Deep neural networks for simultaneous BTEX sensing at high temperatures

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Abstract: In the study of chemical reactions, it is desirable to have a diagnostic strategy that can detect multiple species simultaneously with high sensitivity, selectivity, and fast time response. Laser-based selective detection of benzene, toluene, ethylbenzene, and xylenes (BTEX) has been challenging due to the similarly broad absorbance spectra of these species. Here, a mid-infrared laser sensor is presented for selective and simultaneous BTEX detection in high-temperature shock tube experiments using deep neural networks (DNN). A shock tube was coupled with a non-intrusive mid-infrared laser source, scanned over 3038.6–3039.8 cm⁻¹, and an off-axis cavity enhanced absorption spectroscopy (OA-CEAS) setup of ~100 gain to enable trace detection. Absorption cross-sections of BTEX species were measured at temperatures of 1000–1250 K and pressures near 1 atm. A DNN model with five hidden layers of 256, 128, 64, 32, and 16 nodes was implemented to split the composite measured spectra into the contributing spectra of each species. Several BTEX mixtures with varying mole fractions (0–600 ppm) of each species were prepared manometrically and shock-heated to 1000–1250 K and 1 atm, and the composite measured absorbance were split into contributions from each BTEX species using the developed DNN model, and thus make selective determinations of BTEX species. Predicted and manometric molefractions were in good agreement with an absolute relative error of ~11%. We obtained a minimum detection limit of 0.73–1.38 ppm of the target species at 1180 K. To the best of our knowledge, this work reports the first successful implementation of multispecies detection with a single narrow wavelength-tuning laser in a shock tube with laser absorption spectroscopy.

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1. Introduction

Laser sensors provide quantitative, non-intrusive, and high-temporal resolution measurements of chemical species in high-temperature environments, and thus have proven to be vital for combustion research and development [1,2]. Laser absorption spectroscopy (LAS) has been utilized in various combustion systems, such as shock tubes, rapid compression machines (RCMs), and flow reactors to understand chemical kinetics at elevated temperatures and pressures [3–6]. In particular, shock tubes provide well-controlled, quiescent conditions spanning wide temperature and pressure ranges. Extensive shock tube and RCM studies have been directed towards developing a database of ignition delay times (IDTs) of hydrocarbon fuels. While IDTs provide global validation targets for chemical kinetic models, they are not sufficient to fully test the fidelity of detailed chemical kinetic models. Species concentration measurements during chemical reactions provide such high-fidelity targets. These measurements, particularly simultaneous multi-speciation, are quite scarce in literature [7].

Typically, LAS is used to detect a single species at the resonant wavelength. LAS has been employed for hydrocarbon sensing in both the near- and mid-IR spectral regions. Mid-IR laser sources are increasingly being utilized as absorption strengths of many hydrocarbons are orders of magnitude higher in the mid-IR region compared to the near-IR [8,9]. Previous studies of mid-IR hydrocarbon detection include the use of lead-salt diode lasers that required cryogenic...
cooling [10]. Difference frequency generation (DFG) systems based on nonlinear optics can also be used to access the mid-IR region but these sources are generally quite complex and give out low power [6]. Quantum cascade lasers (QCLs) and inter-band cascade lasers (ICLs), on the other hand, are compact, robust, and user-friendly semiconductor sources, and have thus gained high popularity for hydrocarbon detection [11].

In the presence of more than one absorbing species, differential absorption (peak-minus-valley) strategy takes advantage of narrow spectral features of target species to account for interference from broadly absorbing molecules [12], while multidimensional linear regression (MLR) can be applied over a wavelength range to split the composite spectra into the contributions from absorbing species [13]. However, detection strategies have not been previously designed for multi-species detection in the case of similarly-shaped broad absorbance spectra [14]. Recently, we showed that simultaneous detection of species having similar absorbance spectra is possible by using deep neural networks and wavelength scanning [15]. This was demonstrated by selective sensing of benzene, toluene, ethylbenzene, and xylenes (BTEX) at ambient conditions. Extension of this technique to high temperatures is far from trivial due to the spectral variation with temperature and complex experimental conditions. Such a capability can play an important role in studying reaction kinetics at elevated temperatures which involves several species being simultaneously formed and consumed. For example, pyrolysis/oxidation of the aromatic components of distillate fuels can lead to the formation of a large number of polycyclic aromatic hydrocarbons (PAHs). Understanding the detailed chemistry of these components is crucial to minimize harmful emissions from our current energy infrastructure.

Laser sources targeting the C-H stretching band near 3.4 µm have been utilized in pyrolysis/oxidation speciation studies in shock tubes [16,17]; however, the broad overlapping absorbance spectra of the formed hydrocarbons obfuscate post-processing of the measured composite spectra, and thus preclude interference-free sensing. Multi-color diagnostics have been employed for multi-species measurements using a sufficient number of laser sources, which adds significant complexity and cost to the diagnostic system. For example, a recent study by Cassady et al. addressed the pyrolysis of propane using nine wavelengths (6 laser sources) to quantify the major carbon-containing species [18]. Due to the limited optical access in the shock tube, the experiments had to be repeated two or three times since all wavelengths could not be transmitted simultaneously through the shock tube. Hence, more uncertainty was introduced by the variation of thermodynamic conditions of the repeated shocks.

Aromatic hydrocarbons are present in significant amounts in commercial gasoline, diesel, and kerosene [19]. Building chemical kinetic models of real fuels as well as performing their experimental studies is quite challenging. Alternatively, studies can be performed on surrogate fuels with physical and chemical properties mimicking the real fuels. Benzene, toluene, ethylbenzene, and xylenes (BTEX) are good candidates to represent the aromatic fraction of commercial fuels, such as gasoline [20]. Several combustion studies have been carried out on BTEX species over wide ranges of temperatures and pressures. However, their pyrolysis and oxidation are still far from being understood [21]. Typically, the target species were sampled from the reactor and analyzed using gas chromatography (GC) and mass spectrometric (MS) methods [22,23]. Studying the chemistry of BTEX species would also enable models of PAHs which are vital to the formation of soot particles and the evolution of carbon galaxies [24].

In this work, we report the use of a mid-IR laser source and cavity-enhanced absorption spectroscopy (CEAS) to develop a sensor for simultaneous BTEX measurements at elevated temperatures (1000–1250 K) in a shock tube. We employed deep neural networks (DNNs) to distinguish the similar broadband absorbance spectra of BTEX species. This work provides a novel framework and a new diagnostic strategy which exploits advancements in data processing techniques for the detection of multiple species simultaneously.
2. Laser absorption spectroscopy

Laser intensity attenuation through an absorbing medium gives information about the medium’s temperature, pressure, and/or composition. Beer-Lambert law of laser absorption spectroscopy relates the changes in laser intensity to gas properties [25]:

\[
\alpha_{\text{SP}} = \ln \left( \frac{I_0}{I_t} \right) = \sigma(T, P, \nu) \cdot n(T, P) \cdot L \cdot \chi
\]

where \( \alpha_{\text{SP}} \) is the measured absorbance for a single pass of the laser, \( I_0 \) and \( I_t \) are the incident and transmitted laser intensities, respectively, \( \sigma(T, P, \nu) \) is the temperature- and pressure-dependent absorption cross-section that describes species propensity to absorb light at a frequency \( \nu \), \( n(T, P) \) is the total number density of the gas mixture, \( L \) is the absorption path-length (inner diameter of the shock tube in this work), and \( \chi \) is the mole fraction of the absorbing species. When multiple species absorb at the same frequency, their absorbances are simply added to get the total composite absorbance.

For a given absorption transition and experimental conditions \( (T, P, \nu) \), trace concentrations of absorbing species result in negligibly small absorbance. Increasing the path-length, \( L \), is typically the only option to reliably detect such species [26]. Cavity-based techniques, such as cavity ring-down spectroscopy (CRDS) and cavity-enhanced absorption spectroscopy (CEAS), have made a significant contribution towards the detection of trace species [27]. These techniques amplify the path-length by utilizing two highly reflective concave mirrors to create an optical cavity through multiple reflections of the laser light. Although both techniques observe the light intensity exiting the cavity, their operating principles are different [28]. In CRDS, light intensity builds up inside the cavity until the laser is turned off, and the transmitted signal then decays exponentially with a characteristic time which depends on cavity parameters and gas absorption [29]. In CEAS, a continuous wavelength laser is typically scanned over a specific spectral range to observe a spectrally-resolved absorption feature [30]. Here, cavity absorbance, \( \alpha_{\text{CEAS}} \), is given as [31]:

\[
\alpha_{\text{CEAS}} = \ln \left( \frac{I_0}{I_t} \right) = \ln(1 + G \cdot U)
\]

where \( G \) is the gain factor of the cavity which is derived from mirrors’ reflectivity, \( R \), by \( G = R / (1 - R) \), and \( U = 1 - e^{-\alpha_{\text{SP}}} \). In the case of a weak absorber and high reflectivity (\( \alpha_{\text{SP}} \rightarrow 0 \) and \( R \rightarrow 1 \)), Eq. (2) simplifies to:

\[
\alpha_{\text{CEAS}} \approx G \cdot U
\]

3. Experimental details

3.1. Low pressure shock tube facility

Measurements were performed in the stainless steel, electro-polished, low-pressure shock tube (LPST) facility at King Abdullah University of Science and Technology (KAUST). The LPST has an inner diameter of 14.22 cm and a driven section length of 9.1 m. Driver section length can be varied up to a maximum of 9.1 m, used in this study, with high purity helium (99.99%) as the driver gas. The driven and driver sections were separated by a 0.005" polycarbonate diaphragm. Before each shock, driver and driven sections were pumped down by mechanical vacuum pumps, with the latter connected to a turbo-molecular vacuum pump to ultimately achieve 1 \( \mu \)Torr. Mixtures were prepared in a magnetically-stirred stainless steel tank and left to homogenize for at least one hour to ensure homogeneity. High-purity argon (99.9999%) was used as the bath gas. Chemicals used were as follows: benzene (99.8\%, Sigma-Aldrich), toluene (98\%, VWR Chemicals), ethylbenzene (99.8\%, Acros Organics), xylenes (99.8\%, Acros Organics). Five PCB piezoelectric pressure transducers (Kistler PZT, 603B1), installed over the last 1.3 m of the driven
section, were used to measure incident shock velocity. Reflected shock temperature and pressure were calculated using 1-D shock-jump relations [32,33]. Temperature and pressure uncertainties were calculated to be ±0.7% and ±1%, respectively, and were mainly caused by uncertainties in the measured incident shock speed and mixture composition [6]. Further details of the shock tube facility can be found elsewhere [34,35].

3.2. Wavelength selection

Based on a detailed interference analysis for benzene detection in a previous work [36,37], we selected the C-H stretching bands near 3.3 µm (3039 cm⁻¹) to measure BTEX species. As high-temperature cross-section data are unavailable in literature, Fig. 1(a) shows simulated absorbance spectra of BTEX species at ambient conditions (T = 25 °C, P = 1 atm, L = 30 cm, χ = 1000 ppm) [38]. The zoom-in view in Fig. 1(b) shows that BTEX species exhibit very similar absorption features near 3039 cm⁻¹ due to the common C-H stretching vibrational modes in their aromatic rings. This makes it highly challenging to measure BTEX species selectively in this wavelength region.

![Figure 1](image)

**Fig. 1.** BTEX spectra in the C-H stretching band (T = 25 °C, P = 1 atm, L = 30 cm, χ = 1000 ppm). Spectral data taken from the PNNL database [38], (a) over 3000–3100 cm⁻¹, (b) zoom-in view over 3038.6–3039.8 cm⁻¹.

3.3. Optical setup

Optical layout of the sensor designed in this work is shown in Fig. 2, where we used a DFB interband cascade laser (ICL, Nanoplus) emitting near 3.3 µm with an output power ~ 1 mW. Higher power commercial lasers are not available in this region. The laser was scanned, with a sawtooth injection current, over 3038.6–3039.8 cm⁻¹ at a repetition frequency of 10 kHz. A 670 nm red laser (Thorlabs) was propagated collinearly with the IR laser to facilitate optical alignment. Two ZnSe mirrors of 99.25 ± 0.3% nominal reflectivity, 20 mm diameter, 3 mm thickness, and 1 m radius of curvature were used to form a cavity in the low-pressure shock tube. Mirrors were glued to custom designed plugs and mounted on the shock tube ports located 2 cm away from the shock tube end-wall. Three fine adjustment screws (Thorlabs, FAS100) were used for cavity alignment. In this work, we implemented an off-axis cavity alignment which helps suppress spurious coupling noise compared to an on-axis cavity. The transmitted laser signal was collected via a focusing lens on to a DC-coupled, TE-cooled photodetector (bandwidth of 1.5 MHz, Vigo Systems). A 7.62 cm germanium etalon, with a free-spectral range (FSR) = 0.0164 cm⁻¹, was utilized to convert the scan time to wavenumbers.
4. Experimental results

4.1. Cavity gain evaluation

Cavity gain is determined by the mirrors’ reflectivity. The actual value of reflectivity can deviate significantly from the manufacturer’s nominal specification, resulting in large uncertainty in the cavity gain. Here, the manufacture-specified nominal reflectivity of 99.25\(\pm\)0.3\% results in a gain of 132\(\pm\)89, which is an unacceptably wide range. Thus, a more precise value of the cavity gain (G) is needed. We performed experiments for the evaluation of G using various mixtures of each BTEX species in argon with known compositions (0.05–0.2\%), over \(T = 950–1300\)K and \(P \sim 1\) atm. Cavity gain was determined by plotting \(\alpha_{\text{CEAS}}\) against \(U\), as shown in Fig. 3. Here, cavity gain comes out to be 97\(\pm\)2, with significant improvement in the uncertainty bounds. The uncertainty (\(\pm\)2) was determined based on a 95\% confidence interval of the measured values. This value of cavity gain increases the effective laser path-length from 14.22 cm (shock tube internal diameter) to 13.79 m. Uncertainties of \(\alpha_{\text{CEAS}}\) and \(U\) are obtained from Eqs. (4) and (6) given in Section 4.5.

4.2. Absorption cross-sections

High-temperature absorption cross sections of benzene, toluene, ethylbenzene, and xylenes were measured experimentally behind reflected shock waves over \(T = 1000–1250\)K and \(P \sim 1\) atm with known mole fraction (0.01–0.5\% in argon) of each species. The laser was scanned over 3038.6–3039.8 cm\(^{-1}\) at a repetition rate of 10 kHz. A representative shock for determining cross section of benzene (\(T = 1180\)K, \(P = 1\) atm, \(\chi = 339\) ppm) is shown in Fig. 4. Here, \(I_0\) was measured with the shock tube at vacuum, and \(I_t\) was collected behind the reflected shock wave. The red highlighted part in Fig. 4 refers to the pre-shock conditions, while the green part refers to conditions behind the reflected shock. Time zero indicates the arrival of the reflected shock at the measurement location (2 cm from the end-wall). It was observed that the absorption cross sections obtained from various laser scans were nearly identical, which means that benzene did not react / decompose at these conditions. Absorption cross sections were thus obtained by averaging cross section values of laser scans between 0 and 2 ms. The vertical shift in \(I_t\) is caused...
Fig. 3. Cavity absorbance as a function of U (see Eq. (3)). The slope represents the cavity gain. Measurements were carried out over $T = 950–1300 \text{K}$ and $P \sim 1 \text{ atm}$.

by thermal emission, and was minimized by a 3.3 $\mu$m band-pass filter (Thorlabs, FB3330-150, FWHM = 150 nm). The shift does not affect the features of the signal, and was simply subtracted from $I_t$.

Fig. 4. Detector signals of incident and transmitted laser intensities in pre-shock (red highlighted, $T_1 = 295 \text{ K}, P_1 = 0.05 \text{ atm}$) and post-reflected-shock (green highlighted, $T_5 = 1180 \text{ K}, P_5 = 1 \text{ atm}$) regions. Pressure trace is shown on the right vertical axis. Mixture: 339 ppm benzene in argon.
Temperature-dependent absorption cross sections of benzene, toluene, ethylbenzene, and xylenes were determined by Eq. (1). Figure 5 shows measured cross-sections over 1000–1250 K, which were determined by performing reflected-shock experiments over 950–1300 K, and interpolating measured spectra at increments of 50 K. To compare cross-sections of target BTEX species at the same temperature, a representative plot is shown in Fig. 6(a) at 1180 K. Given the similarly-shaped broad spectra of these species over the investigated wavelength range, the predictive ability of traditional fitting models (e.g., 1-D linear fitting, multi-dimensional linear regression, partial least squares regression, etc.) is deteriorated, so those models are not able to distinguish our target species. Hence, a deep neural networks (DNN) model was employed to overcome this challenge. In addition, absorption cross-sections were normalized (by the peak cross-section over the measured wavelength range) to highlight weak spectral features of the target species. Such a normalization enhances the ability of the DNN model to differentiate these species. The normalized cross-sections are shown in Fig. 6(b).

4.3. DNN prediction model

The similarly-shaped broad absorption spectra of BTEX, shown in Figs. 5 and 6, make it highly challenging to determine mole fractions of individual molecules from a composite spectral measurement. Multi-dimensional linear regression (MLR) was previously used to distinguish the spectra of benzene, ethylene and methane [36]. The three species had varying spectral features over the tuning range of the laser which enabled their selective detection using MLR. However, the predictive ability of MLR is dramatically compromised in the case of BTEX species due to their similar-shaped spectra. Hence, machine learning algorithms are explored. Based on a previous work, we found that the best method to selectively measure BTEX concentrations at ambient conditions is using deep neural networks (DNN) [15,39]. Here, advancements in model training and tuning were needed for the high-temperature application.

To train the DNN algorithm, we assembled a database comprising of 10,000 simulated spectra and 30 measured spectra. The simulated spectra were based on interpolated high-temperature absorption cross-sections to generate a wide range of concentrations. BTEX mole fractions, $x_i$, were randomly varied in the range of 0–1000 ppm, while the total BTEX concentration, $x_{total}$, was fixed to 1000 ppm. We note that the total concentration does not need to be varied as the concentration ratios, $x_i/x_{total}$, are normalized. For the measured spectra used in the training, mixtures were prepared in the lab with various concentration ratios where the total BTEX concentration scanned a range of 200–1000 ppm. Manometric mixtures were prepared using partial pressures measured with high-accuracy pressure transducers. A mixing tank is evacuated using a turbomolecular vacuum pump, then BTEX species are evaporated into the tank. The bath gas (argon) is finally added so the mole fraction of species $i$ is $x_i = P_i/P_{total}$, where $P_i$ is the partial pressure of species $i$ and $P_{total}$ is the total pressure after adding argon. The simulation and measured data were randomly split in 80/20 train/test sets.

Python 3.8 software was utilized to build the prediction models. A random search algorithm was applied to tune the hyper-parameters of DNN, including the number of hidden layers and nodes, activation functions, dropout layer, weight regularization, learning rate, momentum, number of epochs and batch size. An optimal DNN model of five hidden layers with 256, 128, 64, 32, and 16 nodes, respectively, was utilized. ReLU and Adamax (learning rate = 0.01) were opted as the activation function and optimizer, respectively. The model was run on 2000 epochs with a batch size of 64, and its performance was monitored by mean-squared-error values. To avoid overfitting, the validation loss was monitored with a patience of 20 epochs.

4.4. Sensor validation

To assess the performance of this diagnostic strategy, eight new mixtures with varying concentrations (0–600 ppm) of each of the BTEX species were prepared manometrically, and the
Fig. 5. Temperature dependent absorption cross-sections of benzene, toluene, ethylbenzene, m-xylene, o-xylene, and p-xylene over $T = 1000$–$1250$ K and $P \sim 1$ atm.
Fig. 6. (a) Measured absorption cross-sections of BTEX species at $T = 1180\,K$ and $P \sim 1\,\text{atm}$, over $3038.6$–$3039.8\,\text{cm}^{-1}$, (b) Normalized cross-sections at the same conditions to show spectral features.
measured total absorbance was analyzed the DNN model. These mixtures were not part of the training/testing process. Figure 7 elaborates the overall process followed to build the DNN model and to extract the BTEX ratios.

Figure 7 illustrates the overall process followed to build the DNN model and to extract BTEX ratios. Blue arrows correspond to model tuning using the 10,000 simulated and 30 measured spectra, while green arrows correspond to extracting BTEX ratios from the 8 separately measured spectra.

Figure 8 shows a sample composite absorbance spectrum of a shock-heated BTEX/Ar mixture (manometric values: $\chi\text{Benzene} = 275$ ppm, $\chi\text{Toluene} = 232$ ppm, $\chi\text{Ethylbenzene} = 254$ ppm, $\chi\text{Xylenes} = 241$ ppm, $T = 1180$ K, $P = 1$ atm). Normalizing the absorbance spectrum enhances spectral features which enable the model to differentiate absorbing species, thus leading to their selective determination. The measured concentrations retrieved from this normalized spectrum are compared in Fig. 9 to manometric concentrations.

Figure 8. Measured and normalized composite absorbance spectra of a BTEX/Ar mixture at $T = 1180$ K and $P = 1$ atm.
Excellent agreement between the predicted and manometric BTEX molar fractions in Fig. 10 validates the ability of our diagnostic strategy to selectively and simultaneously measure BTEX molecules at high-temperature conditions (T = 1000–1250 K and P ∼ 1 atm). Using a minimum detectable absorbance of 0.1%, effective path-length of 13.79 m, and measured absorbance cross-sections at 1180 K and 1 atm, the minimum detection limits of this sensor are 0.73, 0.79, 0.82, and 1.38 ppm for benzene, toluene, ethylbenzene, and xylenes, respectively. Such a sensor can be highly valuable for real-time multi-species detection in complex reaction kinetic systems.
4.5. Uncertainty quantification

Uncertainty in our measurements comes from uncertainties in reflected-shock temperature (0.7%) and pressure (1%), path-length inside the shock tube (1.4%) [6], and mixture composition (0.2%). Uncertainty in measured absorbance was determined to be 2% using root sum square (RSS) method:

\[
\frac{\partial A}{A} = \left[ \left( \frac{\partial I_0}{I_0} \right)^2 + \left( \frac{\partial I}{I} \right)^2 \right]^{\frac{1}{2}}
\]  

(4)

Those uncertainties were propagated to obtain the Euclidean norm of uncertainty in the measured absorption cross-sections, which comes out to be 2.83%.

\[
\frac{\partial \sigma}{\sigma} = \left[ \left( \frac{\partial T}{T} \right)^2 + \left( \frac{\partial P}{P} \right)^2 + \left( \frac{\partial L}{L} \right)^2 + \left( \frac{\partial \chi}{\chi} \right)^2 + \left( \frac{\partial A}{A} \right)^2 \right]^{\frac{1}{2}}
\]  

(5)

Based on Eq. (1), the uncertainty in \( U \), which is a direct function of the single-pass absorbance (\( \alpha_{SP} \)), was calculated to be 3.32% using Eq. (6).

\[
\frac{\partial U}{U} = \left[ \left( \frac{\partial \sigma}{\sigma} \right)^2 + \left( \frac{\partial P}{P} \right)^2 + \left( \frac{\partial \chi}{\chi} \right)^2 + \left( \frac{\partial T}{T} \right)^2 + \left( \frac{\partial L}{L} \right)^2 \right]^{\frac{1}{2}}
\]  

(6)

The DNN model introduced 10.72% uncertainty (RMSE) in the predicted absorbance ratios of the target species. This uncertainty might increase if there are additional absorbing species with similar spectral features. Hence, the overall uncertainty in the reported mole fractions of the measured species was estimated to be 11.28% using Eq. (7).

\[
\frac{\partial \chi_{measured}}{\chi_{measured}} = \left[ \left( \frac{\partial \sigma}{\sigma} \right)^2 + \left( \frac{\partial G}{G} \right)^2 + \left( \frac{\partial C_{\text{ratios}}}{C_{\text{ratios}}} \right)^2 \right]^{\frac{1}{2}}
\]  

(7)

where \( G \) is the cavity gain and \( C_{\text{ratios}} \) corresponds to the absorbance ratios obtained from the DNN model. The main contribution to uncertainty originated from the DNN model. In future, a wider wavelength tuning range can help capture more spectral features and reduce the overall uncertainty.

5. Concluding remarks

A laser sensor based on cavity-enhanced absorption spectroscopy has been developed to measure low concentrations of benzene, toluene, ethylbenzene, and xylenes (BTEX) at high temperatures. The single-pass absorption increased by two orders of magnitude by the use of high-reflectivity mirrors, enabling a minimum detection limit of 0.73–1.38 ppm of the target species at 1180K. High-temperature absorption cross-sections of all BTEX species were measured over 1000–1250K. The sensor can selectively and simultaneously measure all of these species using deep neural networks (DNN). The sensor was demonstrated for shock-heated BTEX mixtures over a wide range of temperatures and compositions. Agreement between predicted and manometric concentrations motivate the implementation of this multi-species sensing strategy to reacting systems for simultaneous time-history measurement of evolving species.

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.
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