Finding the optimal TDLS wavelength

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We present a mathematical method which allows determination of the optimal spectral range for gas mixture analysis based on theoretical absorption spectra. The algorithm is particularly suited for tunable diode laser spectroscopy (TDLS) and represents a multi-step mathematical calculation which can easily be implemented in almost any programming language. We applied the method to exemplary mixtures of hydrocarbons and present the according results.

Introduction – Laser spectroscopy is nowadays a well-established method for the analysis of gaseous mixtures [1,2]. When designing a laser spectrometer, the definition of the laser's emission wavelength or, if tunable, its spectral range is crucial for its potential applications. In practice the identification of a suited spectral range for a certain application, i.e. for the analysis of a certain mixture of gases, is often an educated guess based on known spectra [2,3]. We present, to the best of our knowledge, the first quantitative method to determine a well suited spectral range for sensitive and selective gas analysis. The procedure is customized for lasers of a certain tuning range, such as semiconductor lasers, and delivers its optimal center wavelength.

Mathematical procedure – Fig. 1 shows the flowchart of the mathematical procedure. Prerequisite for the application is that absorption spectra of all relevant components in the mixture are known. They can be measured beforehand or extracted from according databases.

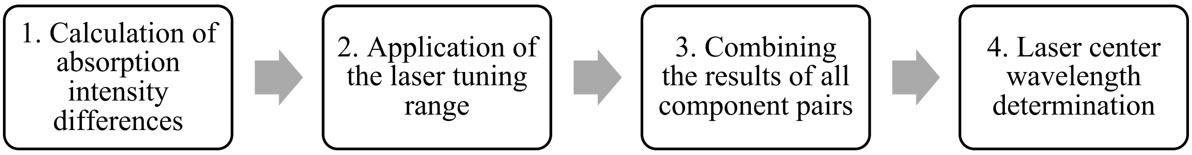

Fig 1. Flowchart of the mathematical procedure.

In order to detect the individual gas components selectively, i.e. with least ambiguity, it is necessary to identify the wavelengths at which the absorption spectra maximally differ from one another [4]. These spectral regions are found in a first step by calculating the intensity differences for each pair of gases. The application of the laser tuning range, approximately 10 nm in case of an interband cascade laser, is implemented in a second step by integrating the single difference spectra over that 10 nm. This integration can be considered a window function that slides over the entire spectral range. In order to combine the contribution of all gas pairs, the "filtered" differences are multiplied. This third step delivers the wavelengths at which the single gas pairs maximally differ and, at the same time, absorption is strong. The wavelength region around the maximum of this function indicates the spectral range in which the center wavelength of the laser should be located. In a fourth step the median of this range is calculated and considered to be the optimum laser center wavelength.

Exemplary results – The mathematical procedure described above was programed in MATLAB and applied to assumptive gas mixtures. Fig. 2 shows the results for a mixture of $^{12}CH_4$ and $^{13}CH_4$. Fig. 3 shows them for a mixture of $^{12}CH_4$, $^{12}C_2H_4$ and $^{12}C_2H_6$. The resulting optimum laser center wavelengths λ_C are 3320.7 nm and 3347.3 nm, respectively. The yellow boxes mark the respective laser tuning ranges.

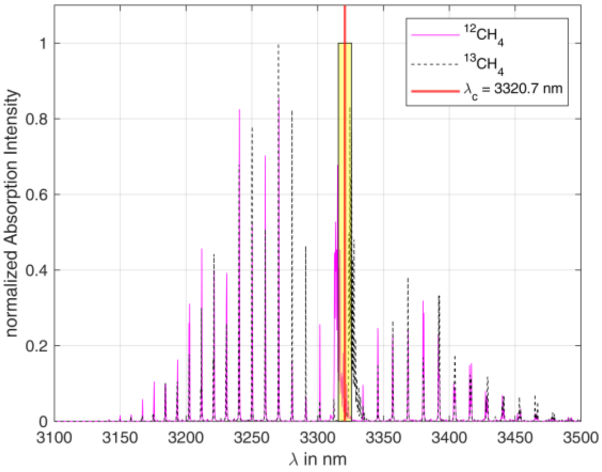

Fig. 2 Mixture of $^{12}CH_4$ and $^{13}CH_4$ [5].

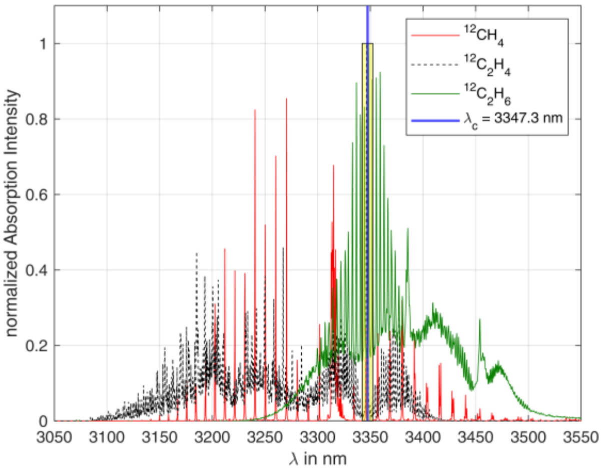

Fig. 3 Mixture of $^{12}CH_4$, $^{12}C_2H_4$ and $^{12}C_2H_6$ [5-7].

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