Passive remote sensing of pollutant clouds by FTIR spectrometry: Signal-to-noise ratio as a function of spectral resolution

Roland Harig

Technische Universität Hamburg-Harburg, 21079 Hamburg, Germany

In a passive infrared remote sensing measurement, the spectral radiance difference caused by the presence of a pollutant cloud is proportional to the difference between the temperature of the cloud and the brightness temperature of the background (first order approximation). In many cases, this difference is of the order of a few Kelvin. Thus, the measured signals are small and the signal-to-noise ratio (SNR) is one of the most important quantities to be optimized in passive remote sensing. In this work, a model for the SNR resulting from passive remote sensing measurements with an FTIR spectrometer is presented. Analytical expressions for the signal-to-noise ratio of a single Lorentzian line for the limiting cases of high and low spectral resolutions are derived. For constant measurement time the SNR increases with decreasing spectral resolution, i.e. low spectral resolutions yield the highest signal-to-noise ratios. For a single scan of the interferometer, a spectral resolution that maximizes the SNR exists. The calculated signal-to-noise ratios are in good agreement with measured signal-to-noise ratios.
Introduction

Passive infrared remote sensing of pollutant clouds is based on the analysis of infrared radiation absorbed and emitted by the molecules of the clouds. The signal, that is the spectral radiance difference caused by a vapor cloud is - in a first order approximation - proportional to the difference between the temperature of the cloud and the brightness temperature of the background. In many cases, this effective temperature difference is of the order of a few Kelvin. Thus, the measured signals are small and the signal-to-noise ratio (SNR) is one of the most important quantities to be optimized in passive remote sensing.

Since the method of Fourier-transform spectrometry was developed, the noise in the spectrum and the signal-to-noise ratio have continually been the subject of studies (e.g. references 1, 2, 3, 4). Flanigan treated the case of the signal-to-noise ratio of a passive infrared remote sensing system for the detection of hazardous vapors theoretically. In passive remote sensing measurements, absorption and emission lines are observed on background radiation with spectral radiances that are typically orders of magnitude greater than the spectral radiance difference caused by the lines. Thus, Flanigan defined the signal-to-noise ratio as the ratio of the radiance difference caused by an absorption or emission band and the noise in the radiance spectrum. In Flanigan’s work, absorption lines and bands were modeled by Lorentz profiles.
calculation of the SNR was performed using a model in which the Lambert-Beer law was used with low-resolution (effective) absorption coefficients, calculated by integration of the Lorentz profile over a spectral interval given by the spectral resolution. Based on Flanigan’s definition of the SNR, a new model for quantitative description of the SNR resulting from measurements with a real spectrometer (FTIR spectrometer) is presented in this work. The model consists of three submodels: a radiative transfer model, a model for the instrument line shape of the spectrometer, and a model for the noise equivalent spectral radiance.

**Radiative Transfer Model**

In order to describe the characteristics of spectra measured by a passive infrared spectrometer, a model may be used\(^6,^7\) in which the atmosphere is divided into plane-parallel homogeneous layers along the optical path. In many cases a model with three layers is sufficient to describe the basic characteristics of the spectra (Figure 1). Radiation from the background, for example the sky or a surface (background layer), propagates through the vapor cloud (cloud layer, a mixture of the released molecules and air), and the atmosphere between the cloud and the spectrometer (atmospheric layer). The radiation containing the signatures of all layers is measured by the spectrometer. The cloud and atmospheric layers are considered homogeneous with regard to all physical and chemical properties. Application of the three layer model\(^6\) yields

\[
L_S = (1 - \tau_{at})B_{at} + \tau_{at}[(1 - \tau_c)B_c + \tau_c L_b]
\]  

\((1)\)
for the spectral radiance at the entrance aperture of the spectrometer $L_S$. Here, $\tau_{at}$ is the transmittance of the atmosphere between the spectrometer and the cloud, $B_{at}$ is the spectral radiance of a blackbody at the temperature of the atmosphere, $T_{at}$, $\tau_c$ is the transmittance of the cloud, and $B_c$ is the spectral radiance of a blackbody at the temperature of the cloud, $T_c$. $L_b$ is the radiance that enters the layer of the cloud from the background. The quantities in Equation (1) are frequency-dependent. Because the scattering coefficient in the infrared spectral region is small under many measurement conditions, the contribution of scattering is neglected in this model. If the assumption of homogeneous layers is not warranted, for example if there are strong temperature gradients within the layers, additional layers may be added.

If the temperatures of the cloud layer and the atmospheric layer are equal, Equation (1) can be simplified:

$$L_S = B_{at} + \tau_{at}\tau_c(L_b - B_{at}). \quad (2)$$

It follows from Equation (2) that in this case layers 1 and 2 may be exchanged without influence on the spectrum. The radiance difference $\Delta L = L_S - L_b$ is given by

$$\Delta L = (1 - \tau_{at}\tau_c)\Delta L_{cb}, \quad (3)$$
where $\Delta L_{cb} = B_c - L_b$ (Because a confusion in terms is unlikely, in this work the term radiance is used as a simplifying synonym for the correct term spectral radiance.).

For the calculation of spectra with atmospheric optical paths (without a pollutant cloud), in particular for the calculation of $L_b$ if the sky is the background, computer codes that apply the theory of radiative transfer such as Modtran\textsuperscript{8} or Fascode\textsuperscript{9} may be used. If the spectrometer is aligned to a topographic target such as a forest or the wall of a house, the radiation entering the cloud $L_b$ contains radiation emitted by the surface and reflected radiation, i.e. ambient radiation and radiation from the sky. However, the emittance of many surfaces is high and is a slowly varying function of the frequency in the range $650 – 1500 \text{ cm}^{-1}$. In these cases, the radiance of a black body may be used as an approximation for $L_b$. In this work, measurements are performed with a black plate as the background, and $L_b$ is modeled by the radiance of a black body.

**Instrument Line Shape**

The spectrum $S^C(\sigma)$, calculated by Fourier transformation of the measured interferogram, may be written as

$$S^C(\sigma) = \int_{-\infty}^{\infty} S(\sigma') A(\sigma - \sigma', \sigma') d\sigma'.$$

(4)
Here, \( S(\sigma) \) is the true spectrum, i.e. the spectrum measured with infinite optical path difference and collimated radiation. \( A(\sigma, \sigma') \) is the instrument line shape (also called apparatus function) at the frequency \( \sigma' \), i.e. the shape of the calculated spectrum of monochromatic radiation with the frequency \( \sigma' \). For an ideal interferometer operating with perfectly collimated radiation, the ideal instrument line shape \( A_0 \) is given either by the Fourier transform of the function describing the finite movement of the mirror or the Fourier transform of the apodization function. If no apodization function is applied, the instrument line shape is given by

\[
A(\sigma, \sigma') = A_0(\sigma) = 2D \text{sinc}(2\pi D \sigma). \tag{5}
\]

where \( D \) is the maximum optical path difference in the interferometer and \( \text{sinc}(x) = \sin(x)/x \).

Here, the instrument line shape \( A(\sigma, \sigma') \) is independent of \( \sigma' \) and the integral in Equation (4) becomes a convolution integral.

In practice, especially in the case of an interferometer optimized for high throughput, non-paraxial rays from a finite source, which subtends a solid angle \( \Omega \) at the interferometer, reach the detector (due to the finite detector area), causing a broader instrument line shape and a frequency shift. In this case, the instrument line shape is given by the convolution

\[
A(\sigma, \sigma') = A_0(\sigma) \ast A_{\text{inh}}(\sigma, \sigma'), \tag{6}
\]

where \( A_{\text{inh}}(\sigma, \sigma') \) is the instrument line shape due to the finite detector area.
where $A_{inh}(\sigma, \sigma')$, the inherent apparatus function\(^{10}\), is a function describing the effect of broadening and the frequency shift. In the case of a homogeneous source and an ideal Michelson interferometer (ideal mirrors etc.), in which the radiation leaving the interferometer is measured by a detector in the focal plane of a condenser lens (or mirror), $A_{inh}(\sigma, \sigma')$ is a rect-function (boxcar) of total width $\frac{\sigma \Omega}{2\pi}$, centered at $\Delta \sigma' = -\frac{\sigma \Omega}{4\pi}$\(^{11,11}\). Steel\(^{10}\) deduced the inherent apparatus function of a simple Michelson interferometer without collimator and condenser. Saarinen and Kauppinen deduced the inherent apparatus functions for the cases of a misaligned cube corner interferometer\(^{12}\) and an off-focus radiation source\(^{13}\). The resulting instrument line shape functions are frequency-dependent, i.e. they are dependent on $\sigma'$. However, in a small spectral range $\Delta \sigma_{SR}$ around a particular frequency $\sigma'$, i.e. $\Delta \sigma_{SR} \ll \sigma'$ the spectrum may be approximated by a convolution of the true spectrum with the apparatus function at $\sigma'$ (Equation (4)):

$$S^c(\sigma) = S(\sigma) * A(\sigma, \sigma'). \quad (7)$$

The inherent apparatus functions cited are valid for special cases. They describe ideal interferometers or the impact of the considered setup (misaligned interferometer, off-focus source) on the line shape. In order to characterize the combined effects of aberrations, misalignment, nonlinear movement of the mirrors (see reference 12) etc., empirical apparatus functions may be used. For active open-path measurements this has been described in reference 14. The instrument line shape may also be characterized by a path difference dependent function describing the distortions in the interferogram (for $\sigma' = \text{const.}$)\(^{15,16}\).
In this work, two instrument line shape functions are applied. For the theoretical calculations, an ideal instrument line shape \( A_0 \) is used. For modeling of measured spectra, an instrument line shape function, calculated using an empirical inherent apparatus function defined by five parameters \( p_1 \ldots p_5 \), is used:

\[
A_{inh}(\sigma, \sigma') = \begin{cases} 
0 & \text{for } \sigma < -p_1 \\
p_2 + p_3 \left( \sigma + p_1 \right)^2 & \text{for } -p_1 \leq \sigma \leq -p_4 \\
p_5 \text{rect} \left( \frac{\sigma + p_4}{2} \right) & \text{for } \sigma > -p_4
\end{cases}
\]  

This model for the inherent apparatus function contains the inherent apparatus function of the ideal Michelson interferometer illuminated by an extended homogeneous source as a limiting case and it contains an approximation for the inherent apparatus function of the interferometer without collimator and condenser. Because only a small spectral range around \( \sigma' \) is considered in this work, the dependence of the inherent apparatus function on \( \sigma' \) is neglected. Fig. 2 shows an instrument line shape function calculated using this model (Equations (6) and (8)).

**Model for the Signal-to-Noise Ratio**

The signal measured at a finite spectral resolution \( \Delta L_M \), that is the measured radiance difference caused by the cloud layer, is modeled by convolution of the true radiance difference
$\Delta L$ calculated using Equation (3) with the instrument line shape, $A(\sigma, \sigma')$ (Equations (6) and (8), $\sigma' = \text{const.}$):

$$
\Delta L_M(\sigma) = \Delta L(\sigma) * A(\sigma, \sigma').
$$

(9)

The signal-to-noise ratio SNR at a particular frequency $\sigma_i$ is given by the ratio of the measured signal and the noise equivalent spectral radiance NESR in this spectral region:

$$
\text{SNR}(\sigma_i) = \frac{|\Delta L_M(\sigma_i)|}{\text{NESR}}.
$$

(10)

In a detector-noise-limited model for a spectrometer, the noise equivalent spectral radiance NESR is given by (see for example references 7, 17)

$$
\text{NESR} = \frac{\sqrt{A_D}}{\Theta \xi \Delta \sigma_E \sqrt{t} \ D^*}.
$$

(11)

Here, $\Delta \sigma_E$ is the equivalent width\textsuperscript{18} of the instrument line shape, $\xi$ is the overall efficiency of the system\textsuperscript{2,17} (also termed overall transmittance: term including reflection losses, transmittance of optical elements such as the beam splitter, modulation efficiency, and other losses due to aberrations, misalignment etc.), $\Theta$ is the étendue, $t$ is the measurement time, $A_D$ is the detector.
area, and $D^*$ is the specific detectivity of the detector. For an ideal interferometer and if no apodization function is applied, the equivalent width is given by $\Delta \sigma_E = \frac{1}{2D}$ ($D$: maximum optical path difference in the interferometer). Equation (11) may also be used to express the NESR in terms of the nominal spectral resolution $\Delta \sigma = 1/D = 2\Delta \sigma_E$. In this case the resulting factor of 2 in comparison to Equation (11) may be included in the definition of $\xi$, as in reference 5, or the factor of 2 is introduced by substituting $\Delta \sigma_E = \Delta \sigma/2$ into Equation (11) (as is done in this work).

In order to calculate the NESR as a function of the spectral resolution for a single (two-sided) scan, Equation (11) is expressed using different quantities because the measurement time $t$ is a function of the spectral resolution:

$$\text{NESR}_{\text{Scan}} = \frac{\sqrt{2A_D f_S}}{\Theta \xi D^* \sqrt{\sigma_L \Delta \sigma}}.\quad (12)$$

Here, $f_S$ is the interferogram sampling frequency and $\sigma_L^{-1}$ is the difference between the optical path differences of two adjacent sampling positions. For a two-sided interferogram the measurement time is given by $t = 2\sigma_L/(\Delta \sigma f_S)$.
SNR for a Single Lorentzian Line

In the lower atmosphere, at a pressure of approximately 1000 hPa, pressure broadening of spectral lines dominates. Thus, the shape of a spectral line may be approximated by a Lorentz profile. The transmittance of a layer of a gas is given by the Lambert-Beer law:

\[ \tau(\sigma) = \exp(-\beta(\sigma)cl). \]  \hspace{1cm} (13)

Here, \( \beta(\sigma) \) is the absorption coefficient, \( \sigma \) is the frequency (wavenumber, expressed in cm\(^{-1}\)), and \( cl \) is the column density of the gas (in this work it is expressed in ppm m, assuming conditions of the lowest layer of the standard atmosphere). For a line causing a minimum transmittance \( \tau_{\text{min}} \), the argument of the exponential function of the transmittance (Equation (13)) may be written as

\[ \beta(\sigma)cl = -\ln(\tau_{\text{min}}) \frac{\gamma^2}{\gamma^2 + (\sigma - \sigma_0)^2}. \]  \hspace{1cm} (14)

Here, \( \sigma_0 \) is the center frequency of the line and \( \gamma \) is the half width at half maximum. In order to calculate the radiance difference caused by the line, Equation (3) is used with the transmittance \( \tau_c \) calculated using Equation (14). The background is modeled by the spectrum of a blackbody at the temperature \( T_b \). Because only a small spectral range is considered, the frequency dependence of \( \Delta L_{cb} \) is neglected in this work. The transmittance of the atmosphere is assumed to be ideal.
(τ_{at} ≈ 1) in the atmospheric window. For the calculation of the spectrum the following parameters were used: $T_c = 283 \text{ K}$, $T_b = 303 \text{ K}$, $\sigma_0 = 930 \text{ cm}^{-1}$, $\gamma = 0.05 \text{ cm}^{-1}$, $\tau_{\text{min}} = 0.8$. 16 spectra with spectral resolutions between $\Delta \sigma_1 = 4 \times 10^{-3} \text{ cm}^{-1}$ and $\Delta \sigma_{16} = 123 \text{ cm}^{-1}$ were calculated. The highest and lowest resolutions that are used cannot be measured with the interferometer used in this work or cannot be used for the identification of gases, respectively. They are used in order to study the limiting cases of the model. The instrument line shape is modeled by the ideal instrument line shape (Equation (5)).

Figure 3 shows the absolute value of the signal $\Delta L_{\sigma}(\sigma)$ calculated using Equation (9) for an ideal FTIR spectrometer as a function of the spectral resolution parameter $\rho = \Delta \sigma/(2 \gamma)$, i.e. as a function of the nominal spectral resolution in units of the full width at half maximum (FWHM) of the line. At low spectral resolutions ($\rho \gg 1$), the signal is inversely proportional to the spectral resolution $\Delta \sigma$. This may be shown by treatment of a line causing a high transmittance. In this case the approximation $e^{-x} \approx 1-x$ is valid and

$$\Delta L(\sigma) = (1 - \tau_c(\sigma)) \Delta L_{cb} = -\ln(\tau_{\text{min}}) \frac{\gamma^2}{\gamma^2 + (\sigma - \sigma_0)^2} \Delta L_{cb}. \quad (15)$$

If the width of the instrument line shape is much larger than the width of the absorption line, $\Delta L(\sigma)$ has only significant contributions in a spectral range within which $A_0(\sigma) = A_0(0) = 2D$. Thus, using $\Delta \sigma = 1/D$ the following approximation for the signal is valid:
Here, the signal is proportional to $\Delta \sigma^{-1}$ (see Figure 3). For lines causing low transmittance, the integral yields a different result but the dependence on $\Delta \sigma$ is the same.

In the case of high spectral resolution, i.e. $\rho \ll 1$ the instrument line shape yields significant contributions in a range within which $\Delta L(\sigma) = \Delta L(\sigma_0)$ is valid. Thus, in this case Equation (9) may be approximated:

$$\Delta L_M(\sigma_0) = \int_{-\infty}^{\infty} \Delta L(\sigma')A_0(\sigma_0 - \sigma')d\sigma' = \int_{-\infty}^{\infty} \Delta L(\sigma_0)A_0(\sigma_0 - \sigma')d\sigma' = \Delta L(\sigma_0). \quad (17)$$

Here, the signal is not dependent on the spectral resolution.

Figure 4 shows the SNR for a single scan measurement. The NESR was calculated using the following values: $D^* = 4 \times 10^{10} (\text{cm Hz}^{1/2}) / W$, $A_D = 0.01 \text{ cm}^2$, $\Theta = 0.0082 \text{ cm}^2 \text{sr}$, $f_S = 70 \text{ kHz}$, $\sigma_L = 15798.5 \text{ cm}^{-1}$, $\xi = 0.1$. Substituting the right-hand sides of the Equations (12) and (17) into Equation (10) yields the signal-to-noise ratio for a single scan at high spectral resolutions ($\rho \ll 1$):

$$\Delta L_M(\sigma_0) = \int_{-\infty}^{\infty} \Delta L(\sigma')A_0(\sigma_0 - \sigma')d\sigma' = \int_{-\infty}^{\infty} \Delta L(\sigma_0)A_0(\sigma_0 - \sigma')d\sigma' = \Delta L(\sigma_0). \quad (16)$$
Here, the signal-to-noise ratio is proportional to $\Delta\sigma^{1/2}$. For high transmittance and low spectral resolutions ($\rho \gg 1$) the signal-to-noise ratio is given by

$$
\text{SNR}_{1\text{Scan}}(\sigma_0) = \frac{|\Delta L(\sigma_0)|}{\text{NESR}_{1\text{Scan}}} = \frac{\Delta L(\sigma_0)|\Theta\zeta D^* \sqrt{\sigma_L \Delta\sigma}}{\sqrt{2A_D f_S}}. \quad (18)
$$

Here, the signal-to-noise ratio is proportional to $\Delta\sigma^{-1/2}$.

The signal-to-noise ratio for constant measurement time ($t = 1\ s$) is shown in Figure 5. The noise equivalent spectral radiance for constant measurement time NESR$_t$ was calculated using Equation (10) with the same values as in the single scan calculations.

Substituting the right-hand sides of the Equations (11) and (17) into Equation (10) yields the signal-to-noise ratio for constant measurement time at high spectral resolutions ($\rho \ll 1$):

$$
\text{SNR}_t(\sigma_0) = \frac{|\Delta L(\sigma_0)|}{\text{NESR}} = \frac{|\Delta L(\sigma_0)|\Theta\zeta D^* \Delta\sigma \sqrt{t}}{2\sqrt{A_D}}. \quad (20)
$$
Here, the signal-to-noise ratio is proportional to $\Delta \sigma$. For high transmittance and low spectral resolution ($\rho >> 1$) the signal-to-noise ratio is given by

$$\text{SNR}_t (\sigma_0) = \frac{-2\pi \ln(\tau_{\text{min}})}{\Delta \sigma \text{ NESR}} = \frac{-\pi \ln(\tau_{\text{min}})}{\Delta L_{cb} | \Theta | D^* \sqrt{\xi}} \xi D^* \sqrt{\tau} \sigma_{\tau \pi \gamma} \ln(\text{NESR}) \ln(2) \frac{\delta}{t} \text{SNR}_{\text{min min}}^0.$$  \hspace{1cm} (21)

Here, the signal-to-noise ratio is not dependent on the spectral resolution.

For constant measurement time the SNR increases with decreasing spectral resolution, i.e. low spectral resolutions yield the highest signal-to-noise ratios (Figure 5). For a single scan, a spectral resolution that maximizes the signal-to-noise ratio of a single line exists (Figure 4).

**Measurement and Numerical Calculation of the SNR**

In order to determine the signal-to-noise ratio as a function of spectral resolution experimentally, a gas cell was mounted in front of the entrance window of an interferometer (Bruker OPAG, Bruker Daltonik, Leipzig, Germany). The length of the steel cell was 0.15 m, the window material was NaCl. A heated black plate (active area 25×25 cm$^2$) was used for the radiometric calibration and as radiation source for the measurements. For each spectrum, a single interferogram (two-sided), corresponding to a nominal spectral resolution of 0.6 cm$^{-1}$ was measured. Spectra were calculated by Fourier-transformation (fast Fourier-transformation) of the appropriate number of samples of these interferograms.
In order to calculate the signal, spectra were calculated by convolution of a spectrum of ammonia (with an ideal black body as the background, see Equation (3)) with the instrument line shape. The absorption coefficient $\beta(\sigma)$ of ammonia was calculated with the use of Hitran$^{20}$ and Fascode$^9$ under conditions of the standard atmosphere. For the calculation of the instrument line shape, the model for the inherent apparatus function was used (Equation (8)). The temperature of the ammonia-sample $T_c$ and the difference between the brightness temperature$^6$ of the background $T_{Brb}$ and $T_c$, $\Delta T = T_{Brb} - T_c$ were determined by a nonlinear least squares quantification method$^{21}$ (principle of the method described in reference 22) using a spectrum with the highest spectral resolution ($\Delta \sigma = 0.6 \text{ cm}^{-1}$).

Various methods for the determination of noise have been described (for example in references 2, 4). In this work, the noise equivalent spectral radiance NESR was determined under the assumption that the data are ergodic. First, the difference between two spectra of the black plate that were measured under the same conditions (temperature of the black plate $T_b = 305$ K) was calculated in the range 900 - 1100 cm$^{-1}$. In order to remove baseline shifts which may be caused by various effects, such as a temperature drift of the radiation source, or a temperature drift of the interferometer$^{1,23}$, a baseline correction by linear regression was applied. The noise equivalent spectral radiance was calculated by division of the standard deviation of the resulting spectra in this spectral range with the responsivity of the spectrometer at $\sigma = 1000 \text{ cm}^{-1}$. In order to calculate the noise in a single spectrum, the results were divided by $\sqrt{2}$.
Figure 6 shows measured spectra with different spectral resolutions. All spectra were calculated using data of the same interferogram. Moreover, calculated spectra (using Equations (3) and (9)) and the difference spectra between the measured spectra and the calculated spectra are shown.

Figure 7 shows the results for the NESR in the range 900 - 1100 cm\(^{-1}\) as a function of spectral resolution. As shown in Figure 7, the measured NESR may be approximated by a function \(f(\Delta \sigma) = \text{const.} \times \Delta \sigma^{-1/2}\). This confirms that the NESR may be described by the detector-noise limited model (Equations (11) and (12)). The efficiency \(\xi\) of the system was determined by a least squares fit of the model function (Equation (12)) to the measured NESR. A calculation with \(D^* = 4 \times 10^{10} \text{(cm Hz}^{1/2})/W\), \(A_D = 0.01 \text{ cm}^2\), \(\Theta = 0.0082 \text{ cm}^2\text{sr}\), \(f_S = 70 \text{ kHz}\) und \(\sigma_L = 15798.5 \text{ cm}^{-1}\) yields \(\xi = 0.08\).

The detection and identification algorithm\(^{24}\) of the remote sensing system used in this work analyzes brightness temperature spectra and does not require background spectra. In order to minimize measurement time, the detection algorithm is currently only applied to spectra which are calculated using single-scan interferograms. Moreover, the algorithm contains a baseline correction method. Thus, the NESR calculated by the method described may be interpreted as the noise that limits the detection of pollutants with such an algorithm.

Figure 8 shows the measured signal-to-noise ratio and the calculated signal-to-noise ratio (Equation (10)) for \(\sigma_i = 931 \text{ cm}^{-1}\). The relatively small signal-to-noise ratio at \(\Delta \sigma = 15 \text{ cm}^{-1}\) is due to the position of the absorption band of ammonia relative to the center of the spectral

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resolution element (see Figure 6). However, it is in good agreement with the signal-to-noise ratio calculated using the model. This effect could be compensated by calculation of the Fourier-integral at the center of the band of ammonia, which may also be performed by a fast Fourier transformation after zero-filling\(^{39}\) of the interferogram. This is not performed in this study because the calculation of the Fourier integral for smaller increments of the frequency as well as the calculation of the spectra after zero-filling will strongly increase the computing time. Especially in imaging applications with real-time data analysis\(^{22}\), the calculation time should be minimized.

The good agreement between the calculated spectra and the measured spectra at all spectral resolutions shows that the signal may be described by the model presented in this work. The good approximation of the measured NESR with the detector-noise limited model for the NESR shows that this model may be used for the description of the NESR as a function of spectral resolution.

The measurements and the calculations show that the signal-to-noise ratio of the investigated transition of ammonia increases with decreasing spectral resolution within the range of spectral resolutions considered (except at \(\Delta\sigma = 15\ \text{cm}^{-1}\)), although the measurement time is inversely proportional to \(\Delta\sigma\). However, the relation between the signal-to-noise ratio and the spectral resolution is dependent on the absorption band considered because many absorption lines may contribute to a single resolution element of the spectrum at low spectral resolutions, as described by the convolution of the true spectrum with the instrument line shape.
Conclusions

The model for the signal-to-noise ratio presented in this work allows the quantitative prediction of the signal-to-noise ratio in a passive FTIR measurement. The signal-to-noise ratios calculated using the model are in good agreement with experimentally determined signal-to-noise ratios. The model may be applied to other types of spectrometers by substituting the appropriate instrument line shape into the model equations.

The results of this study confirm theoretically and experimentally that the choice of the spectral resolution is a compromise between more spectral information at high spectral resolutions and higher signal-to-noise ratios at low spectral resolutions (for constant measurement time and a detector-noise limited system). In order to maximize the signal-to-noise ratio, the lowest spectral resolution that yields the required spectral information for a specific analytical task is optimal. For single scan measurements, a spectral resolution that maximizes the signal-to-noise ratio exists. The spectral resolution of this maximum is dependent on the transition considered.

Another important quantity to be optimized is the measurement time. In particular, if measurements are performed from a moving platform or a scanning imaging remote sensing system is used. In these applications, the measurement time should be minimized due to either the movement of the platform or the large number of spectra to be collected. The minimum time required for the acquisition of an interferogram is inversely proportional to $\Delta\sigma$. This makes low resolution spectra well suited for these and other applications that require high data rates.
The calculations and the experiment described in this work were performed for constant system parameters, in particular for a constant étendue $\Theta$. Because the maximum solid angle (from which radiation is detected) allowed in the interferometer is proportional to $\Delta \sigma$ (see for example reference 25), the solid angle and consequently the étendue may be increased at lower resolutions. Thus, the SNR may be increased further at low spectral resolutions.

In order to increase the accuracy of the model, the model for the NESR that neglects all noise sources except detector noise may be replaced by a model that considers additional noise sources such as photon noise.

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Fig. 1.
Fig. 2.
Fig. 3.
Fig. 4.
Fig. 5.
Fig. 6.
Fig. 7.
Fig. 8.
**Fig. 1.** Illustration of the measurement setup of passive infrared remote sensing of airborne pollutants.

**Fig. 2.** Instrument line shape calculated using Equations (6) and (8) ($\Delta \sigma = 2 \text{ cm}^{-1}$, $\sigma' = 1000 \text{ cm}^{-1}$, no apodization).

**Fig. 3.** Absolute value of the signal of a single absorption line as a function of spectral resolution parameter ($\times$) ($\Delta \sigma$ in units of the full width of the line) and approximation for low spectral resolution calculated using Equation (16)(dashed).

**Fig. 4.** Signal-to-noise ratio of a single absorption line for measurement of a single scan as a function of spectral resolution ($\times$)(in units of the width of the line), approximation for high spectral resolution (Eq. (18)) (dashed), and approximation for low spectral resolution (Eq. (19)) (dash-dotted).
**Fig. 5.** Signal-to-noise ratio of a single absorption line for constant measurement time (1 s) as a function of spectral resolution ($\times$), approximation for high spectral resolution (Eq. (20)) (dashed), and approximation for low spectral resolution (Eq. (21)) (dash-dotted).

**Fig. 6.** Spectra of ammonia with different spectral resolutions calculated by Fourier-transformation of the appropriate number of samples of the same interferogram (solid line), simulated spectra (dashed), and the difference (dash-dotted, offset subtracted). All simulated spectra were calculated with the same parameters ($c l_{NH3} \approx 600 \text{ ppm m, } \Delta T \approx 12 \text{ K}$).

**Fig. 7.** Measured and calculated (Eq. (12): $f(\Delta \sigma) = \text{const.} \times \Delta \sigma^{-1/2}$) noise equivalent spectral radiance for a single scan as a function of spectral resolution $\Delta \sigma$ (error bars: standard deviation, 10 measurements).

**Fig. 8.** Measured and calculated signal-to-noise ratio for a single scan as a function of spectral resolution $\Delta \sigma$ ($c l_{NH3} \approx 600 \text{ ppm m, } \Delta T \approx 12 \text{ K, } \sigma_i \approx 931 \text{ cm}^{-1}$, error bars: standard deviation).