Artificial intelligent framework for the detection of gasoline residues in fire debris samples: Transforming gas chromatography/mass spectrometry data into image presentation for transfer learning

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ABSTRACT

This poster presents a novel artificial intelligence (AI)-powered framework to detect gasoline residues from neat gasoline and fire debris samples. The framework consists of image transformation of gas chromatography and mass spectrometry (GC/MS) data and transfer learning of a pre-trained convolutional neural network (CNN). The classifiers based on the framework are easy to develop and feature an automatic analytical process and accurate results.

INTRODUCTION

According to National Fire Protection Association (NFPA) annual fire report [1], Ignitable liquids (ILs) accounted for the largest share of civilian deaths/injuries and direct property damages in arson fires. Because gasoline is readily available on the market and easily transported, it has become the most widely used IL by arsonists. The detection of gasoline residues therefore assists with the determination of fire origin and cause. Modern test method for identifying gasoline residues in fire debris samples is GC/MS [2].

The recent advances in deep learning have made image analysis a powerful tool for classification tasks. Convolutional neural network (CNN) dominates image processing among all deep learning algorithms. A CNN uses multiple layers to extract and recognize features from input data. Instead of training a CNN from scratch, transfer learning improves the computational efficiency and performance by re-training a pre-trained CNN [3].

In this study, an AI-powered framework was proposed to process GC/MS data and develop an intelligent classifier for gasoline detection in fire debris samples. The GC/MS data was transformed into 2-dimensional scalograms and utilized to re-train an existing CNN. The framework provides promising classification performance to facilitate the detection of gasoline residues based on GC/MS analysis.

MATERIALS AND METHODS (1/2)

Sample preparation To prepare neat gasoline samples, the stock solution was prepared by using gasoline standard (20,000 µg /mL in methanol). The working solutions were prepared by serial dilution of the stock solution in the concentration range of 78 - 10,000 µg /mL in methanol (N = 8). Five µL of each calibrator sample was transferred to a 20-mL headspace (HS) vial (Supelco Inc.) for HS-solid phase microextraction (SPME)-GC/MS analysis.

Prior to preparing spiked samples, approximately 16 cm2 of a Nylon carpet was burned by a butane torch (Bernzomatic, Chilton, WI) for 1 min in the air. Then, 5 µL of each calibrator sample was added to 250 g of the burned carpet in a 20-mL HS vial for HS-SPME-GC/MS analysis.

RESULTS AND DISCUSSION

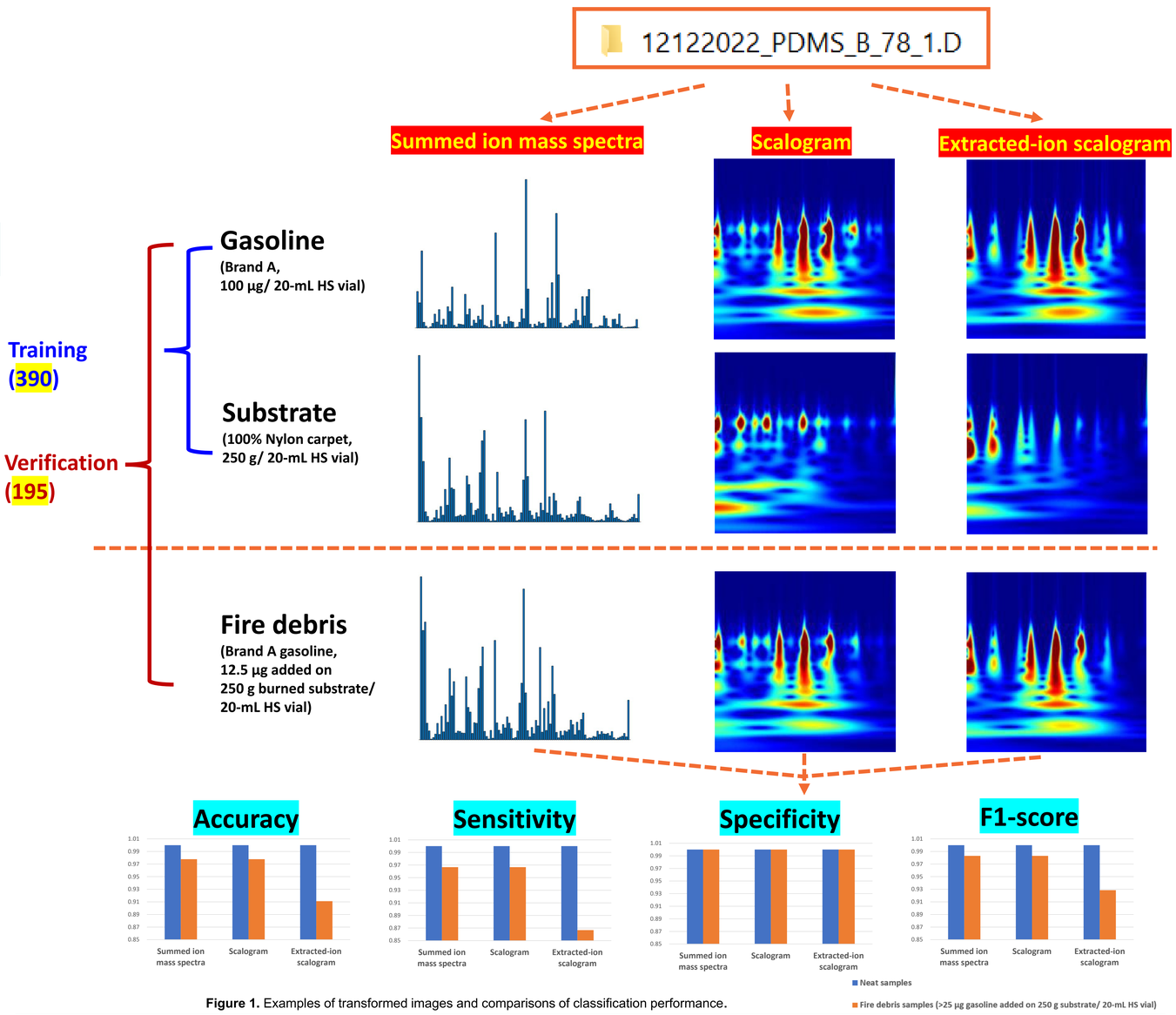

Figure 1. Examples of transformed images and comparisons of classification performance.

CONCLUSIONS

- Summed ion mass spectra and scalograms provided characteristic features of gasoline chemical profiles for transfer learning.
- Classification performance: summed ion mass spectra = scalograms > extracted-ion scalograms.
- The AI-powered classifiers have limitations on predicting fire debris samples (LOD = 25 µg gasoline added on 250 g burned substrate/ 20-mL HS vial)
- The re-training of CNNs did not require manual feature extraction.
- The re-trained CNNs achieved outstanding performance without big-scale training data.

MATERIALS AND METHODS (2/2)

Instrumental analysis The HS-SPME-GC/MS analysis was performed on an Agilent 7890B gas chromatograph coupled with a 5975A mass spectrometer (Agilent Technologies, Santa Clara, CA). The settings are shown in Table 1 and 2.

There was a total number of 390 GC/MS data (315 neat gasoline and 75 burned carpet data) collected for model training; 195 GC/MS data (90 neat gasoline, 90 fire debris, and 30 burned carpet data) collected for model verification.

Image transformation and transfer learning The GC/MS data were first converted into summed ion mass spectra (*m/z* 55-156). Second, the summed ion mass spectra were transformed into scalograms using a continuous wavelet transform (CWT) filter bank. Then, the training scalograms were fed into a pre-trained CNN, GoogLeNet, to create a classifier for discriminating "gasoline present" and "gasoline absent" samples. The settings for CWT and transfer learning are shown in Table 3. Both CWT and transfer learning were performed on MATLAB (The MathWorks, Natick, MA).

Table 1. GC/MS settings

Oven program steps	Condition
GC oven initial temperature	40 °C
Hold time	2 min
Rate #1, Oven temperature #1, Hold time #1	10 °C/min, 150 °C, 0 min
Rate #2, Oven temperature #2, Hold time #2	30 °C/min, 300 °C, 0 min

Table 2. HS-SPME settings

HHS-SPME step	Condition
Pre-fiber conditioning temperature	250 °C
Pre-fiber conditioning time	60 s
Pre-incubation time	300 s
Incubation temperature	80 °C
Extraction time	120 s
Desorption time	120 s
Post-fiber conditioning temperature	250 °C
Post-fiber conditioning time	600 s

Table 3. Image transformation and transfer learning settings

Analysis type		Condition
CWT	Signal length	1000
	Sampling frequency	Fs
	Voice per octave	12
Transfer learning	Mini batch size	15
	Max epochs	20
	Initial learn rate	1e-4
	Validation frequency	10

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