

# **Combustion diagnostics at a biomass-fired grate furnace using FT-IR absorption spectroscopy for hot gas measurements**

**Thomas Fleckl<sup>1</sup>, Helmut Jäger<sup>2</sup>, Ingwald Obernberger<sup>1,3</sup>**

<sup>1</sup>Institute of Chemical Engineering Fundamentals and Plant Engineering,  
Technical University Graz, A-8010 Graz, Austria  
email: fleckl@glvt.tu-graz.ac.at

<sup>2</sup>Institute of Experimental Physics,

Technical University Graz, A-8010 Graz, Austria

<sup>3</sup>BIOS – Bioenergy Systems, Sandgasse 47/13, A-8010 Graz, Austria

## **Abstract**

In-situ Fourier transform infrared (FT-IR) absorption spectroscopy has been applied as a combustion diagnostic tool to a biomass-fired travelling grate furnace with the purpose of obtaining information about the volatilisation of gaseous compounds from the fuel bed as well as the further reactions of these compounds during the combustion process. For these aims FT-IR in-situ measurements are carried out directly in the hot furnaces. The main advantage of this procedure is that it is considerably quicker and easier than conventional suction probe measurements. The key issues of the work are the achievement of highly automated FT-IR hot gas measurements for selected gaseous compounds as well as the minimisation of errors caused by measuring through unknown and fluctuating temperature and concentration profiles in the turbulent flame.

For quantitative analysis it is important to obtain the absorption coefficients of the gaseous components to be measured at high temperatures. Therefore, a calibration cell was constructed to gain calibration spectra for H<sub>2</sub>O, CO, CO<sub>2</sub> and CH<sub>4</sub> at temperatures up to 1,100 °C. Moreover the HITRAN/HITEMP database was used to calculate synthetic high temperature spectra for H<sub>2</sub>O, CO and CO<sub>2</sub> in order to compare them with the spectra measured.

First measurements performed at a pilot-scale travelling grate furnace with wood chips and waste wood as fuels showed that quantitative and qualitative detection of the gaseous compounds H<sub>2</sub>O, CO, CO<sub>2</sub> and CH<sub>4</sub> is possible in reducing and oxidising zones of the furnace up to temperatures of 1,100 °C in spite of the significant amount of water vapour in the flue gas. The results achieved will be used as a basis for chemical kinetic simulations concerning NO<sub>x</sub> reduction by primary measures as well as to verify and check the results achieved by CFD simulations of the combustion process.

## **Keywords**

Biomass, combustion, FT-IR in-situ measurements, HITRAN, travelling grate furnace

## Introduction

The gas composition is a parameter of great importance in any combustion system. Fourier transform infrared spectroscopy (FT-IR) is a technique often used for investigating the composition of the flue gas by extracting the gas to a measuring cell. This technique has the disadvantage that the gases have to be cooled and filtered before entering the cell. Due to the temperature dependence of thermodynamic and chemical equilibria the composition of a gas prepared in this way may change. One way to avoid such problems is for measurements to be made directly in the combustion chamber (in-situ). An additional advantage of this method is that the measurements can be made with significantly higher spatial resolution in comparison to the extraction method, where the natural gas flow is disturbed by probe extraction. FT-IR spectroscopy has been previously used for various in-situ analyses of recovery boilers [1] and combustion of black liquor [2], pulverised coal [3] and straw [4]. The present paper describes the application of FT-IR in-situ absorption spectroscopy to a biomass-fired travelling grate furnace with waste wood and wood chips as fuels, the determination of the relevant absorption coefficients and results obtained from test runs at a pilot-scale furnace.

## Theory

The absorption of infrared radiation by a gas is given by the Beer-Lambert law[5].

$$\tau(\nu) = e^{-\alpha(\nu) \cdot n \cdot \ell} \quad \text{Equation (1)}$$

Where  $\alpha(\nu)$  is the absorption coefficient as a function of the wavenumber  $\nu$ ,  $\tau(\nu)$  the spectral transmittance and  $\ell$  the path length of radiation through the absorbing medium. In the case of a gas the concentration  $n$  (number of absorbing particles per unit volume) can be replaced by

$$n = \frac{c \cdot p}{k_B \cdot T} \quad \text{Equation (2)}$$

where  $c$  is the volume part (volume ratio) of the absorbing gas in the gas mixture,  $T$  the temperature,  $p$  the total pressure and  $k_B$  the Boltzmann constant. If  $\ell$  and  $\alpha(\nu)$  are known, the gas concentration can be derived from the absorption spectrum. Every infrared active gas component has a specific spectral absorption coefficient which depends on gas temperature, gas concentration, gas composition and total pressure. To obtain an absorption coefficient as a function of these quantities, synthetic calibration spectra have been calculated on the one hand and spectra have been measured for different gases at various concentrations and temperatures on the other.

The data required for the calculation of the synthetic spectra, such as line positions, line intensities and line broadening coefficients, were taken from the spectral database HITRAN. The 1996 edition of the database contains a high temperature database called HITEMP for CO, CO<sub>2</sub> and H<sub>2</sub>O. With these data it is possible to calculate  $\alpha(\nu)$  [6] according to:

$$\alpha(\nu) = S(T) \cdot g(\nu - \nu_0) \quad \text{Equation (3)}$$

The line intensity  $S$  and the line position  $\nu_0$  can be directly taken from the database. Voigt profiles [6, 7] and the broadening coefficients were used for the calculation of the normalised line shape function  $g(\nu - \nu_0)$  which takes into consideration that a spectral line at high temperatures and near atmospheric pressure is Doppler as well as pressure broadened.

Using Equations 1-3 it is possible to calculate transmittance spectra of CO, CO<sub>2</sub> and H<sub>2</sub>O for defined temperatures, concentrations, pressures and path lengths. To compare the calculated spectra with the measured values, it is necessary to take into consideration that a spectrometer has a finite resolution and the measured line shape of a spectral line is distorted by the instrument line shape function (ILS) [5]. The transmittance of a real spectrometer  $\tau_m(\nu)$  can be calculated by the convolution of the calculated transmittance spectrum with the ILS function.

$$\tau_m(\nu) = \int_0^{\infty} \tau(\nu) \cdot \text{ILS}(\nu - \nu_0) \cdot d\nu \quad \text{Equation (4)}$$

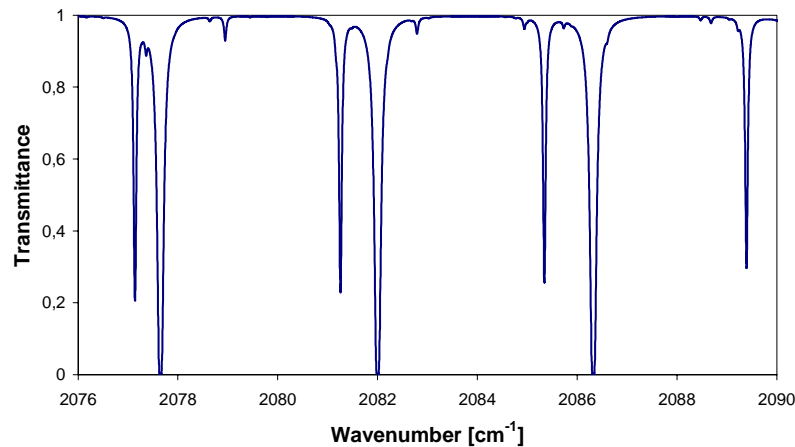
The absorbance  $A_m(\nu)$  is given by

$$A_m(\nu) = -\log_{10}(\tau_m(\nu)) \quad \text{Equation (5)}$$

The ILS function depends on the resolution  $R$  of the spectrometer and on the applied apodization function. Using a triangular apodization, the ILS function is given by [5, 6]:

$$\text{ILS}(\nu - \nu_0) = \frac{2 \cdot \sin^2[\pi(\nu - \nu_0) / R]}{R \cdot [\pi(\nu - \nu_0) / R]^2} \quad \text{Equation (6)}$$

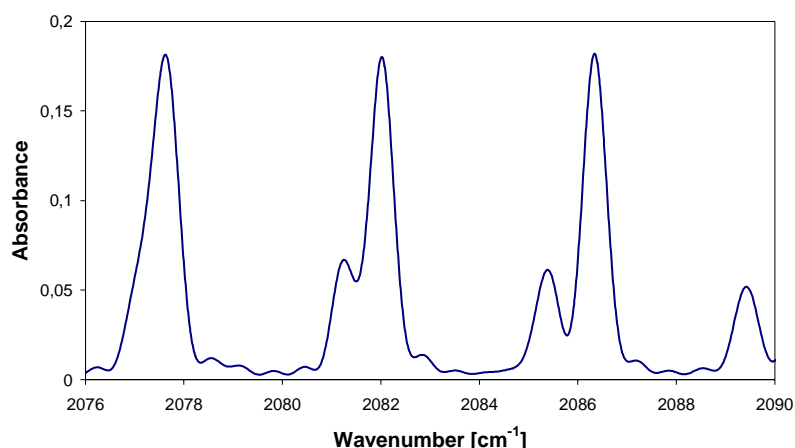
An example of the effect of the convolution applied on a calculated transmittance spectrum (Figure 1) is illustrated in Figure 2. It can be seen that narrow lines in the transmittance spectrum, which cannot be resolved by the spectrometer, may appear as one peak in the absorbance spectrum. A special convolution method described in [6] was used for all calculations performed.



**Figure 1:** Transmittance of CO as a function of the wavenumber

*Explanations*

Spectrum calculated at 1,000 °C, 1 Vol% CO and 80 cm path length



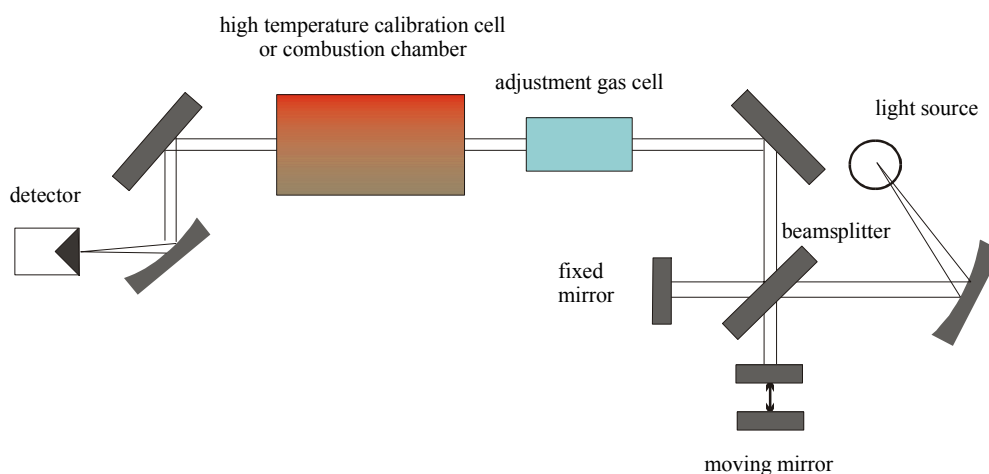
**Figure 2:** Absorbance of CO as a function of the wavenumber

## Experimental results

A Midac M2401-C spectrometer with a maximum resolution of  $0.5 \text{ cm}^{-1}$  equipped with a MCT detector was used for all experiments. The velocity of the moving mirror of the spectrometer was set at  $5.1 \text{ cm/s}$  to obtain high modulating frequencies[5] and to minimise the measuring time as well as the noise induced either by particles passing the line of sight or by flame fluctuations. For each spectrum 60 scans were averaged. Triangular apodization and 16 x zero-filling were used to obtain a spectrum. The data collection time was about 1 minute. Measurements were performed at a pilot-scale furnace (nominal boiler load  $440 \text{ kW}_{\text{th}}$ ) and at a high temperature calibration cell.

### a) Measurements at a calibration cell

The calibration cell was a 9.6 cm long stainless steel tube with wedged sapphire windows on each end. It could be heated up to  $1,100 \text{ }^\circ\text{C}$  and guaranteed small temperature gradients along the line of sight.



**Figure 3:** Experimental set-up for the FT-IR absorption spectroscopy

The experimental set-up is shown in Figure 3. This arrangement provides modulation of the light by the moving mirror and therefore ensures that only radiation from the light source and not radiation emitted from the hot furnace is measured.

An adjustment gas cell (Figure 3) was used to obtain a repeatable ILS function of the spectrometer at any time when the system was newly adjusted. The cell was filled with a defined concentration of CO at ambient temperature and pressure. With the help of the CO spectrum obtained in this way it was always possible to change the adjustment of the spectrometer to the same order of resolution.

Synthetic spectra of CO, CO<sub>2</sub> and H<sub>2</sub>O have been calculated for different concentrations of these gases in air of temperatures up to 1,100 °C. The same mixtures using nitrogen as carrier gas have been prepared experimentally and spectra of these were taken at different temperatures. A comparison of the broadening coefficients of air and nitrogen showed that they are of the same order of magnitude, which is also stated in [8,9]. Concerning CH<sub>4</sub> only experimental data were used due to a lack of data for calculations. The concentrations in the calibration experiments were set high enough to reach the same orders of magnitude for the product of the concentration and the path length as used in the calculations. The validity of the Beer-Lambert law was tested for all cases investigated by changing the concentrations of the gases. Spectral sections of each gas were chosen so that overlapping with bands from the other flue gas compounds and bands of CO<sub>2</sub> and H<sub>2</sub>O of the absorbing gas outside the furnace had a minor influence. For each spectral section a three dimensional calibration function connecting concentration, temperature and absorbance was fitted to the data measured and calculated. With these functions it was possible to obtain the concentration for a given temperature and absorbance. The gas concentrations used and spectral sections chosen are summarised in Table 1.

**Table 1:** Spectral sections and concentrations used for the calibration measurements

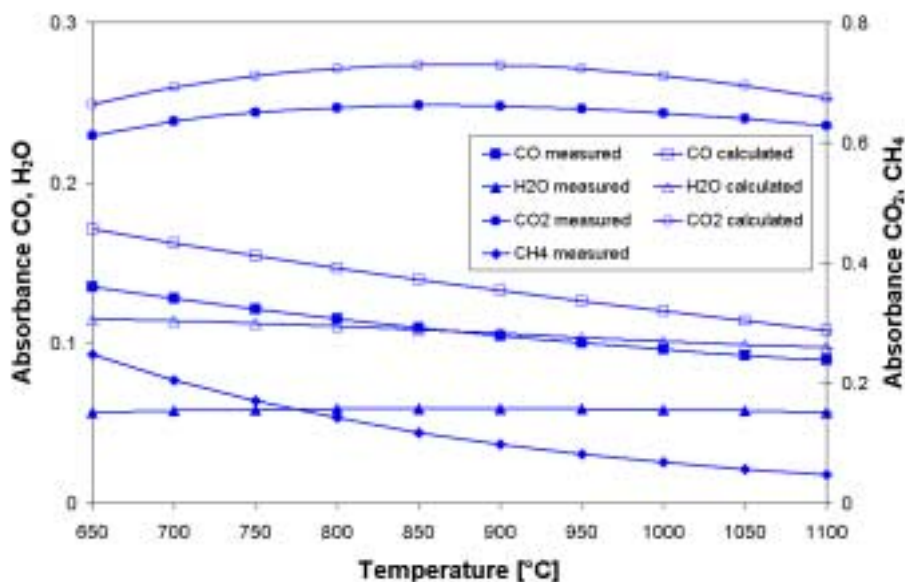
*Explanations*

A section interval is  $\pm 0.05 \text{ cm}^{-1}$  of the given wavenumber.

Species	Centres of spectral sections [ $\text{cm}^{-1}$ ]	Concentration in nitrogen [Vol%]
H <sub>2</sub> O	2065.80, 2078.45, 2087.30	0-50
CO <sub>2</sub>	2393.03, 2394.43, 2396.04	0-100
CO	2073.25, 2086.32, 2094.85, 2099.07	0-20
CH <sub>4</sub>	3002.06, 3007.61, 3017.50	0-5

All results of measured data were converted to data of 80 cm path length. The measured and calculated absorbance as a function of the temperature at a constant concentration are illustrated for one spectral section of each component in Figure 4. The absorbance errors for the spectra calculated were estimated from the errors of the spectral data to be  $\pm 10-20 \%$  at least. That means that the differences between the measured data and the calculated values were smaller than the errors expected. Concerning the absorbance measurements of CO and CH<sub>4</sub> reactions of these gases with the cell wall may take place at high temperatures [2]. Therefore, the absorbance measured can be too low for a given concentration. The H<sub>2</sub>O values measured had estimated errors of about  $\pm 10-15\%$  due to higher uncertainties in the determination of the concentration compared to the other gases. Considering the errors of the

measured and calculated absorbance, CO and CO<sub>2</sub> show a satisfying correspondence. The larger differences of the H<sub>2</sub>O values could not be explained. It seems that either the errors in the experiments or in the calculations are higher than estimated. This fact is valid for all sections investigated nearly independent of temperature and concentration.



**Figure 4:** Measured and calculated absorbance as a function of the temperature at a path length of 80 cm

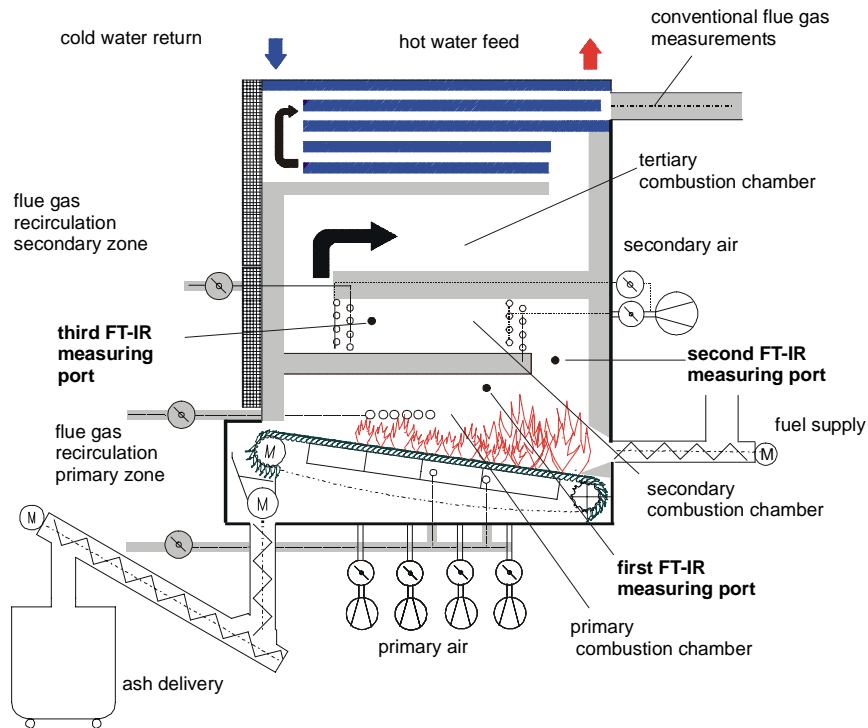
*Explanations*

Concentrations: CO<sub>2</sub> and H<sub>2</sub>O 10 Vol%, CO 5,000 vppm, CH<sub>4</sub> 6,000 vppm  
Spectral sections: CO<sub>2</sub> 2,393.43 cm<sup>-1</sup>, H<sub>2</sub>O 2,078.45 cm<sup>-1</sup>, CO 2,086.32 cm<sup>-1</sup>, CH<sub>4</sub> 3,017.50 cm<sup>-1</sup>

Furthermore it was observed that the absorbance of the selected H<sub>2</sub>O and CO<sub>2</sub> lines showed only a moderate temperature dependence between 700 and 1,100 °C. This proves to be advantageous because it minimises the influence of temperature gradients and errors in temperature measurements on the determination of concentrations.

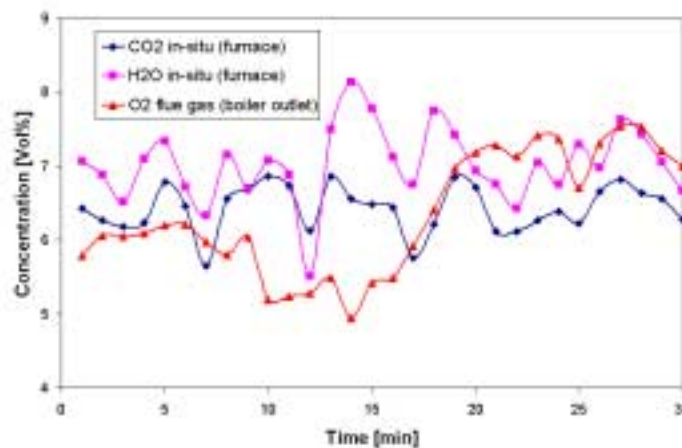
**b) Measurements at a pilot-scale furnace**

Measurements were made along a line of sight at three different locations in a pilot-scale furnace shown in Figure 5. Within these zones thermocouples were placed for temperature measurements. The adjustment of the spectrometer and the background spectrum recording was performed at the cold furnace. Observation zinc selenide windows were mounted on tubes and placed 40 cm away from the furnace wall. These tubes were purged with dry air during the measurements. In addition to the optical diagnostic measurements, conventional flue gas measurements were applied to measure O<sub>2</sub>, CO and NO in the flue gas.



**Figure 5:** Schematic overview of the travelling grate furnace

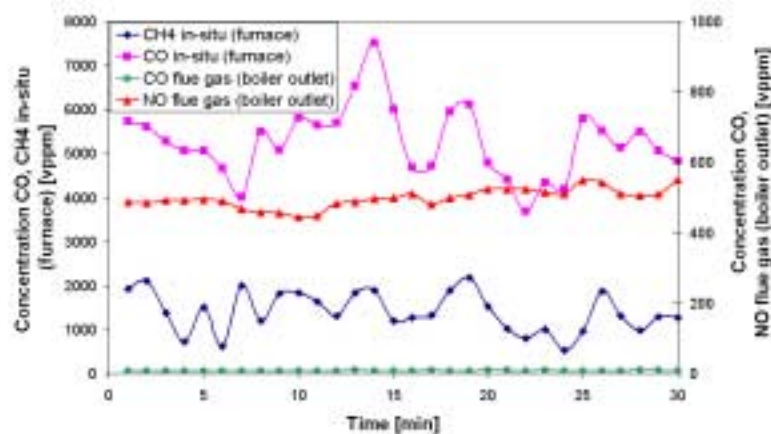
The results achieved are illustrated in Figures 6 to 12. The concentrations were determined on the basis of the calibration functions measured. It should be noted that the results are averaged values due to unknown concentration and temperature profiles along the line of sight. The results in Figures 6 and 7 show that above the fuel bed the combustion was quite stable and had a high combustion efficiency. The fluctuations of the measured in-situ values of CO, CO<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub> were due to changing conditions in the fuel bed as well as of the flow pattern.



**Figure 6:** Concentrations of CO<sub>2</sub> (in-situ - furnace) and H<sub>2</sub>O (in-situ - furnace) measured at the first measuring port as well as of O<sub>2</sub> (boiler outlet) as a function of time

**Explanations**

Boiler load: 350 kW, stoichiometric primary air ratio: 1.1, water content of fuel: 30 weight%<sub>wb</sub>, fuel: waste wood



**Figure 7:** Concentrations of CO (in-situ - furnace) and CH<sub>4</sub> (in-situ - furnace) measured at the first measuring port as well as of CO (boiler outlet) and NO (boiler outlet) as a function of time

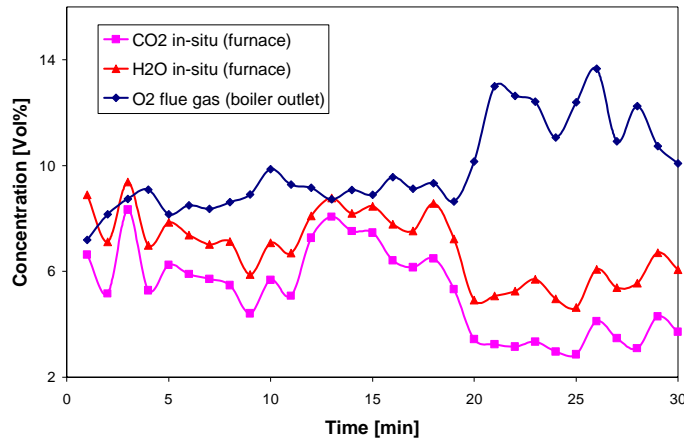
*Explanations*

Boiler load: 350 kW, stoichiometric primary air ratio: 1.1, water content of fuel: 30 weight%<sub>wb</sub>, fuel: waste wood

Figures 8 and 9 show results obtained at the second measuring port situated at the beginning of the secondary combustion chamber. The combustion was stable for the first 20 minutes. Then the flue gas concentration of O<sub>2</sub> increased significantly which is an indication for deteriorating combustion conditions. At the same time the in-situ concentrations of CO, CO<sub>2</sub> and H<sub>2</sub>O decreased, which could be caused by changes in the flow pattern as well as by a decreased release of gaseous compounds from the fuel bed. In spite of the decreasing in-situ CO concentration the CO concentration in the flue gas increased due to reduced temperatures in the secondary combustion chamber, resulting in a worse burn-out. The decrease of the NO concentration in the flue gas can be interpreted as an increase of the residence time and the reduced CO burn-out. In Figure 10 simulated iso-surfaces of H<sub>2</sub>O concentrations using the CFD (computational fluid dynamics)-software FLUENT™ are illustrated. The results show that the concentrations simulated were in the same order of magnitude as the measured ones. Another effect observed from the simulation was that the second measuring port was placed in a region of steep concentration gradients. Therefore, the concentrations measured at this location are likely to be sensitive to the position of the measuring port as well as to changes in flow conditions.

Measurements performed (Figures 11 and 12) at the end of the secondary combustion chamber (third measuring port) showed that under stable furnace conditions, the in-situ CO concentrations were close to detection limits (100-200 vppm). Steady combustion lasted 23 minutes. After that an increase of the in-situ CO and flue gas O<sub>2</sub> and a decrease of the CO<sub>2</sub> and H<sub>2</sub>O concentrations was observed. The time shift and the concentration difference between increasing CO concentrations in the furnace and at the boiler outlet were caused on the one hand by reactions still taking place in the tertiary combustion chamber and on the other hand by the decrease of furnace temperature. The latter mentioned fact is mainly responsible for the time shift.

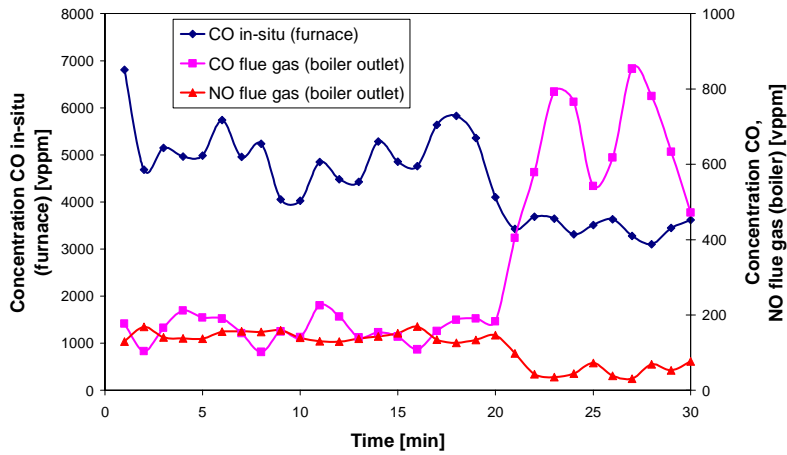
CH<sub>4</sub> was observed neither at the second nor at the third measuring port.



**Figure 8:** Concentrations of CO<sub>2</sub> (in-situ - furnace) and H<sub>2</sub>O (in-situ - furnace) measured at the second measuring port as well as of O<sub>2</sub> (boiler outlet) as a function of time

*Explanations*

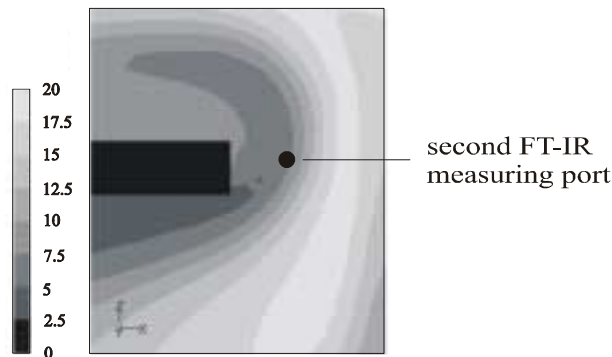
Boiler load: 440 kW, stoichiometric primary air ratio: 1.6, water content of fuel: 15 weight%<sub>wb</sub>, fuel: beech



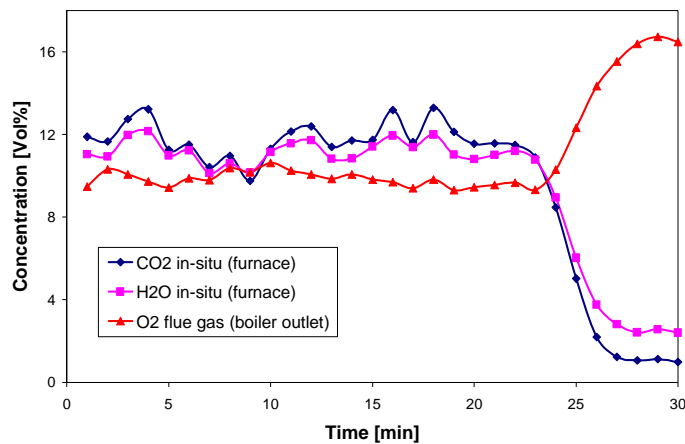
**Figure 9:** Concentrations of CO (in-situ - furnace) measured at the second measuring port as well as of NO (boiler outlet) and CO (boiler outlet) as a function of time

*Explanations*

Boiler load: 440 kW, stoichiometric primary air ratio: 1.6, water content of fuel: 15 weight%<sub>wb</sub>, fuel: beech



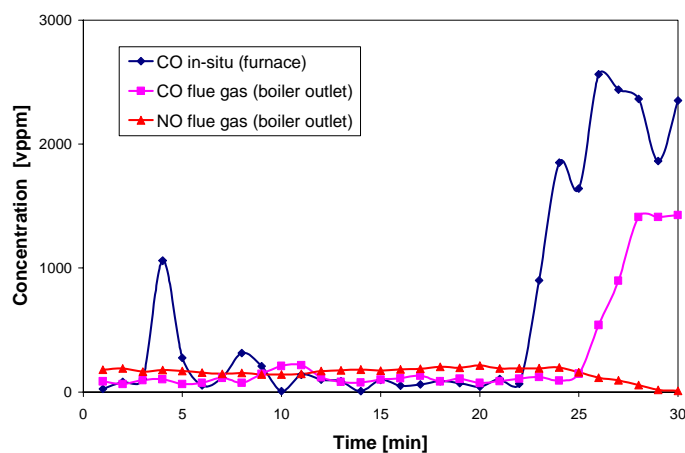
**Figure 10:** Iso-surfaces of H<sub>2</sub>O concentrations [Vol%] calculated with the CFD software FLUENT™



**Figure 11:** Concentration of CO<sub>2</sub> (in-situ - furnace) and H<sub>2</sub>O (in-situ - furnace) measured at the third measuring port as well as of O<sub>2</sub> (boiler outlet) as a function of time

*Explanations*

Boiler load: 440 kW, stoichiometric primary air ratio: 2.1, water content of fuel: 15 weight%<sub>wb</sub>, fuel: beech



**Figure 12:** Concentration of CO (in-situ - furnace) measured at the third measuring port as well as of CO (boiler outlet) and NO (boiler outlet) as a function of time

*Explanations*

Boiler load: 440 kW, stoichiometric primary air ratio: 2.1, water content of fuel: 15 weight%<sub>wb</sub>, fuel: beech

## Conclusions and future approach

A FT-IR spectrometer has been successfully applied for measuring in-situ gas concentrations of CO, CO<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub> in different zones of a biomass-fired travelling grate furnace. The determination of the concentrations was based on measured calibration functions for temperatures up to 1,100 °C. A comparison to calculated calibration functions using the spectral database HITRAN/HITEMP showed that calculated spectra of H<sub>2</sub>O may have higher uncertainties than CO and CO<sub>2</sub> spectra which should be considered for their application in quantitative analysis. In summary, the results show that FT-IR spectroscopy can be used as a diagnostic technique in biomass furnaces for high temperature process control as well as for verification of CFD simulations of the combustion.

Future work will include measurements at a laboratory scale reactor for investigating the release of gaseous compounds directly from the fuel bed under defined conditions. The reactor will also be used for improved calibration measurements of CO and CH<sub>4</sub> by applying a ceramic retort (C/SiC) to minimise wall reactions. Furthermore, a comparison between calculated and measured data of mixtures of CO, CO<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub> in air will be performed for investigating the mutual influences of the gas compounds and effects on the spectra obtained. The application of commonly used statistical methods in spectroscopy, like the PLS (partial least squares) algorithm, should result in further improvements. After these optimisations it should be possible to indicate definitely the accuracy, the detection limits for different gaseous compounds and temperatures and the applicability of FT-IR absorption spectroscopic hot gas in-situ measurements.

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