Real-time adaptive noise cancelling for signal-to-noise enhancement in direct absorption spectroscopy

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An adaptive filter for cancelling noise contained in the direct absorption spectra is reported. This technique takes advantage of the periodical nature of the repetitively scanned spectral signal, and requires no prior knowledge of the detailed properties of noises. An experimental system devised for measuring CH_4 is used to test the performance of the filter. The measurement results show that the signal-to-noise (S/N) value is improved by a factor of 2. A higher enhancement factor of the S/N value of 5.4 is obtained through open-air measurement owing to higher distortions of the raw data. In addition, the response time of this filter, which characterizes the real-time detection ability of the system, is nine times shorter than that of a conventional signal averaging solution, under the condition that the filter order is 100.

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Direct absorption spectroscopy has the advantages of high sensitivity, rapid time response, and relatively lower cost compared with modulation spectroscopy; it is also employed in environmental monitoring and industrial process gas analysis[1−6]. This technique determines the concentration of the analyte by measuring the absorbance through the continuous scanning of the molecular absorption line. Absorbance sensitivities in 10^{-5}–10^{-6} range are required for many atmospheric trace-gas measurements[7]. A high signal-to-noise (S/N) value is required to achieve such low sensitivities, because the detection limit of a spectrometer is determined by the S/N of absorption spectra. Moreover, the enhancement of absorption signal is limited by the low concentration level or a finite optimum absorption path length[8]; thus, noise suppression is a better choice for S/N enhancement. Digital signal processing techniques are widely applied in spectroscopic measurements for noise reduction[9−14]. Those filtering approaches performed on concentration values, such as Kalman filtering[11,12] or α-β-γ filtering[13], seem to be extremely effective in enhancing S/N values. However, the filtering results of concentration values have limited accuracy, as demonstrated by the analysis that follows.

Typical noise sources in a laser spectrometer include electronic thermal and shot noises, laser excess noise, and optical feedback noise[15]. The optical feedback noise can be effectively eliminated by careful alignment or background subtraction; thus, only the three former types of noises are considered[9]. In terms of dependence on laser power incident on the detector, P_D, these noises are given by $N_{TN}^2 = $ constant, $N_{SN}^2 = \alpha P_D$, and $N_{EX}^2 = \beta P_D^2$, where N_{TN}, N_{SN}, and N_{EX} are the root-mean-square (RMS) detector noise currents due to thermal, shot, and excess noises, respectively; α and β are the proportionality coefficients[8]. It is assumed that noises are within the system detection bandwidth. Thus, total signal current from the detector is given by $P_D R + \sqrt{N_{TN}^2 + \alpha P_D + \beta P_D^2}$, where R is the detector responsivity. According to the Beer-Lambert law[16], the relationship between P_D and the incident power in the absence of an absorber, P_0, is given by $P_D(k) = P_0(k) \exp[-c\sigma(k)L]$, where $\sigma(k)$ is the absorption cross section, L is the absorption length, and c is the concentration of the gas species. Given that the laser intensity is detected in time sequence, the frequency scale is replaced by a discrete time scale k for convenience. Thus, the true concentration c is calculated by

$$c = -\frac{\ln[P_D(k)/P_0(k)]}{\sigma(k)L}. \tag{1}$$

Replacing $P_D(k)$ with $P_D(k)R(k) + \sqrt{N_{TN}^2(k) + \alpha P_D(k) + \beta P_D^2(k)}$ and considering the unit of denominator in the logarithmic term in Eq. (1), we obtain

$$c_N = -\frac{\ln\left\{\exp[-c\sigma(k)L] + \frac{\sqrt{N_{TN}^2(k) + \alpha P_0(k)\exp[-c\sigma(k)L] + \beta P_0^2(k)\exp[-2c\sigma(k)L]}}{P_0(k)R(k)}\right\}}{\sigma(k)L},$$

where c_N is the calculated concentration value. Obviously, the relationship between c_N and c is so complicated that c_N cannot be simply indicated by a model of c plus an additive noise. Therefore, approaches to post-process concentration values using linear optimal filters are invalid. A potentially more accurate method is to cancel the noise before the calculation, i.e., to filter the direct absorption spectral data output of the detector[12]. To date, the most commonly used method in direct absorption spectroscopy is the simple averaging of previous n measurements. This technique, which is effective in improving S/N values by reducing the electronic systems
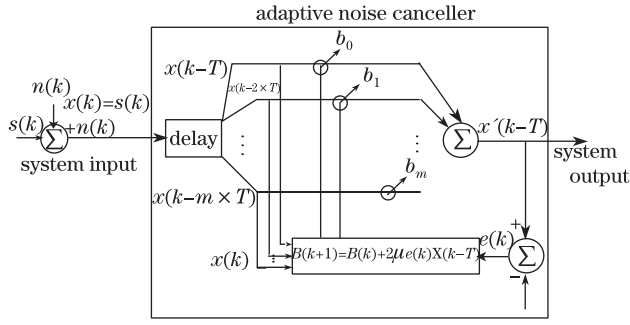
Fig. 1. Adaptive filtering approach for removing noise in direct absorption spectral signal.

bandwidth, is limited by its low duty cycle[17]. As such, this technique is not extremely practical in a system where rigorous real-time monitoring ability is necessary.

The primary objective of the current study is to develop a real-time noise filtering technique for direct absorption spectral signal. We report an adaptive noise-cancelling technique based on the least mean squares (LMS) algorithm. Preliminary experimental results indicate that this adaptive filter can recover the absorption profile from a severely corrupted signal, thereby enhancing the S/N value.

The pioneering work of adaptive noise cancelling is firstly developed by Widrow *et al.*[18]. Although this filter system is successfully applied to several additional problems, a reference noise signal is rarely available from a second sensor in absorption spectroscopy. Therefore, we take another form of adaptive filter, the reference input of which is also the contaminated signal. This improved adaptive filter is originally developed by Sambur[19] to improve the quality of quasi-periodic speech signal. The direct absorption signal is periodic because of the repetitive tuning of laser currents. Thus, this filter can also be used in removing noise in spectral signal, requiring only small modifications in the system input. The principle and structure of this adaptive filter are illustrated in Fig. 1, where $s(k)$ is the absorption signal $P_0(k)\exp[-c\sigma(k)L]R(k)$, $n(k)$ is the noise signal $\sqrt{N_{\mathrm{TN}}^2(k)+\alpha P_{\mathrm{D}}(k)+\beta P_{\mathrm{D}}^2(k)}$, $e(k)$ is the error signal, and T is the signal period. Here, $s(k)$ and $s(k-T)$ are highly correlated because the absorption signal is periodic, but $n(k)$ and $n(k-T)$ are not correlated with themselves and the spectral signal. We assume that $n(k)$ is statistically stationary and has zero mean. Taking the expectation of $e^2(k)$ yields

$$E\left[e^2(k)\right] = E\left\{\left[s(k)-x'(k-T)\right]^2\right\} + E\left[n^2(k)\right]$$
$$+ 2E\left[n(k)s'(k-T)\right] + 2E\left[n(k)n'(k-T)\right]$$
$$= E\left\{\left[s(k)-x'(k-T)\right]^2\right\} + E\left[n^2(k)\right]. \quad (2)$$

As can be concluded from Eq. (2), when the filter is adjusted so that $E\left[e^2(k)\right]$ is minimized, the finite impulse response (FIR) of the filter is given by

$$x'(n-T) = \sum_{i=0}^{m} b_i x(k-i\times T), \quad (3)$$

where b_i represents the weight coefficients and m is the filter order. Meanwhile, the weight vector $B(k) = |b_0,b_1,\cdots,b_m|$ is updated by the LMS algorithm[20] as

$$B(k+1) = B(k) + 2\mu e(k)\mathrm{X}(k-T), \quad (4)$$

where $\mathrm{X}(k-T) = |x(k),x(k-T),\cdots,x(k-m\times T)|^{\mathrm{T}}$. In addition, μ is a factor limited by $0 < \mu < 1/\lambda_{\max}$ for the sake of stability, where $\lambda_{\max}$ is the largest eigenvalue of the matrix $E[\mathrm{X}(k)\mathrm{X}(k)^{\mathrm{T}}]$.

The process of this algorithm is divided into two steps in time sequence. The first step is to choose the appropriate values of μ and m. The value of μ is not extremely significant, because the quality of the filtered spectral signal is insensitive to the exact value of μ as long as μ is sufficiently small[19]. A good compromise value for μ in this study is 10^{-6} considering the convergent time and filtering precision. However, the value of m should be chosen with caution. An overlarge value of m results in filter lags behind the real absorption lineshape, which impairs detection sensitivity. The consuming time for convergence is also affected by m. Usually, convergence is inversely proportional to m and is less than $m/10$ periods. When m is determined, the adaptation begins at $(m+1)$ period once the m periodical signals have been collected. Given that the weight vector $B(k)$ is originally set to 0, the filtered data eventually converges on the real data from 0 with the feedback of $e(k)$.

Figure 2 presents a schematic diagram of the setup used for CH_4 concentration sensing. This portable measuring system was developed by our research team for the purpose of monitoring CH_4 in environments such as oil fields and mine tunnels[13]. The laser source used was a commercial DFB laser (NEL Electronic) driven by a temperature controller and a current controller (ILX Lightwave). The laser wavelength was slowly scanned from 1.6536 to 1.6538 μm by a 56-Hz sawtooth waveform produced by a microcontrol unit (Silicon Labs).
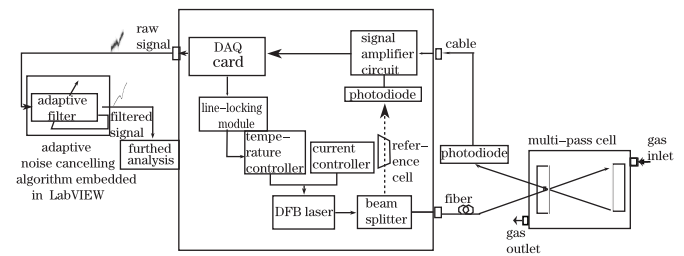

Fig. 2. Schematic diagram of the setup used for monitoring CH_4.
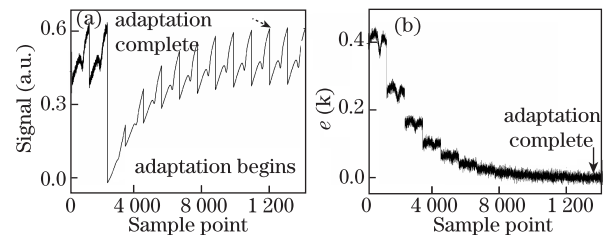

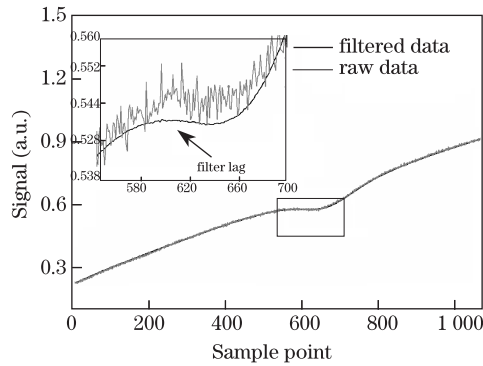Fig. 3. Adaptation processes in (a) absorption signal and (b) error signal.

Fig. 4. Filter lag phenomenon.

The laser light was transmitted by a single-mode fiber to the reference cell and the outside Herriott multi-pass sample cell (29-m total optical length) after undergoing collimation. The multi-pass cell was placed in a constant temperature (296 K) case with a gas inlet and outlet so that the reference cell was a sealed glass tube the thermal expansion interference could be minimized[21]. with a small quantity of CH_4 in it. This cell is used so that the line-locking scheme can relieve the impact of drift. The absorption signals from two cells were detected by two InGaAs photodiodes (GPD Corp.), which were decoupled to two wide gain bandwidth (5 MHz) operational amplifiers. After a current-to-voltage conversion, the data were digitized by a 16-bit DAQ card (WWLAB) at a sampling rate of 200 kS/s. Data analysis and experimental control were performed by a program written in LabVIEW 2010 software. The adaptive noise-cancelling algorithm was embedded into the software as a form of a MATLAB script. Although approximately 1 780 points could have been sampled every period by the DAQ card, only 1 100 points were recorded to avoid the nonlinear response region of operational amplifiers[22]. This process was accomplished by synchronizing the DAQ card with a TTL output. Both raw and filtered data were stored for further analysis.

A noisy raw signal and a relatively clean signal achieved after undergoing filtration are shown in Fig. 3(a). The raw data of 850 direct absorption spectra were recorded after a quantity of approximately 70-ppm CH_4 had been injected into the Herriott cell. Figure 3(b) shows the variation trend of error signal $e(k)$. The process of convergence can be seen clearly in both figures. The filter order is 750 in this case, and the minimum mean-squared error $E\left[e^2(k)\right]_{\min}$ is realized after 9 signal periods. By comparison, two periods of raw absorption signal are illustrated before the beginning of adaptation.

The S/N values of both sets of raw and filtered data were calculated in order to indicate the effectiveness of this filtering technique in noise suppression. Although the absorption signal quantified by $\sqrt{P_0^2 - \overline{P_D^2}}$ (the bar denotes an average value) is more appropriate to be taken as the signal value in calculating the S/N[7] , the exact value of P_0 is difficult to achieve. Usually, P_0 is estimated by fitting the zero absorption wings of each scan using a low-order polynomial[16]. However, strong noises in direct absorption spectra (e.g., Fig. 5(a)) lead to a poor fit. Thus, the S/N value is not accurate and is de-

pendent on the goodness of fit. In fact, the definition of the signal value $\left(\sqrt{\overline{P_0^2} - \overline{P_D^2}} \text{ or } \sqrt{\overline{P_D^2}}\right)$ is not extremely significant in this letter, because we focus only on how well the noise is suppressed. We calculate the S/N value by $10\log_{10}\left[\overline{P_D^2}\Big/\left(P_D - \sqrt{\overline{\overline{P_D^2}}}\right)^2\right]$. Through this process, we obtain 27 and 55 as the S/N values of the raw and filtered data, respectively. Thus, a S/N enhanced by a factor of about 2 is observed in this example.

Shorter converging time and higher S/N enhancement are acquired by some specific larger filter orders. However, as described previously, an overlarge filter order causes filter lags and increases the measuring uncertainties. An obvious filter lag phenomenon can be seen in Fig. 4.

In this case, the filter order is 800, and the relative error is 2.4% in terms of peak absorbance. This phenomenon occurs especially when the absorption signal is extremely small, which tends to distort the absorption profile. Thus, the choice of filter order must be a balance between consuming time and filtering solution precision. The sum of the weights is always approximately 1 after convergence; hence, the adaptive noise canceller is essentially a kind of recursive averaging algorithm. In relation to this, an alternative solution to find an optimum filter order with a maximum absorption signal fidelity is to calculate the Allan variance[14] or to use the experimental results.

In this letter, the optimum filter order in the measuring system is approximately 500 according to the experimental results. A higher S/N enhancement magnitude is achieved after determining the optimum order. A severely corrupted spectral signal is recorded in an open-air CH_4 measuring experiment conducted by our research team, and the details of this experiment can be seen in Ref. [23]. Raw and filtered data by an optimum filter order of 500 are presented in Figs. 5(a) and (b), respectively. The raw signal is heavily interfered mainly by turbulence in the air, and the absorption profile is difficult to recognize. After being filtered, the absorption profile can be recovered from the corrupted raw signal although it is slightly noisy. The S/N values of the raw data and filtered data are 6 and 32.6, respectively. Thus, the value of S/N is improved by a factor of approximately 5.4 in this case.

Response time, which characterizes the real-time detection ability of the system, is another key aspect that should be considered. Here, we take the process of averaging 100 scans as an example. In this letter, this takes approximately $100/56 \approx 1.8$ s. By comparison, only
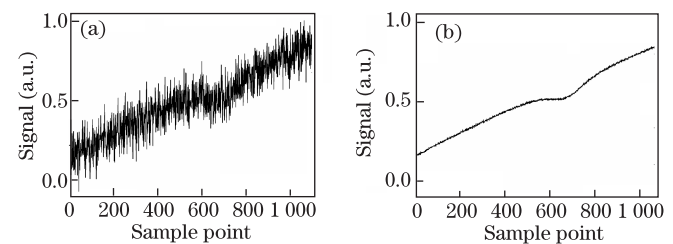

Fig. 5. (a) Severely corrupted signal; (b) filtered signal.

200 ms was needed by an adaptive filter with an order of 100, which was run on a 3.3-GHz CPU. Therefore, the consuming time is shortened by a factor of 9. A shorter computing time is achieved using a language like C or FORTRAN, because the original program is written by a language that is not optimized for speed.

In conclusion, an adaptive noise-cancelling algorithm for filtering direct absorption spectra and the merits of the filtering solution are discussed in detail. Several experiments are performed to investigate the effectiveness of the filter. A S/N enhancement factor of 5.4 is observed with an optimum filter order. The response time of an adaptive filter with a 100 filter order is 9 times shorter than signal averaging of 100 scans. To our knowledge, this is the first time an adaptive filter is used for noise cancelling in direct absorption spectroscopy. This filtering technique can be applied to all branches of direct absorption spectroscopy, especially where a high S/N value is needed. In the future, the use of this filter technique can be extended to modulation spectroscopy to obtain more accurate measurement results and a lower detection limit.

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