers are commonly used for the measurement of atmospheric pollutants and of gases in industrial processes. Spectral interpretation for the determination of gas concentrations is based on the HITRAN database line-by-line modeling method. This article describes algorithms used to model gas spectra and to determine gas concentration under variable temperatures. Integration of individual rotational lines has been used to reduce the impact of spectrometer functions on the comparison of both measured and synthetic modeled spectra. Carbon monoxide was used as an example. A new algorithm for gas concentration retrieval consisting of two ensemble methods is proposed. The first method uses an ensemble of local models based on linear and non-linear PLS (partial least square) regression algorithms, while the second is an ensemble of a calibration set built for different temperatures. It is possible to combine these methods to decrease the number of regression models in the first ensemble. These individual models are appropriate for specific measurement conditions specified by the ensemble of the calibration set. Model selection is based on comparison of gas spectra with values determined from each local model.

Keywords: ensemble method, FTIR, open path, temperature variation.

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1. Introduction

Optical methods for the measurement of gases in industrial processes and in the atmosphere typically measure absorption using lasers or spectrometers. The ability to measure multiple constituents simultaneously is the main advantage of FTIR spectrometry. FTIR spectrometers generate an interferogram, which is transformed to a spectrum mathematically [1]. Because measurement of the entire spectrum by an FTIR spectrometer is relatively fast, this property is used to increase the signal to noise ratio by measuring and averaging multiple spectra.

FTIR spectrometry permits extractive (out of object) [2] as well as remote and in-situ measurement [3]. Extractive measurements consist of gas sampling from the facility and analysis in a cuvette placed in the spectrometer. Depending on gas concentrations, the measurement path can have different lengths. For low gas concentrations long path multipass cells are used. In the laboratory, reproducible conditions can be provided. Quantitative analysis requires the construction of a calibration model based on the analysis of a specified number of reference samples. This model is then used to estimate the contents of the test samples. In absorption spectroscopy, as well as measuring the spectra of the samples, background spectra are also required in order to determine the spectral characteristics of the radiation source. In extraction spectroscopy, background spectra are determined from cells filled with an inert gas such as nitrogen.

Remote detection is based on measurements taken from a different location than the test samples [4]. Thus, measurement takes place from a distance, and does not interfere with the

object tested. In such measurements, the efforts of the experimenter are focused not on the preparation of samples for calibration and measurement but on creating appropriate algorithms for data analysis. Spectrophotometric absorption measurements in some industrial environments should also take into account the possibility of multiple scattering in the particle phase (e.g., due to dust, water vapor, etc.). Dispersive media can significantly increase the systematic error of measurement of absorption coefficients [5,6].

2. Open path spectroscopy

OP-FTIR spectrometers can be used in active or passive modes. Active open path analysis involves using an external source independent of the spectrometer and the measurement of absorption between these items. In this configuration, determination and correction of the background spectra are problematic [7, 8]. Moreover, interference from water vapor and carbon dioxide is a problem in long-path atmospheric measurements [9]. Optical paths in the atmosphere can have a length of up to several hundred meters.

In passive techniques, there is no additional source of radiation. The thermal radiation emitted by hot gases due to temperature differences between the observed layers is analyzed. Radiometric calibration is an additional operation necessary in the analysis of the spectrometric data. Passive spectrometry is typically 100-1000 times less sensitive than active spectrometry [10]. In addition to determining the concentration, passive methods also allow the determination of the temperature of gases [11].

Spectroradiometric measurements may be carried out under industrial conditions if access can be provided to the interior of the test object. Fiber-optic probes are one solution to these difficulties, for instance in measuring gas concentrations and temperatures inside waste incinerators [12]. An optical system allowing multipass FTIR measurement of gas turbine exhaust is another interesting example [13].

However, CLS (Classical Least Squares) and PLS (Partial Least Squares) are the most frequently applied methods for quantitative analysis of OP-FTIR spectra [14, 15]. The former method minimizes the residue of each wavelength. The spectra are matched by linear addition of the reference spectra; therefore, requirements for the linearity of the absorbance spectra and for knowledge of all components of the mixture are limitations of this method. For open-path measurements, modifications of the original CLS method are proposed. One of these improvements limits the range of solutions. Thus, the predicted concentrations do not exceed the range of true values [16]. Adding physical constraints to the reconstruction of measured quantities improves the quality of solutions [17]. The PLS method, in turn, requires measurement not of the spectra of pure substances but of a set of mixtures with compositions similar to the test samples. Synthetic spectra are often used for calibration instead of reference measurements. If nonlinearity occurs, it can cause additional errors, most frequently in estimation of lower concentration levels. Adding more latent variables in PLS calibration is the simplest method for dealing with slight nonlinearity. Otherwise, if it is possible, weaker absorption bands might be utilised.

As an alternative to chemometric methods, automated, iterative, non-linear least square fitting of spectral windows ($100\text{-}200\text{ cm}^{-1}$) can be applied [18]. In this method, the inverse problem is solved by simulation of the direct problem [19, 20]. For OP-FTIR spectrometry, spectral modeling based on HITRAN and spectrometer ILS (Instrumental Line Shape) is a direct problem [21]. Iterative methods utilize a rather small range of the spectrum, in which no interference from other components occurs. A wide spectral range and low resolution (8 cm^{-1}) was used in one analysis of combustion gases [22], in which calibration was performed by measuring gases at $100\text{ }^{\circ}\text{C}$. This implies that if the temperature changed during measurement, related additional errors would appear. Comparison of CLS and iterative fitting

of spectra suggests the superiority of the latter [23]. The CLS method gives large errors, especially at low concentrations.

3. Modeling of gas spectra

The spectra in this article have been modeled on the basis of HITRAN [24]. Carbon monoxide, one of the main gases produced during the gasification of biomass [25, 26], is considered (Fig. 1). High levels of CO may appear in the observed path in industrial processes like the burning and gasification of biomass. For example, in measurements of atmospheric pollutants, CO values range from 20 to 6400 ppm·m [27]. The CO spectrum shown in [28] gives a value of 10136 ppm·m. High levels of CO also appear in thermogravimetric analyses, ranging up to 5% [29] or even 16%, which for a 0.12 m path length yields a value of 19200 ppm·m [30]. Optical *in situ* methods used in this type of measurement avoid the disadvantages of extractive methods, such as changes in composition during sampling or condensation of gases during cooling. In this article, simulations were performed for very high CO concentrations of up to 50000 ppm·m. Such values are possible only in the biomass gasification process. Such high concentrations permit the verification of modeled nonlinear relationships between absorbance and concentration.

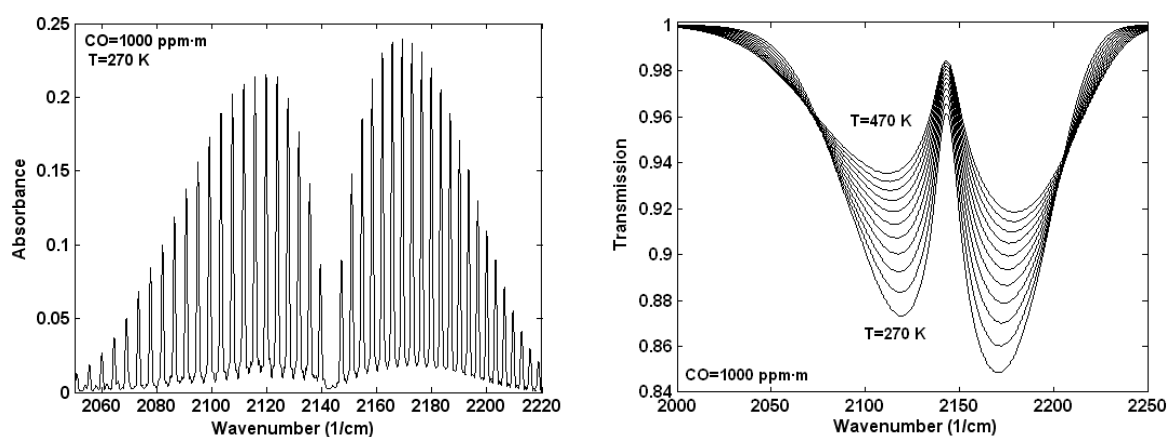


Fig. 1. CO spectrum, 1 cm⁻¹ resolution, triangular apodisation (left); temperature-induced CO transmissivity changes, 5 cm⁻¹ resolution, triangular apodisation (right).

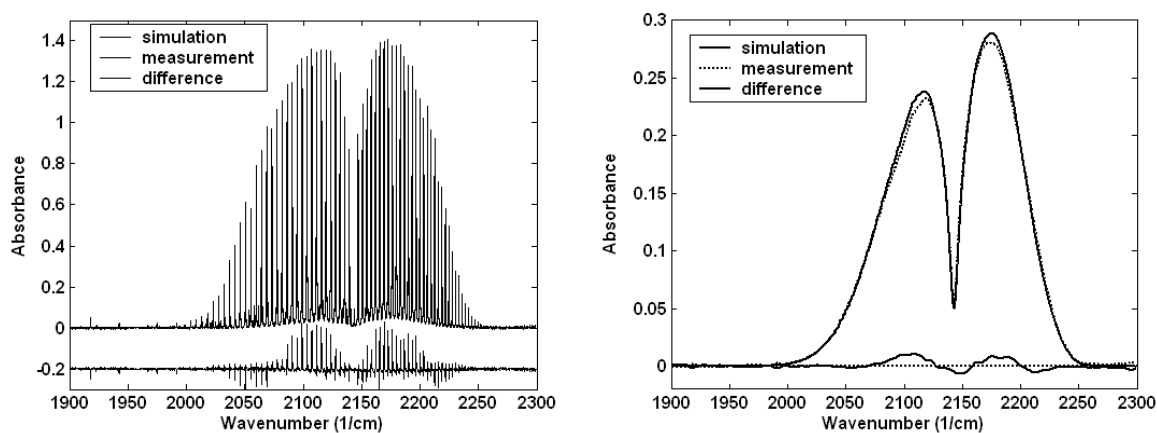


Fig. 2. Comparison of simulated and experimental spectra [28]: 0.25 cm⁻¹ resolution, triangular apodisation (left); 5 cm⁻¹ resolution and Gaussian apodisation (right).

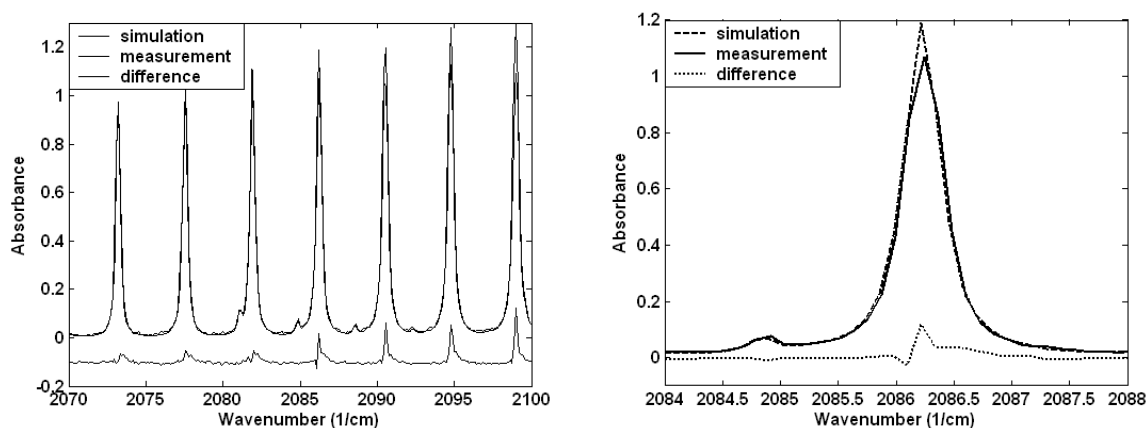


Fig. 3. Comparison of rotational lines between measured [28] and simulated CO spectra for 0.25 cm^{-1} resolution and triangular apodisation.

In Figures 2 and 3, the measured [28] and modeled spectra are compared. The differences confirm the correctness of the spectral model. A similar approach using HITRAN and ILS was also confirmed experimentally at temperatures of up to $1100 \text{ }^\circ\text{C}$ [31].

Appropriate ILS modeling is the main problem in the generation of OP-FTIR synthetic spectra. Errors due to a lack of knowledge about ILS during synthetic calibration have been considered in detail in the literature [32]. In the simplest approximation, ILS is a Fourier transform of apodisation functions [33], also called windows [34]. CO retrieval is very sensitive to instrument field-of-view, which influences the ILS instrumental line shape of FTIR spectrometers [27]. The synthetic calibration method belongs to the inverse problem group [35, 36]. Neural networks used for CO gas retrieval served as calibration models, but errors of up to 50% occurred. The authors suggested that instrumental effects (ILS) in the model caused this large error [37]. The integration of absorption in the specified range solves this difficulty; the area of a spectral line, which is not influenced by ILS, is analyzed instead of its shape. In calculation, the integrated absorption of individual rotational lines of finite extent at lower resolutions should be considered. However, if the integration width is greater than 3 cm^{-1} , the error resulting from the ILS width is less than 1% [38]. Figures 4 and 5 show the ranges of the spectrum for which absorption was integrated. The individual ranges correspond to the CO rotational lines, similarly as in [38].

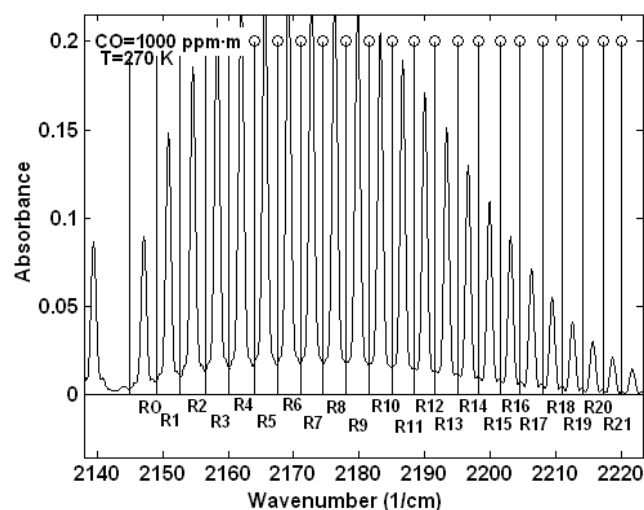


Fig. 4. Definition of areas for each rotational line (R-branch).

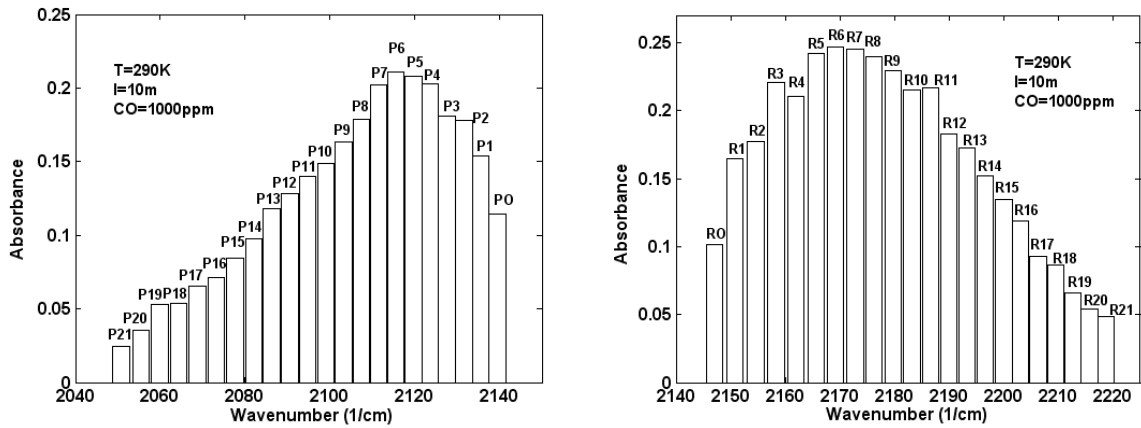


Fig. 5. Integrated CO rotational lines (P-branch and R-branch).

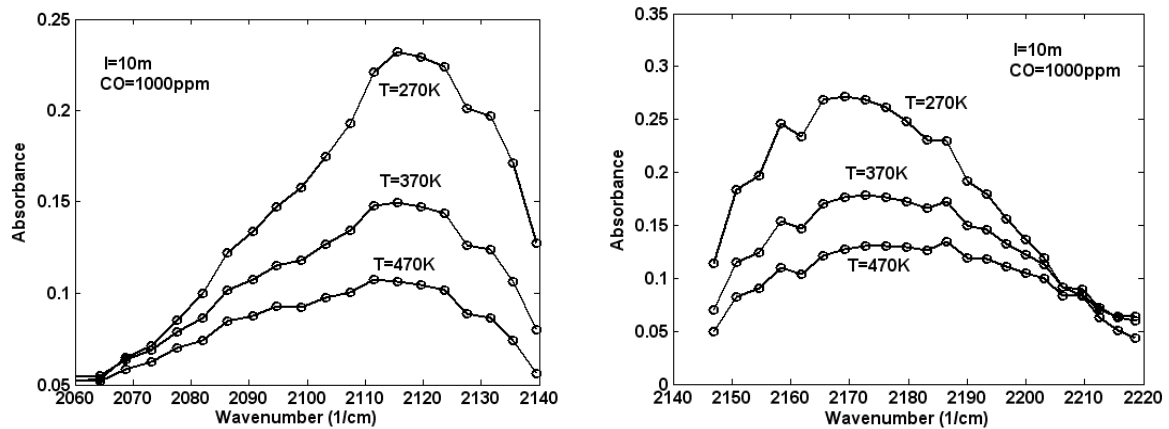


Fig. 6. Influence of temperature on integrated rotational lines (P-branch and R-branch).

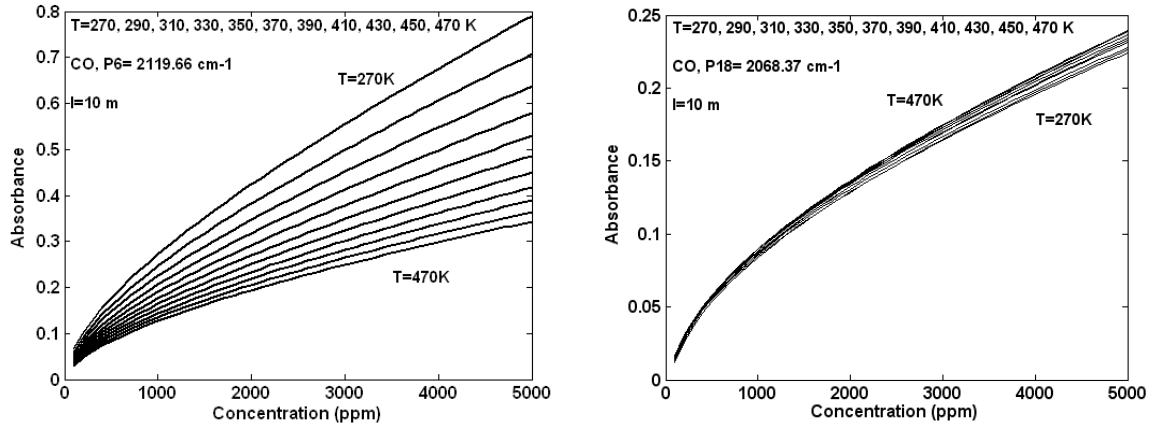


Fig. 7. Influence of temperature on the relationship between absorbance and CO concentration: integrated lines P6, 2119.66 cm^{-1} (left) and P18, 2068.37 cm^{-1} (right).

4. Algorithm for the determination of gas concentrations based on integrated spectral lines.

Changes in measurement conditions can cause significant errors in prediction using models built for other conditions. Difficulty with temperature variations in the open path occur in both industrial and atmospheric measurements. Degraded predictive performance of calibration models in which the temperatures of calibration and prediction differ is a known

problem [39, 40]. Quantitative interpretation of spectra at varying temperatures is difficult [41]. Mathematical modeling of spectra enables assessment of the impact of additional influences on the calibration model, whereas simulation allows determination of properties of the model that cannot be examined directly. This is an important part of the cognitive process in metrology [42]. As depicted in Figures 6 and 7, temperature change influence on the spectrum of carbon monoxide is significant. For very precise measurements, even changes of temperature below 1 °C are noticeable [43]. There are two types of situation: those with known temperatures and those in which the temperature is unknown [44]. Using some spectroscopic techniques, it is possible to measure temperature and include it as a secondary variable [45]. However, in some cases, such as atmospheric remote sensing, direct temperature measurement is not possible.

The problem of temperature changes in CLS calibration is simplified by using reference spectra for average temperatures. For measurement of the products of biomass pyrolysis, a reference spectrum at 400 K has been used [25]. If the actual temperature was 500 K, the CLS method based on this reference spectrum at 400 K gives an error of 30%. In some cases, such high values are acceptable [25]. A calibration set was prepared using the HITRAN database and spectrometer ILS modeling. A similar method was applied for atmospheric gas measurement, and a CLS regression method was also used as a calibration model for CO measurement, with a spectral range of 2020-2265 cm^{-1} [46]. The method of gas determination proposed in this article creates a calibration model using spectra calculated with the HITRAN database and integrated in specific bands (Figs. 4 and 5). Spectra prepared in this way can be used to build a PLS calibration model. In practical gas measurements of the biomass gasification process carried out by the author, significant CO concentrations were present [26]. Due to this, the relationship between absorbance and concentration is nonlinear. Linearity is obeyed for weak absorbances above 0.5 [47]. Nonlinearity typically occurs when absorbance exceeds a value of 1.0. If the measurements are carried out over a wide range of gas concentrations, the calibration set can be divided into segments for which separate PLS models are built [48]. In this article, instead of separate models for the different areas of concentration, we propose the use of the PLS method and its nonlinear version, Radial Basis Functions-Partial Least Squares (RBF-PLS) [49]. It is worth to consider other nonlinear methods e.g. SVM and robustness of such model when a noise component can be induced by spectra measurements of various accuracy [50]. When the spectra of the selected quantities are measured some other indicators of gas presence can be considered which do not always require intense computing [51].

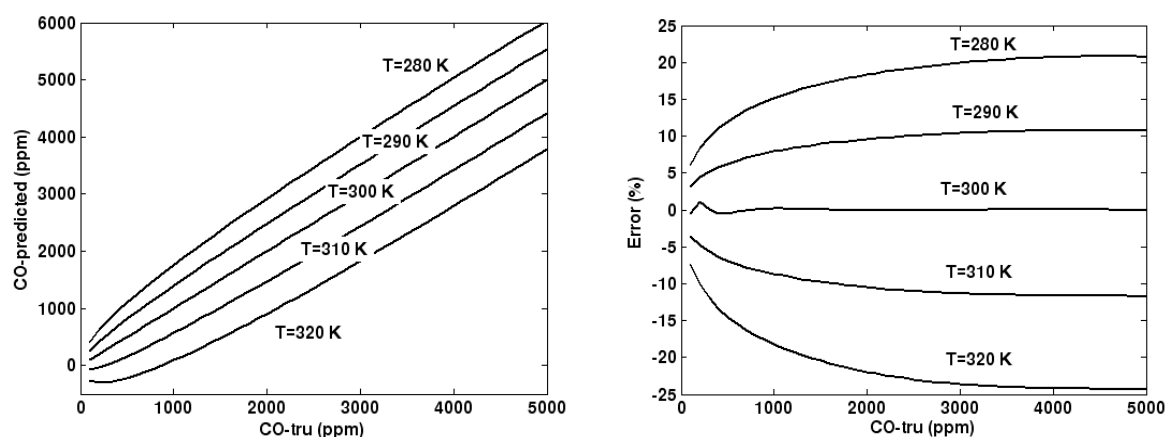


Fig. 8. The effect of temperature on the PLS model for 300 K.

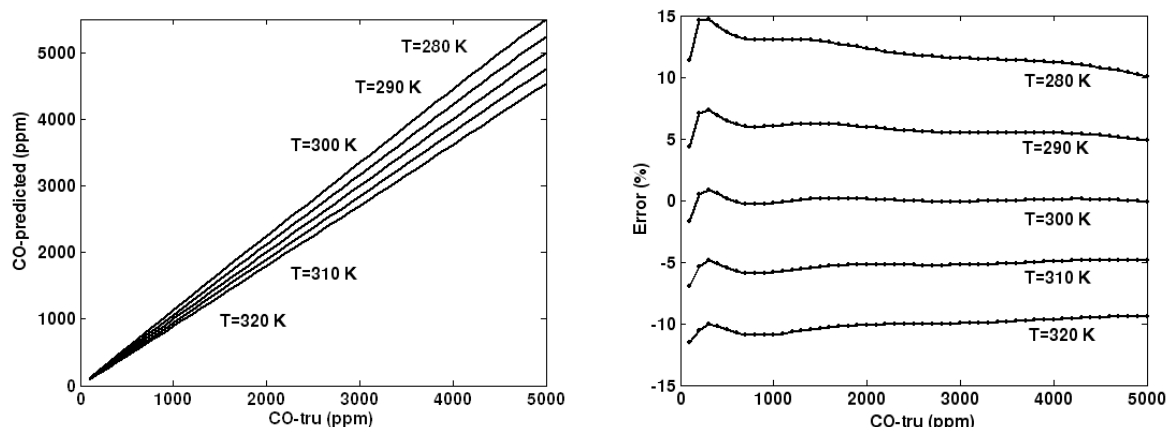


Fig. 9. The effect of temperature on the PLS-RBF model for 300 K.

Both PLS (Fig. 8) and PLS-RBF (Fig. 9) models built for temperatures other than that measured yield significant errors. In cases where robust regression is needed, ensemble methods can be used, in particular the recently proposed selection-based strategy (SBS) [52]. There are many different approaches to ensemble regression [53]. SBS is based on selection of the best available estimation methods for the current prediction. In the original version, a classifier selecting the best estimation was used. For open-path gas measurement on the basis of simulations, spectra are created that are suitable for local models (RBF-PLS) and adequate for specific temperature ranges. The measured spectrum is introduced into individual local models. On the basis of the resulting predictions, the direct models calculate spectra for the local temperature. Based on the difference between the measured and calculated spectra (Fig. 11), the local model with the smallest difference is selected.

Each local model is created for a specific range of temperatures (Fig. 10). It can be based on various regression models. For a linear relationship between absorbance and concentration, the classic PLS method is adequate, while the PLS-RBF method is more suitable for pronounced nonlinearity.

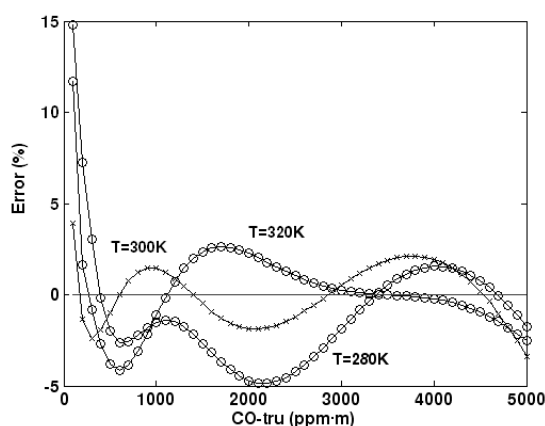


Fig. 10. Model errors for temperatures inside (300 K) and outside (280 K, 320 K) the calibration range.

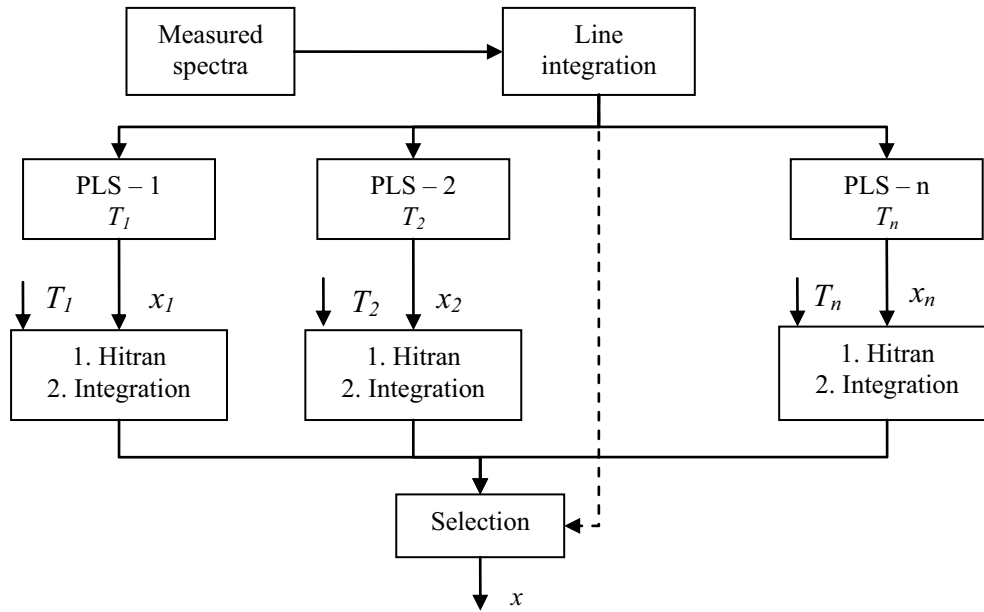


Fig. 11. Algorithm for determination of gas concentrations based on the local model ensemble method.

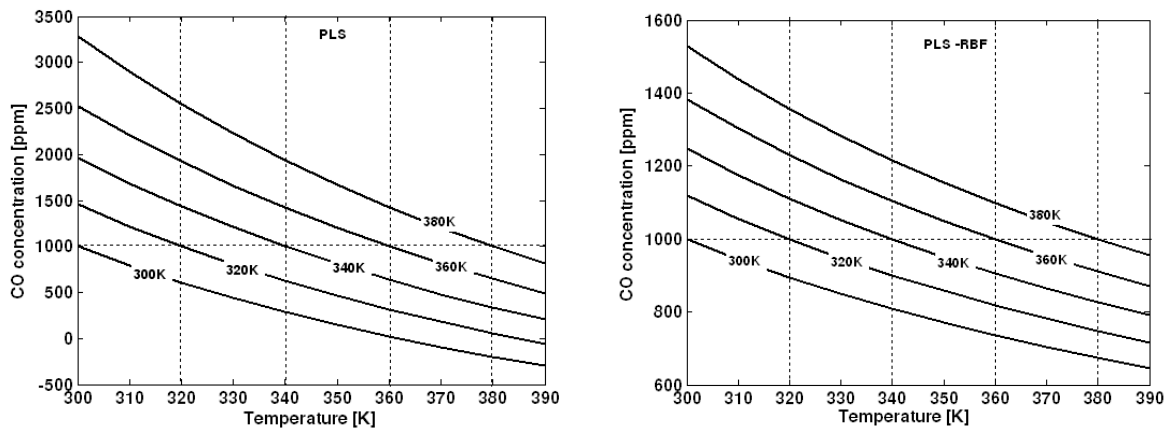


Fig. 12. Local model properties (single-temperature calibration).

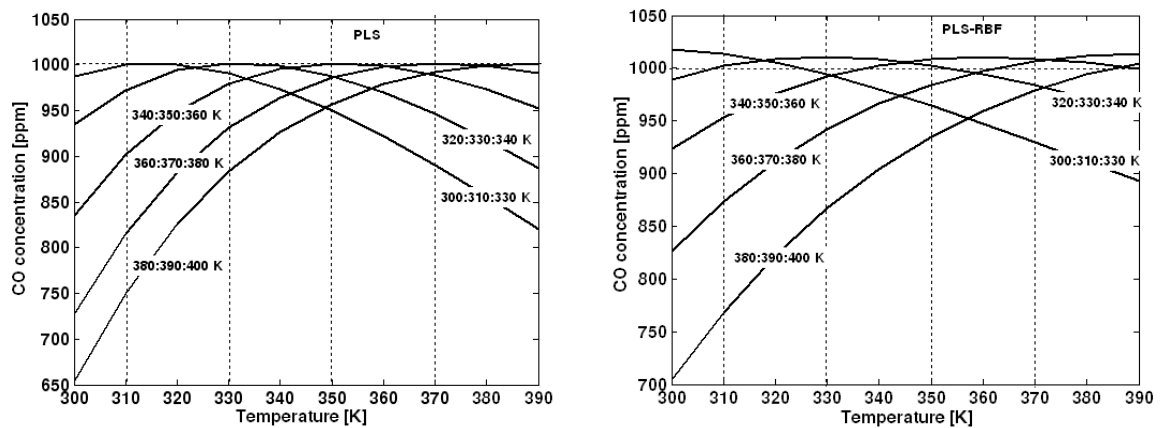


Fig. 13. Local model properties (calibrated at 3 temperatures over a 30 K range).

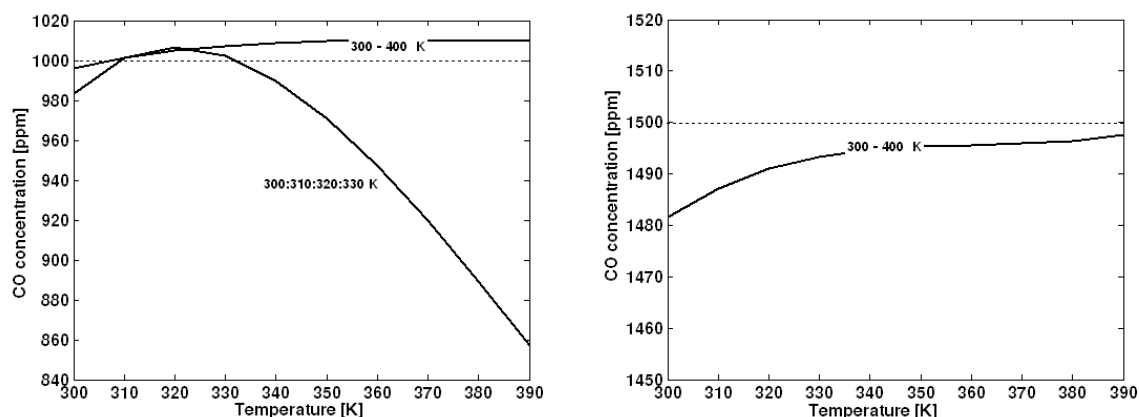


Fig. 14. Properties of models based on a calibration set ensemble for different temperatures.

The calibration set ensemble is an alternative to building several local models. It involves the creation of a calibration set containing a specific temperature range. In Fig. 12, the properties of models built for a specific temperature are shown. In all cases, the test concentration was 1000 ppm; this value is also representative of other concentrations. Even a relatively small deviation from the temperature of the calibration set generates significant inverse model errors. The next step is to use a 30 K temperature range in the calibration set, which lessens the required number of inverse models in the ensemble, and also makes the models less sensitive to temperature changes within the specified range (Fig. 13). As in the previous case (Fig. 12), the CO concentration in the test set was 1000 ppm (10 m length). A calibration set with a temperature range from 300K to 400K was used to build the PLS model presented in Fig. 14. As can be seen, for the two test sets used (1000ppm and 1500ppm), the PLS model can cope with temperature changes.

6. Conclusions

OP-FTIR spectrometers are often used with *in-situ* gas measurement methods. In many processes, especially the gasification and pyrolysis of biomass, significant CO concentrations are present. Moreover, in these processes the temperature of the produced gases often changes. A common method for building a calibration model under these conditions is to use synthetic spectra generated by the line-by-line method, and then match them to the resolution of the spectrometer. However, imprecise knowledge of ILS can cause significant errors in determining gas concentrations. This error can be reduced by comparing spectra in which individual rotational lines are integrated. When there are changes in the measured gas temperature, fitting measured and synthetic spectra with iterative methods is most common. This article presents a method for the solution of the inverse problem in determination of gas concentrations from open path measured spectra that uses many local models built for specific temperatures or a temperature range. If the temperature can additionally be measured, the corresponding local model can be selected on that basis. If the temperature is unknown, the choice of model for concentration determination is based on comparison of measured and calculated spectra from the individual submodels. Alternatively, methods using calibration set ensembles are proposed. For the temperature and concentration ranges studied here, these methods perform similarly. For other gases and measurement applications, the proposed solution may vary, depending on both the number of local models and the range of temperatures a particular calibration set covers.

The results of these calculations are valid not only for open path measurements but also for other spectroscopic methods, particularly in industrial environments. The influence of temperature on the performance of the most commonly used chemometric methods is

noticeable. The average value of this error is 1%/K under the typical conditions used in this article, and fluctuations of 1-2 K can occur even under strictly controlled conditions in the laboratory. Therefore, even for extraction methods of gas measurement where samples are cooled, it might be beneficial to use a calibration set for a specific range of temperatures. However, in calibration the temperature does not have to be very precisely controlled. As a result, a model or set of models can be built with fixed properties for all possible temperature ranges. Another conclusion that may emerge is that there is no need to build several models if one with a suitable calibration set can be used. On the other hand, ensembles of models can be used for diagnostic purposes, such as determining or increasing the accuracy of the result.

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