

An Artificial Intelligence-Based Detection of Ignitable Liquid Residues in Fire Debris Using a Deep Convolutional Neural Network

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ABSTRACT

This poster presents an intelligent workflow that utilized transfer learning with deep convolutional neural networks (CNNs) for fire debris analysis. Pre-trained image classifier was re-trained to classify scalogram images transformed from headspace solid phase microextraction (HS-SPME) - gas chromatography and mass spectrometry (GC/MS) data. The performance of the workflow on predicting trained class type and untrained class type of data is presented.

INTRODUCTION

Incendiary fires usually begin with the ignition of various items, such as trash, paper, mattress, etc. As reported by the National Fire Protection Association (NFPA) [1], ignitable liquids (ILs) contributed to the majority of fatalities, injuries, and direct property losses among all the intentional structure fires between 2014 and 2018. The detection of neat ILs and ILs in fire debris is crucial during the process of fire investigation since the result of IL analysis assists in the determination of the cause of a fire. The gold standard for interpreting the result of GC/MS analysis of ILs in fire debris is based on the American Society for Testing and Materials International (ASTM International) E1618-19 [2]. Due to the complex chemical composition of ILs and matrix interferences, chemometric tools are used to process and extract analytical signals based on mathematical algorithms to assist in interpreting sample attributes [3]. Convolutional neural networks (CNNs) have been one of the remarkable artificial intelligence (AI) algorithms for solving image classification tasks for the past few years [4]. Transfer learning is to re-train an existing CNN and leverage knowledge to another task [5], with noticeable performance in an efficient training fashion.

In this study, two hypotheses were proposed and experimental results were presented: 1) an AI-based workflow via transfer learning with a CNN could be utilized to classify GC/MS data based on scalogram images and detect neat ILs and IL residues from synthetic sample matrices; 2) the proposed AI workflow could be applied to analyze inter-laboratory data without retention time alignment.

MATERIALS & METHODS (1/2)

Intra-laboratory sample preparation 1) Neat samples: Gasoline samples were collected from five brands of gasoline stations in Huntsville, Texas. Stock solutions were prepared by dissolving 20 mg of each brand of gasoline in 1 mL of 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-SPME-GC/MS analysis; 2) Spiked samples: 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 & DISCUSSION

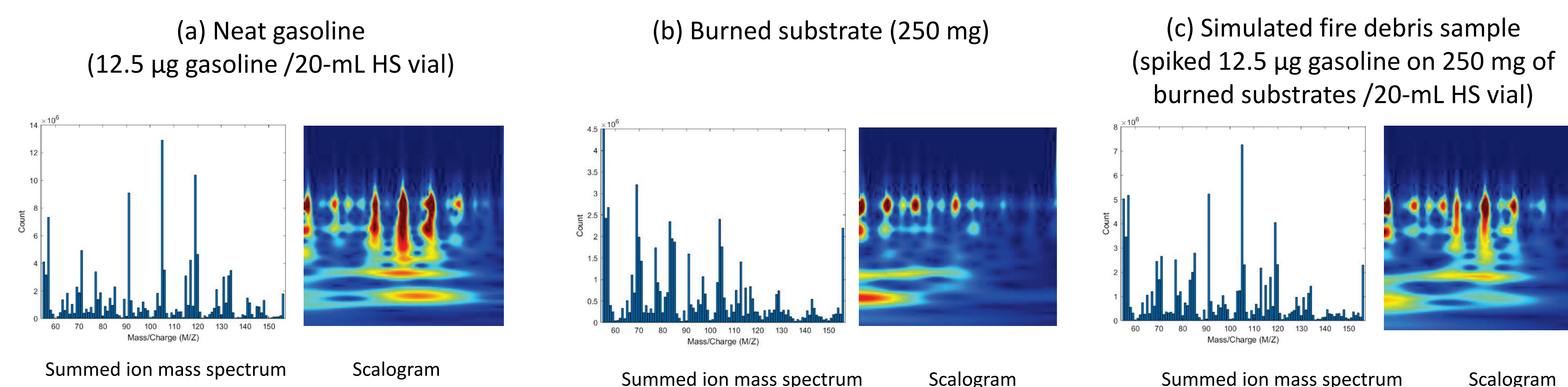


Figure 1. Examples of scalogram images.

Table 4. classification performance of the CNN on the intra-laboratory data.

ResNet-50	Accuracy	Precision	Sensitivity (TPR)	Specificity (TNR)
Neat gasoline 1.6-100 µg gasoline / 20-mL HS vial vs. burned substrates	1 ± 0	1 ± 0	1 ± 0	1 ± 0
Simulated fire debris samples (spiked 1.6-100 µg gasoline on 250 mg of burned substrates /20-mL HS vial) vs. burned substrates	0.41 ± 0.01	1 ± 0.04	0.31 ± 0.03	1 ± 0
Simulated fire debris samples (LOD of ResNet-50) vs. burned substrates	0.91 ± 0.01	1 ± 0.02	0.86 ± 0.01	1 ± 0

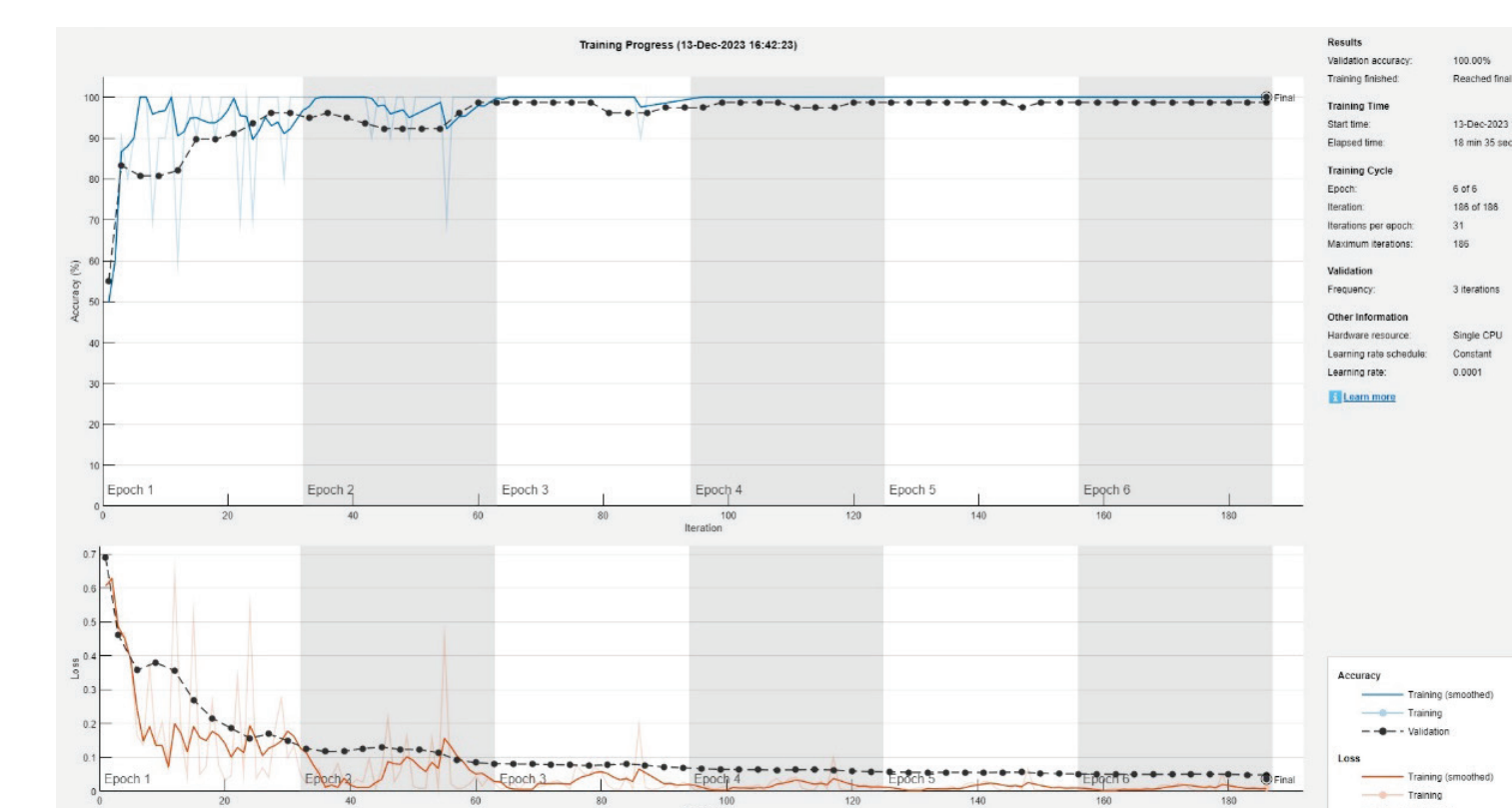
Table 5. classification performance of the CNN on the inter-laboratory data (National Center for Forensic Science database).

ResNet-50	Accuracy	Precision	Sensitivity (TPR)	Specificity (TNR)
Neat gasoline vs. burned substrates	0.88 ± 0.01	0.89 ± 0.01	0.94 ± 0.01	0.76 ± 0.03
Simulated fire debris samples vs. burned substrates	0.84 ± 0.01	0.86 ± 0.02	0.89 ± 0.02	0.76 ± 0.03

Figure 2. Training progress of the CNN.

Training summary of ResNet-50:

- Training time = 18 min 35 sec.
- Epoch maintaining the highest validation accuracy = Epoch 6.
- Validation accuracy = 100%.



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MATERIALS & METHODS (2/2)

Inter-laboratory data collection Samples were downloaded from the Ignitable Liquids Database and Reference Collection (ILRC) [6], the Substrate Database [7], and the Fire Debris Database [8] from the National Center for Forensic Science. More than 36 neat gasoline, 17 burned substrates, and 28 simulated fire debris samples GC/MS data were obtained.

Instrumental analysis An Agilent 7890B gas chromatograph coupled with a 5975A mass spectrometer (Agilent Technologies, Santa Clara, CA) was used to perform HS-SPME-GC/MS analysis of the intra-laboratory samples. The settings of HS-SPME-GC/MS analysis 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). A continuous wavelet transform (CWT) filter bank was used to transform the summed ion mass spectra into scalogram images. Those images were fed into a pre-trained CNN, ResNet-50. The re-trained ResNet-50 was used to discriminate "positive of gasoline" and "negative of gasoline" 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	10
	Max epochs	6
	Initial learn rate	1e-4
	Validation frequency	3

CONCLUSIONS

- Scalogram images preserved characteristic features of gasoline chemical profiles for transfer learning with ResNet-50.
- The re-training of ResNet-50 did not require manual feature extraction.
- ResNet-50 achieved appropriate performance by using less than 400 training data.
- The LOD for intra-laboratory data of fire debris samples was 25 µg gasoline added on 250 mg burned substrate/ 20-mL HS vial.

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