



Class-conditional feature modeling for ignitable liquid classification with substantial substrate contribution in fire debris analysis



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ABSTRACT

Forensic chemical analysis of fire debris addresses the question of whether ignitable liquid residue is present in a sample and, if so, what type. Evidence evaluation regarding this question is complicated by interference from pyrolysis products of the substrate materials present in a fire.

A method is developed to derive a set of class-conditional features for the evaluation of such complex samples. The use of a forensic reference collection allows characterization of the variation in complex mixtures of substrate materials and ignitable liquids even when the dominant feature is not specific to an ignitable liquid. Making use of a novel method for data imputation under complex mixing conditions, a distribution is modeled for the variation between pairs of samples containing similar ignitable liquid residues. Examining the covariance of variables within the different classes allows different weights to be placed on features more important in discerning the presence of a particular ignitable liquid residue.

Performance of the method is evaluated using a database of total ion spectrum (TIS) measurements of ignitable liquid and fire debris samples. These measurements include 119 nominal masses measured by GC–MS and averaged across a chromatographic profile. Ignitable liquids are labeled using the American Society for Testing and Materials (ASTM) E1618 standard class definitions. Statistical analysis is performed in the class-conditional feature space wherein new forensic traces are represented based on their likeness to known samples contained in a forensic reference collection.

The demonstrated method uses forensic reference data as the basis of probabilistic statements concerning the likelihood of the obtained analytical results given the presence of ignitable liquid residue of each of the ASTM classes (including a substrate only class). When prior probabilities of these classes can be assumed, these likelihoods can be connected to class probabilities. In order to compare the performance of this method to previous work, a uniform prior was assumed, resulting in an 81% accuracy for an independent test of 129 real burn samples.

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1. Introduction

Forensic fire debris analysis requires the analyst to first investigate if a sample contains ignitable liquid residue (ILR). If ILR is assumed to be present, the analyst will further identify the class of ignitable liquid. The process of ILR detection and classification is complicated by the complex composition of many ignitable liquids, the large number of commercially available liquids, weathering of the liquid during the fire, and the presence of background contributions from substrate pyrolysis [14,23,24].

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Sample extraction from fire debris can be accomplished by a variety of techniques [4,9,19]; however, none of the methods are selective for ILR relative to pyrolysis products. Gas chromatography–mass spectrometry (GC–MS) is employed for sample analysis in modern laboratories. Mass spectrometry is information-rich and allows the data to be visualized as total ion chromatograms or extracted ion profiles. Target compounds may be identified based on a combination of retention times relative to standards and mass spectral profiles. The digital format of GC–MS data facilitates the analysis of fire debris; nonetheless, the analyst commonly relies on visual pattern recognition for statements concerning the presence of ILR and classification of the liquid. Visual pattern recognition is subjective and an error rate is unknown or based on a limited number of audits or experiments.

Electronic databases are available to assist fire debris analysts with the identification of ILR and the presence of substrate pyrolysis product contributions.¹ Electronic library searches can be complicated by chromatographic retention time shifts from inter-laboratory method variability. Retention time matching programs, which are available to assist with this problem, do not work well when the compared chromatographic profiles differ dramatically [12]. Alternatively, retention-time independent methods have been examined that utilize covariance mapping [22] and the summed mass spectrum across the chromatographic profile [21].

The work described here addresses the problem of calculating the likelihood of an analytical observation under the assumption that the sample contains a complex mixture of substrates along with the possibility of a certain type ignitable liquid. Ignitable liquid classes are defined by the American Society for Testing and Materials [3] (ASTM E1618). Previous methods aimed at classification into these classes report generally low correct rates of classification. We approach this problem by seeking an improved feature space which leverages the chemical characteristics of these classes. The method makes use of a reference collection of both neat and partially evaporated ignitable liquids, and substrate materials pyrolyzed in laboratory conditions, to derive a feature space based on the total ion spectrum (TIS). In this space the classification of ILR is facilitated despite the above-mentioned complicating factors. Using a reduced feature space, class specific covariances are calculated using a bootstrap-like sampling of intact and evaporated ignitable liquids weighted and mixed with substrate contributors. By using the TIS representation of the samples, retention time shifts in the chromatographic analysis are removed. Furthermore, this space allows interpolation of sample mixtures in terms of relative ion abundances in a fairly straightforward manner.

This *in silico* mixing procedure, similar to a method proposed in earlier work [25], is employed to emulate substantial contributions from a highly complex substrate mixture and is described in Section 3.1. This data is used to define a feature space for each class. A new sample may be described in terms of the likelihood of observing a specific in-class similarity (by pairwise comparison with labeled samples in the forensic reference collection) given that the new sample belongs to a specific class. This space proves advantageous for classification, as samples are now characterized by their relative similarity to known ignitable liquids.

Cross-validation is used to optimize the method and final performance testing of the model is performed by assessing classification rates for a completely independent set of fire debris data. For this testing set, ground-truth is based on a sample's location relative to the known ignitable liquid pour trail and subsequent examination of the analytical data by an analyst with access to the ignitable liquid used in the burns. Assigning each new

sample to the class showing highest likelihood (i.e. assuming uniform priors) yields overall classification accuracy of 81% when considering 9 distinct classes defined by the ASTM standard.

2. Motivation and previous work

The average mass spectrum across the chromatographic profile (TIS) has been shown to exhibit relatively high specificity for ignitable liquids [21]. Similarities and differences among ignitable liquids based on the ASTM E1618 defined classes are also reflected in the hierarchical clustering of ignitable liquid TIS [26]. Self-organizing feature maps have revealed similar grouping behavior based on a sub-set of ions from the TIS of ignitable liquids [8]. These studies demonstrate the value of the TIS as a basis for identifying and grouping ignitable liquids. The challenge of identifying the presence of ILR and classifying the liquid from which the residue was derived is much more difficult than classification of the neat liquid. Several promising approaches have been reported for determining the presence of ILR in fire debris samples and correct classification of the ignitable liquid present in the residue. Of these, many adopt a multi-step classification scheme where correct binary classification results are achieved between 71.8% and 99.0% depending on the specific classes examined and substrate contribution [25,27]. In some work [15,22], not all ASTM classes are included or no *substrate only* classification is considered.

Previous work has focused on *hard* classification (i.e. assigning a sample to a single class) and, to a lesser extent, on *soft* classification (i.e. assigning probabilities of belonging to each considered class). The overall classification performance of 81% observed in this work is comparable to an 83% classification performance previously reported for multi-class classification [29]; however, the two methods differ significantly. The previous work also relied on the TIS, but required that data for multiple samples taken from a single fire scene be concatenated and analyzed by target factor analysis while making use of the TIS, from the previously mentioned ignitable liquids reference collection (ILRC), as target factors. The method reported here allows for classification of a single sample and therefore is more generally applicable. Previous work did not explicitly model TIS of substrates, whereas the method reported here relies on an estimate of the covariance structure of substrate TIS. While requiring a knowledge of the covariance structure of the TIS may appear a disadvantage, the model allows for classification of a sample into the SUB category, which is an indication that ignitable liquid residue is not present. The likelihood of membership in the SUB class was not directly provided by the previously reported method; however, the method was implemented as a soft classifier with the option of not assigning the fire debris to any of the ASTM E1618 classes if the likelihood of class membership was exceptionally low for all classes [28]. Preliminary work demonstrating the potential of computational mixing of the TIS signals to generate signals resembling fire debris was performed focused on a step-wise classification paradigm [27].

3. Materials and methods

Reference ignitable liquid sample preparation was performed by depositing 20 μ L of ignitable liquid into a vial with 1 mL (1000 μ L) of carbon disulfide (Fisher Scientific, Waltham, MA, USA). Weathered ignitable liquids were prepared by placing 10 mL of ignitable liquid into a graduated microvial. The vial was placed into a dry bath in which the height of vial and temperature of dry bath were adjusted according to the percent volume evaporated. Nitrogen flowed gently above the ignitable liquid and a vacuum pump was used to remove the ignitable liquid vapor above the vial. The nitrogen needle and vacuum tubing were cleaned between

¹ Ignitable Liquids Reference Collection: <http://ilrc.ucf.edu>; Substrate Reference Database: <http://ilrc.ucf.edu/substrate>.

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