Selective BTEX Measurements Using Deep Neural Networks

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Abstract: A laser sensor is developed for selective and simultaneous BTEX measurements. It is based on a DFB-ICL near 3.3 μm and deep neural networks (DNNs) to differentiate broad absorbance spectra of BTEX species.

1. Introduction

Emissions of volatile organic compounds (VOCs) are linked to petrochemical industries. Particularly, engine exhaust, gasoline fuel, refineries, painting and rubber industries [1] cause significant emissions of benzene, toluene, ethylbenzene and isomers of xylene (BTEX). Short exposure (5 – 10 min) to 10,000 – 20,000 ppm of benzene can lead to death, while 70 – 3000 ppm can cause unconsciousness, dizziness or drowsiness [2]. Inhaling 600 – 5000 ppm of toluene can result in severe damages to the brain, liver and kidneys [3]. Irritation of eyes and the respiratory tract have been reported after exposure to 1000 – 5000 ppm of ethylbenzene for a few seconds [4]. Scientists have found that the three isomers of xylene have similar health effects, where exposure to 700 – 10,000 ppm can cause lack of muscle coordination and distortion in the nervous system [5]. Therefore, there is a dire need for new selective BTEX sensors as the existing ones are limited in terms of selectivity due to the similar BTEX molecular structures. In this paper, we report the use of a mid-IR laser to develop a sensor for selective measurements of BTEX species with deep neural networks (DNNs) to distinguish their similar broadband absorbance spectra.

2. Sensor Description

The best wavelength region to measure BTEX is near 14 μm [6]; however, commercially available semiconductor laser sources cannot span this region. Therefore, we selected ro-vibrational BTEX bands near 3.3 μm which are the result of C-H stretching motion. A detailed discussion about choosing this region is shown in a previous work on benzene sensing [7]. Simulated absorbance spectra of all BTEX species in this range are shown in Fig. 1 (T = 25 °C, P = 1 atm, L = 30 cm, χ = 1000 ppm) [6]. Similar C-H stretching of the aromatic rings makes ro-vibrational spectra of BTEX to be very similar. Therefore, we implemented deep neural network (DNN) algorithm and wavelength-scanning to selectively measure the concentration of each of the BTEX species simultaneously. The sensor uses a DFB interband cascade laser (DFB-ICL, Nanoplus) emitting near 3.3 μm with an output power ~ 1 – 2 mW. Two ZnSe windows (Thorlabs) were used in a 30 cm sampling cell. The transmitted signal was collected with a DC-coupled, TE-cooled photodetector (bandwidth of 1.5 MHz, Vigo Systems).

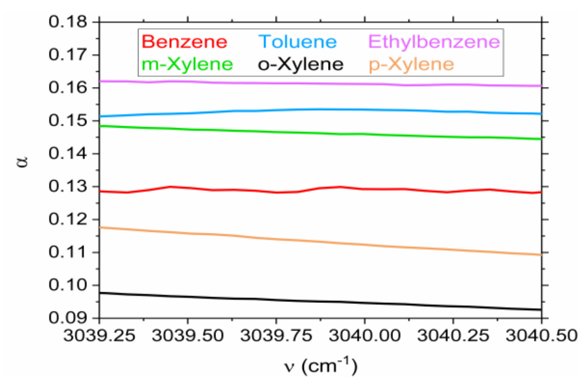

Fig. 1. BTEX absorbance spectra at T = 25 °C, P = 1 atm, L = 30 cm, χ = 1000 ppm over 3039.25 – 3040.5 cm^{-1} [6].

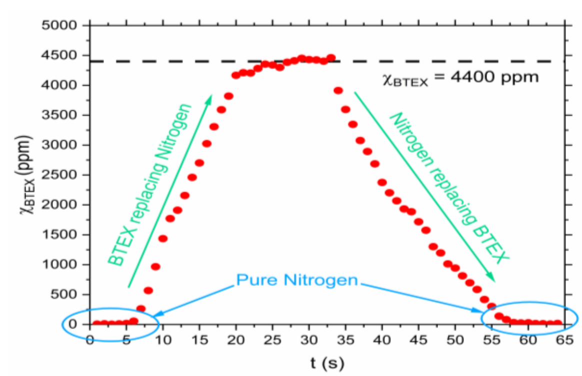

Fig. 2. Real-time measurement of total BTEX flow through a sampling cell (T = 25 C, P = 1 atm, L = 30 cm, χ = 4400 ppm).

3. Results and Discussion

Known absorbance cross-sections and multi-dimensional linear regression (MLR) can be used to measure total BTEX concentration. However, the predictive ability of MLR is affected by the similarly-shaped broad BTEX spectra, and MLR algorithm cannot distinguish among the various species. Therefore, other machine learning methods like support vector machines (SVM), gradient boosting (XGB) and deep neural networks (DNNs) were explored here. Gas samples with known BTEX concentrations were prepared to validate the capability of this diagnostic for simultaneous BTEX measurements. Table 1 shows the 10-fold cross validation results of these methods performed on 5400 simulated and

132 measured BTEX absorbance spectra with varying concentrations of each species. DNN with 3 hidden layers of 64, 32 and 16 nodes, respectively, performs best in terms of the root mean square error (RMSE) and R^2 values of these methods, and thus DNN was used for training and testing models based on a random 80/20 split. A real-time validation test was performed with a 4400 ppm BTEX mixture by flowing BTEX/N_2 continuously through the cell, as shown in Fig. 2. Finally, Fig. 3 shows the results of applying DNN on 12 mixtures containing various BTEX concentrations. Excellent agreement between the measured and manometric concentrations shows the capability of our sensor to perform selective and simultaneous BTEX measurements.

Table 1: 10-fold cross validation results of MLR, SVM, XGB and DNN.

Fitting parameter	MLR	SVM	XGB	DNN
RMSE	0.096	0.093	0.041	0.024
R^2	0.722	0.774	0.945	0.985

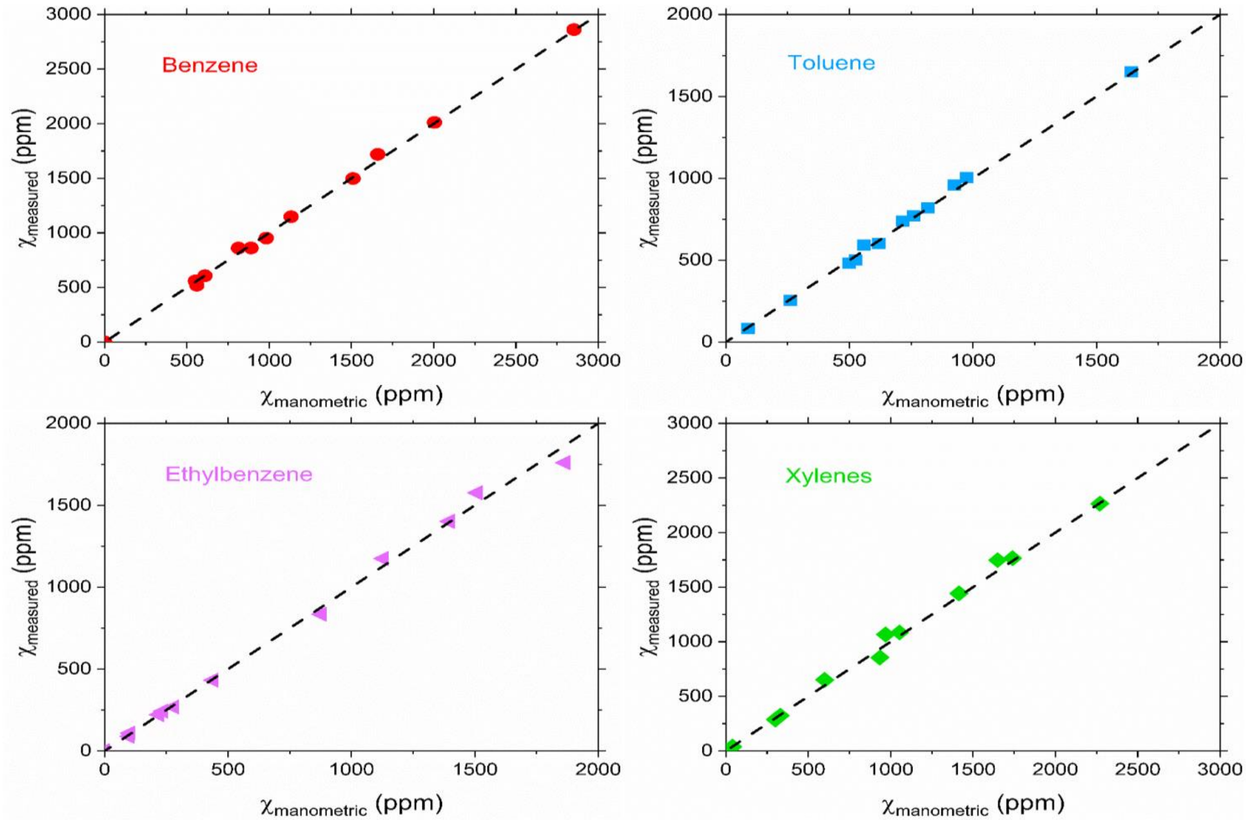

Figure 3: BTEX predicted concentrations using DNN versus manometric concentrations.

4. Conclusions

A laser-based absorption sensor has been developed for selective measurements of BTEX species. The sensor was validated by gas samples prepared in the lab, and can selectively and simultaneously measure all BTEX species with a DNN algorithm. The sensor can be utilized to measure BTEX in petrochemical, painting and rubber industries where the concentrations of these species are elevated and can lead to severe health risks.

5. References

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