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Develop a Hazard Index Using Machine Learning Approach for the Hazard Identification of Chemical Logistic Warehouses

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Abstract

With the rapid development of chemical process plants, the safe storage of hazardous chemicals become an essential topic. Several chemical warehouse incidents related to fire and explosion have been reported recently. Therefore, an accurate hazard identification method for the logistic warehouse is needed not only for the facility to develop a proper emergency response plan but also for the residents who live near the facility to have an effective hazard communication. Furthermore, the government can better allocate the resources for first responders to make fire protection strategies, and the stakeholders can lead to improved risk management. Hazard index is a helpful tool to identify and quantify the hazard in a facility or a process unit. The challenge for this research is to improve the current method with the novel technique to implement our purpose.

The first objective of this research is to develop a "Storage Hazard Factor" (SHF) to evaluate and rank the inherent hazards of chemicals stored in logistic warehouses. In the factor calculation, the inherent hazard of chemicals is determined by various parameters (*e.g.*, the NFPA rating, the flammability limit, and the protective action criteria values, *etc.*) and validated by the comparison with other indices. The current criteria for flammable hazard ratings are based on flash point, which is proved to be insufficient. Two machine learning based methods will be used for the classification of liquid flammability considering aerosolization based on DIPPR 801 database. Subsequently, SHF and other warehouse safety penalty factors (*e.g.*, the quantity of the chemicals, the distance to the nearest fire department, *etc.*) are utilized to identify the Logistic Warehouse Hazard Index (LWHI) of the facilities. In the last chapter, this method is applied to real-time data from Houston Chronicle, and several statistical analyses are used to prove the hazard index is helpful for hazard identification to emergency responders and hazard communication to the public.

Keywords: Hazard identification, Hazard index, Machine learning classification

1. Introduction

Since entering the 21st century, people enjoy the benefits of the rapid development of the industry. With the innovations of the new chemical process, process safety must also be up to date and accommodate the new chemical process.

Many industrial cities around the world are facing a dilemma between economic growth and population growth. With the blooming development of chemical process plants, the safe storage of hazardous chemicals become an essential topic. People should understand that some inherent properties of a chemical which makes it profitable to our society may be hazardous in the meantime. The researcher lived in Tianjin for five years, which is one of the economic centers in the north of China. Tianjin has developed a sub-provincial district named Binhai New Area, which is near the largest port in northern China, and where more than 1800 facilities are related to the storage of hazardous chemicals [1]. This thesis is focused on hazard identification for chemical logistics warehouses, which is inspired by the Tianjin explosion that happened on August 12, 2015 [2].

Based on the investigation reports of the storage facilities related to safety incidents, some hazardous chemicals are mentioned more than one time, such as ammonium nitrate. Former researchers in Mary Kay O'Connor Process Safety Center (MKOPSC) have investigated the thermal decomposition and runaway reaction characteristics of some hazardous chemicals [3-5] while few studies have explored the hazard identification applications.

The storage of hazardous chemicals in a warehouse is a complex problem. The potential hazards include flammability, reactivity, and interaction among different types of hazardous chemicals. Hazard index is a helpful tool to identify and quantify the hazard in a facility or a process unit. Various hazard indices are developed in history. Dow's Fire and Explosion Index is the most famous and widely used one, and others like Mond Index, Dow's Chemical Exposure Index, IFAL Index, Weighted Average Risk Rating Index, etc. are developed or modified based on different scopes and purposes [6]. The first edition of Dow's F&EI was issued in 1964 and used within Dow Chemical Company. After the development over half a century, F&EI has been widely used in Dow and outside Dow and becoming the leading hazard index recognized by the chemical industries.

The first objective of this research is to develop a "Storage Hazard Factor" (SHF) to evaluate and rank the inherent hazards of chemicals stored in logistic warehouses. In the factor calculation, the inherent hazard of chemicals is determined by various parameters (*e.g.*, the NFPA rating, the flammability limit, and the protective action criteria values, *etc.*) and validated by the comparison with other indices. Machine learning attracts much attention in recent years and has been applied in process safety in several aspects. Numerous works applied supervised learning to predict lower flammable limit (LFL), upper flammable limit (UFL), minimum ignition energy (MIE), and autoignition temperature [7-12]. Mage et al. utilized unsupervised learning to cluster the thermal stability of organic compounds into seven groups [13]. Therefore, with the lack of study in liquid flammability considering aerosolization and the tendency of the machine learning approach, it is worthful to implement machine learning algorithms to liquid flammability rating. Two machine learning based methods will be used for the classification of flammability. Subsequently, SHF and

other warehouse safety penalty factors (*e.g.*, the quantity of the chemicals, the distance to the nearest fire department, *etc.*) are utilized to identify the hazard index of the facilities.

The index can be used not only for the facility to develop a proper emergency response plan but also for the residents who live near the facility to have an effective hazard communication. Furthermore, the government can better allocate the resources for first responders to make fire protection strategies, and the stakeholders can lead to improved risk management.

2. Methodology

2.1. Data collection

The Design Institute for Physical Properties (DIPPR) 801 is a project sponsored by AIChE, which provides more than 30 constant properties and nearly 50 thermophysical properties as well as molecular structure, hazard properties, physical constants for more than 2000 compounds. This database is widely used in chemical properties classification and prediction [7, 8]. After data cleaning, 823 organic compounds will be used in this research.

2.2. Storage hazard factor (SHF)

Based on the literature reviews, various hazard indices are developed or modified based on different scopes and purposes. Considering that the index will be applied to the chemical logistic warehouse, the overall index function can be represented as follows in Equation 1.

$$Logistic\ Warehouse\ Hazard\ Index\ (LWHI) = \sum F_i \times SHF \qquad (Eqn.1)$$

where F_i represents different penalty factors such as quantity, population density, SHF represent the inherent hazard of the chemicals stored in the warehouse.

Based on the MKOPSC's PCHP project, the formula for calculating the SHF can be modified as follows in Equation 2.

$$SHF = 2^{Modified\ NF} + 2^{NR} + 2^{Modified\ NH} \qquad (Eqn.2)$$

where NR represents the degree of reactivity, which will be determined by the original NFPA rating; NH represents the degree of health hazard, which will be modified by PAC-3 value; NF represents the degree of flammability, which will be modified by two machine learning methods using DIPPR 801 database.

2.2.1. Modified NH

Protective Action Criteria (PACs) values are an exposure limit system, and this system is commonly used as the guideline for an emergency response to the concentration of the accidental release of the hazardous chemicals.

NH represents the degree of health hazard. The original NFPA rating criteria are based on LC_{50} and LD_{50}, which is more focus on emergency conditions for the working area. Since PAC-3 is the maximum airborne exposure resulting in the most severe consequence, which is life-threatening effects, PAC-3 will be used to modify the NH value for our purpose.

The Department of Energy 's (DOE) current PAC dataset is Revision 29, published in May 2016 [14]. It provides chemical exposure limit values for 3146 chemicals.

2.2.2. Modified NF

The most widely used chemical classification method is NFPA 704, GHS, and OSHA (29 CFR 1910.106). However, both of these criteria are based on flash points only [15]. (Table 1) Evidence shows that liquid can be ignited below its flash point if it is in some particular condition, such as aerosol form [16, 17]. In this research, flash point, autoignition temperature, surface tension, and viscosity are selected to modify the classification, using K-Mean and hierarchical clustering with PCA.

Table 1. Current standards for liquid flammability rating and classification

Standard	Flammability rating and classification	Criteria
	0	Materials will not burn in air when exposed to a temperature of 1500°F for a period of 5 minutes
	1	Flash point at or above 200°F
	2	Flash point between 100 and 200 °F
	3	Flash point between 73 and 100°F
	4	Flash point below 73°F
GHS classification and labeling of chemicals	1	Flash point < 23°C and boiling point ≤ 35°C
	2	Flash point < 23°C and boiling point > 35°C
	3	Flash point ≥ 23°C and ≤ 60°C
	4	Flash point > 60°C and ≤ 93°C
OSHA (29 CFR 1910.106)	1	Flash point < 73.4°F and boiling point ≤ 95°F
	2	Flash point < 73.4°F and boiling point > 95°F
	3	Flash point ≥ 73.4°F and ≤ 140°F. When a category 3 liquid with a flash point ≥ 100°F is heated for use to within 30°F of its flashpoint, it shall be handled in accordance with the requirements for a Category 3 liquid with a flash point < 100°F.
	4	Flash point > 140°F and ≤ 199.4°F. When a category 4 liquid is heated for use to within 30°F of its flashpoint, it shall be handled in accordance with the requirements for a Category 3 liquid with a flash point < 100°F.
	5	When a liquid with a flash point > 199.4°F is heated for use to within 30°F of its flashpoint, it shall be handled in accordance with the requirements for a Category 4 flammable liquid.

In this study, the KC and HC algorithm is implemented through the Python package, Scikit-Learn [18]. The number of clusters is determined by the elbow method, which plots the within-cluster sum of square (WCSS) with respect to the number of clusters [19]. Figure 1 shows the example of the elbow plot when implementing the KC algorithm on liquid flammability clustering based on flash point and autoignition temperature. The number of clusters is 5 in this thesis.

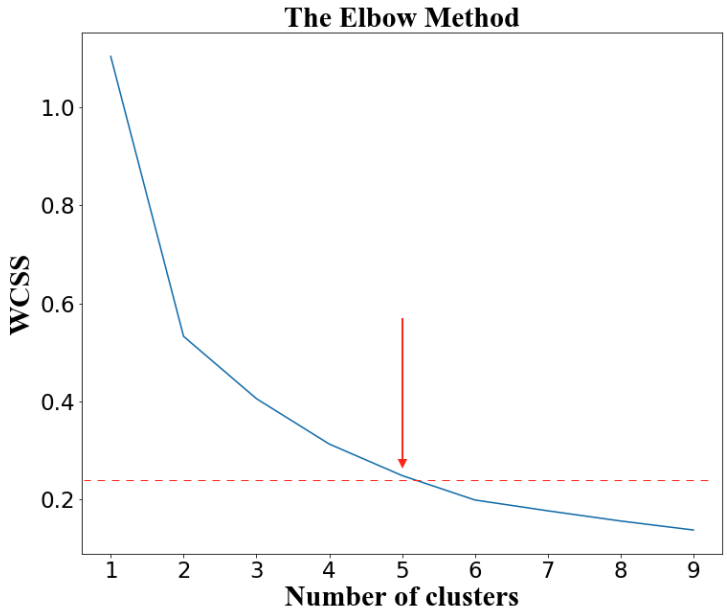

Figure 1. Within-cluster sum of square (WCSS) and the number of clusters

This modification method is reliant on the availability of the data. Despite the lack of data, the original NFPA rating with simple update (if UFL – LFL > 10%, then NF + 1 with a maximum of 4) can be used for SHF calculations.

2.3 Penalty factors

The other important part of Equation 1 is $\sum F_i$, which represents different penalty factors. In this study, quantity, population density, and distance to the nearest fire station are selected to be the penalty factors. The determination guides for each factor are described in this section.

2.3.1. Quantity

Quantity is an important factor that should be considered first when designing a hazard index. Besides the inherent hazard of a hazardous chemical, the amount of chemicals stored in the facility also reveals the level of hazardous.

The following table shows the determination guide of the quantity penalty value. (Table 2)

2.3.2. Population density

Besides the inherent hazards of a chemical and the quantity of the facility stored, another important factor is the safety impact to the public. Given the coordinate of a facility, we defined the population in a radius of two miles near the facility that can be used to represent the population density factor in Equation 1.

Population density information is retrieved on LandView 6.0, a geographic information system software. The following table shows the determination guide of population density penalty value. (Table 3)

Table 2. Penalty value of quantity determination guide

Original code	Min (Pounds)	Max (Pounds)	Penalty value
1	0	99	1.2
2	100	499	1.4
3	500	999	1.4
4	1,000	4,999	1.6
5	5,000	9,999	1.6
6	10,000	24,999	1.8
7	25,000	49,999	1.8
8	50,000	74,999	1.8
9	75,000	99,999	1.8
10	100,000	499,999	2
11	500,000	999,999	2
12	1,000,000	9,999,999	2
13	10,000,000	…	2

Table 3. Penalty value of population density determination guide

(in a radius of two miles near the facility)

Min	Max	Penalty value
10	100	1.2
100	1000	1.4
1000	10000	1.6
10000	100000	1.8
100000	…	2

2.3.3. Distance to the nearest fire station

In the previous sections, we considered the inherent hazard, quantity, and the potential impact to the public. And last but not least, we choose a factor that can reflect the mitigation process, which is an essential point for a storage facility.

Distance to the nearest fire station (FS) is retrieved from HazardHub, a provider of property-level hazard risk database [20]. The following table shows the determination guide of distance to the FS penalty value. (Table 4.)

Table 4. Penalty value of distance to FS determination Guide

Min (Miles)	Max (Miles)	Penalty value
0	1	1.2
1	2	1.4
2	3	1.6
3	4	1.8
4	…	2

3. Results and discussions

3.1 NF modification

3.1.1 Database visualization

Before conducting the liquid flammability rating with the inclusion of aerosolization, we would like to investigate the distribution of observations for each liquid property, and the scatter plots of each pair of liquid properties. The figure 2 shows the aggregated scatter plots, distribution plots, and heatmap of liquid properties. The diagonal of figure 2 shows the distribution of observations for each liquid property. For example, Figure 3 shows the distributions of flash point and surface tension are normally distributed. However, the distributions of autoignition temperature and viscosity are right-skewed.

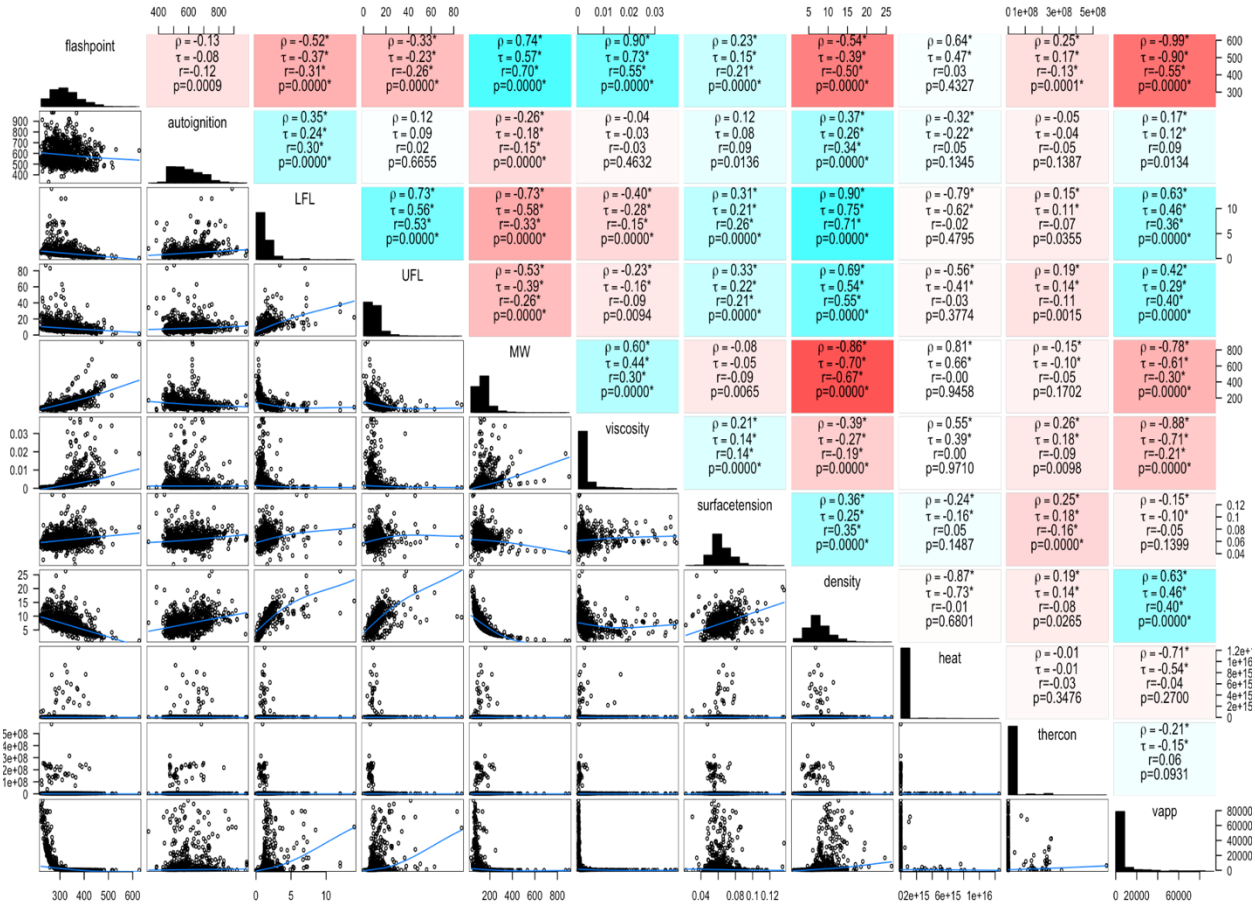

Figure 2. Scatter plots, distribution plots, and heatmap of liquid properties

The left part of figure 2 is the scatter plot of each pair of liquid properties. For example, a positive slope is plotted for the relationship between flash point and molecular weight, shown in the 5th plot from the top in the first column on the left part of figure 2, and the magnified plot in Figure 4.

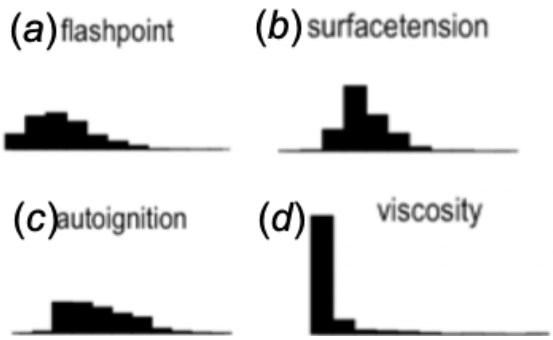

Figure 3. Distributions of liquid properties: (a) flash points; (b) surface tension; (c) autoignition temperature; (d) viscosity

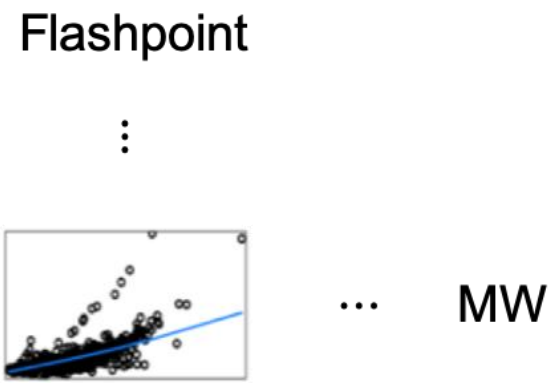

Figure 4. Scatter plot for flash point and molecular weight

The right part of figure 2 shows the statistical correlation between each pair of liquid properties, including Pearson coefficient (ρ), Kendal coefficient (τ), Spearman coefficient (r), and the P-value for Pearson coefficient (p). For example, the statistical correlation between flash point and vapor pressure is found in the upper rightmost location. The Pearson coefficient between flash point and vapor pressure is -0.99, which means a completely negative correlation.

3.1.2. KC and HC algorithm

As discussed before, the number of clusters determined by the elbow method is 5 in this thesis. Thus, the 823 organic compounds from DIPPR 801 are split into five groups and rated from 0 to 4 as in the NFPA rating. The KC clustering is based on flash point and autoignition temperature, which is different from the NFPA rating. The compounds in the group with a rating of 4 are the compounds with the highest flammability. On the other hand, compounds with a rating of 0 have the lowest flammability. Figure 5 shows the data distribution.

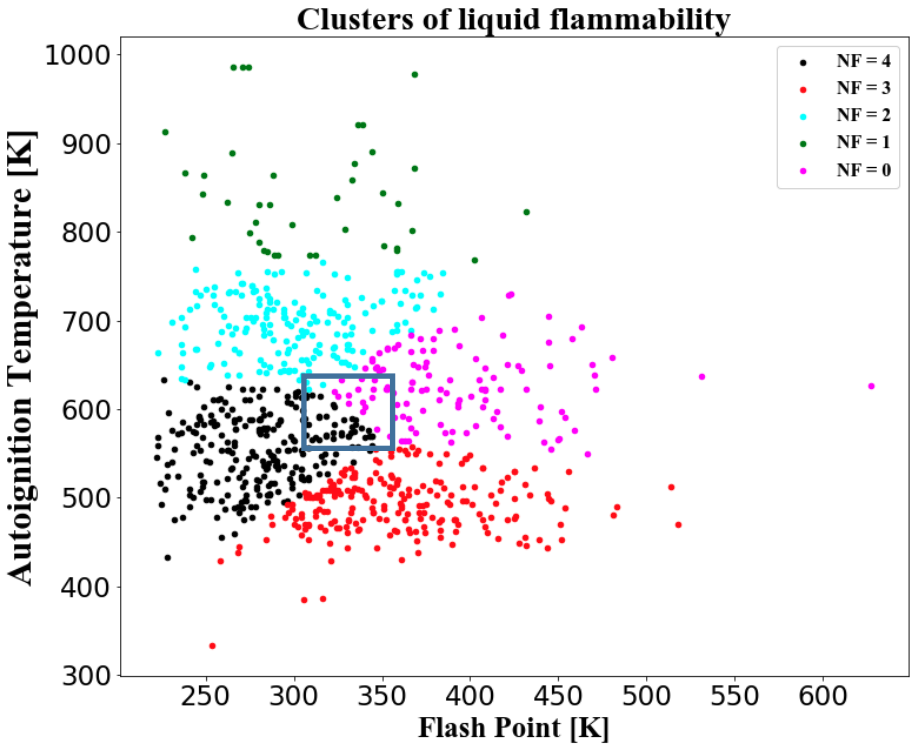

Figure 5. Clusters of liquid flammability using KC algorithm

In Figure 5, some data points labeled black have a medium flash point and medium autoignition temperature comparing to the neighbor points labeled red and cyan. Those points either have a high flash point and low autoignition temperature, or have a low flash point and high autoignition temperature. However, the black label means NF = 4, which is higher than the red (NF = 3) and cyan (NF = 2) label. Similar results and doubts show at the boundary of different clusters in the circled area.

Similarly, Figure 6 displays the dendrogram of clustering through the HC algorithm. Also, 823 organic compounds from DIPPR 801 are split into five groups and rated from 0 to 4 as the same criteria with the HC algorithm. The agglomerative clustering result will assign to each data point. Figure 7 shows the visualized plot in Cartesian coordinates.

In Figure 7, the results located in the controversial boundary between the black (NF = 4) and the red (NF = 3) regions are more reasonable. But this time, a misclassification may happen in the circled area. With a similar flash point, the black labeled data points have the medium autoignition temperature comparing to the red and magenta labeled data points. However, these data points are classified as NF = 4, which is the most hazardous material among all. On the other hand, some

points with the lower autoignition temperature are classified as NF = 3, which is less dangerous than black labeled points.

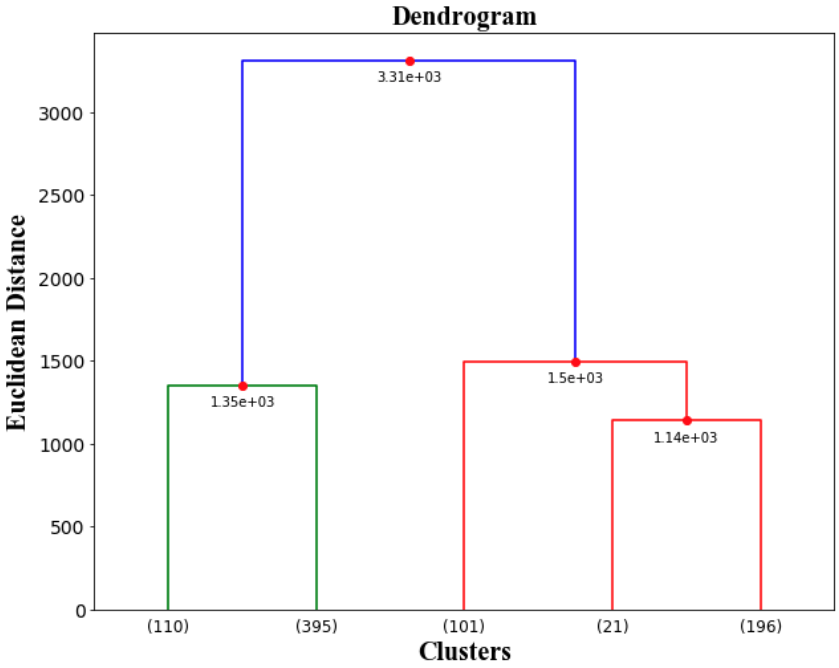

Figure 6. Truncated dendrogram of clustering of liquid flammability

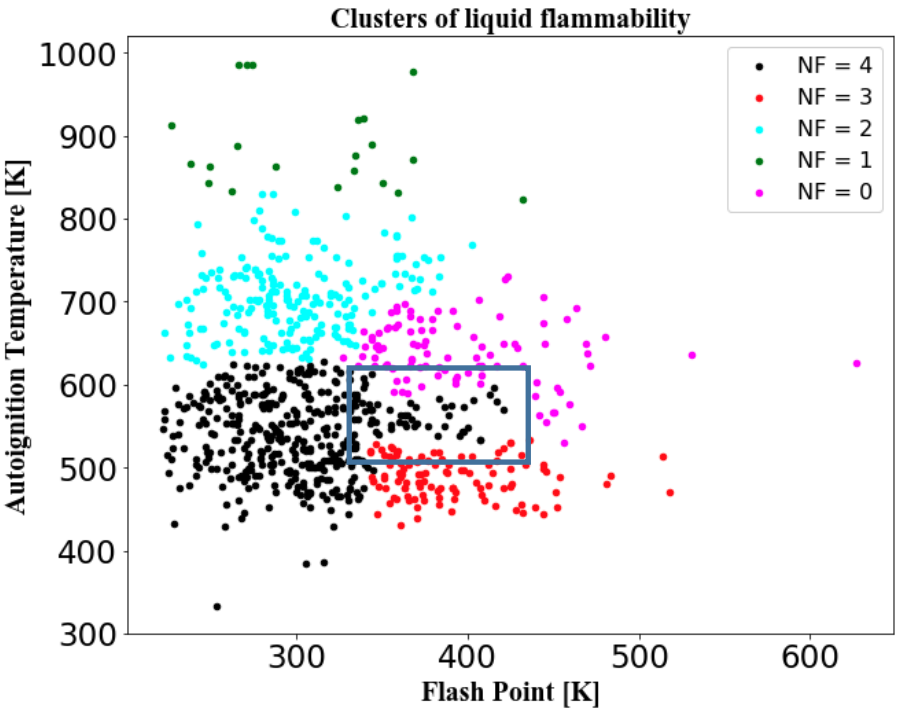

Figure 7. Clusters of liquid flammability using HC algorithm

Comparing the KC and HC algorithms, there are 653 out of 823 compounds with the same rating for liquid flammability in both algorithms. Table 5 shows the liquids with significantly different ratings between the two algorithms. Those liquids in Table 5 require more attention when conducting a risk assessment with inherent flammability.

Table 5. Liquids with significant different ratings between KC and HC algorithm

Substance name	Flammability rating (KC)	Flammability rating (HC)
o-ethylaniline	2	0
hexylene glycol	0	4
cetyl methacrylate	3	0
3-methyl-1-pentene	4	2
1-dodecanol	3	4
4-methyl-1-octanol	0	4

As a result, the KC algorithm has a more reasonable rating for the clustering of liquid flammability, because the circled area is smaller in Figure 5 compared with Figure 7. Another reason is that the misclassification in the KC algorithm is more likely to happen on the boundary of two clusters, whereas the misclassification in HC algorithm is more likely to happen in an area. These results are considering the flash point and autoignition temperature in two dimensions. Therefore, the results are highly interpretable since the X and Y axis both have physical meaning.

But if we want to consider liquid aerosolization probability at the same time, we need to reduce the features for visualization and easier calculation. The PCA method will be applied in the next section.

3.1.3. PCA with KC and HC algorithm

The main purpose of NF modification is to consider aerosolization. In the previous chapter, we conclude that viscosity and surface tension can be used as two indicators of aerosolization. To reduce the flash point, autoignition temperature, viscosity, and surface tension into two principal components (PCA1 and PCA2), we applied the RBF kernel function when reducing four features. Another advantage is that PCA does not need to specify the weight of contributions of liquid aerosolization and flammability. Figure 8 shows the clustering results by the KC and HC algorithm based on PCA1 and PCA2. Besides the advantages of PCA, one thing that needs to keep in mind is that both X and Y axes in Figure 11 have no physical meaning. This is the main disadvantage of the PCA method.

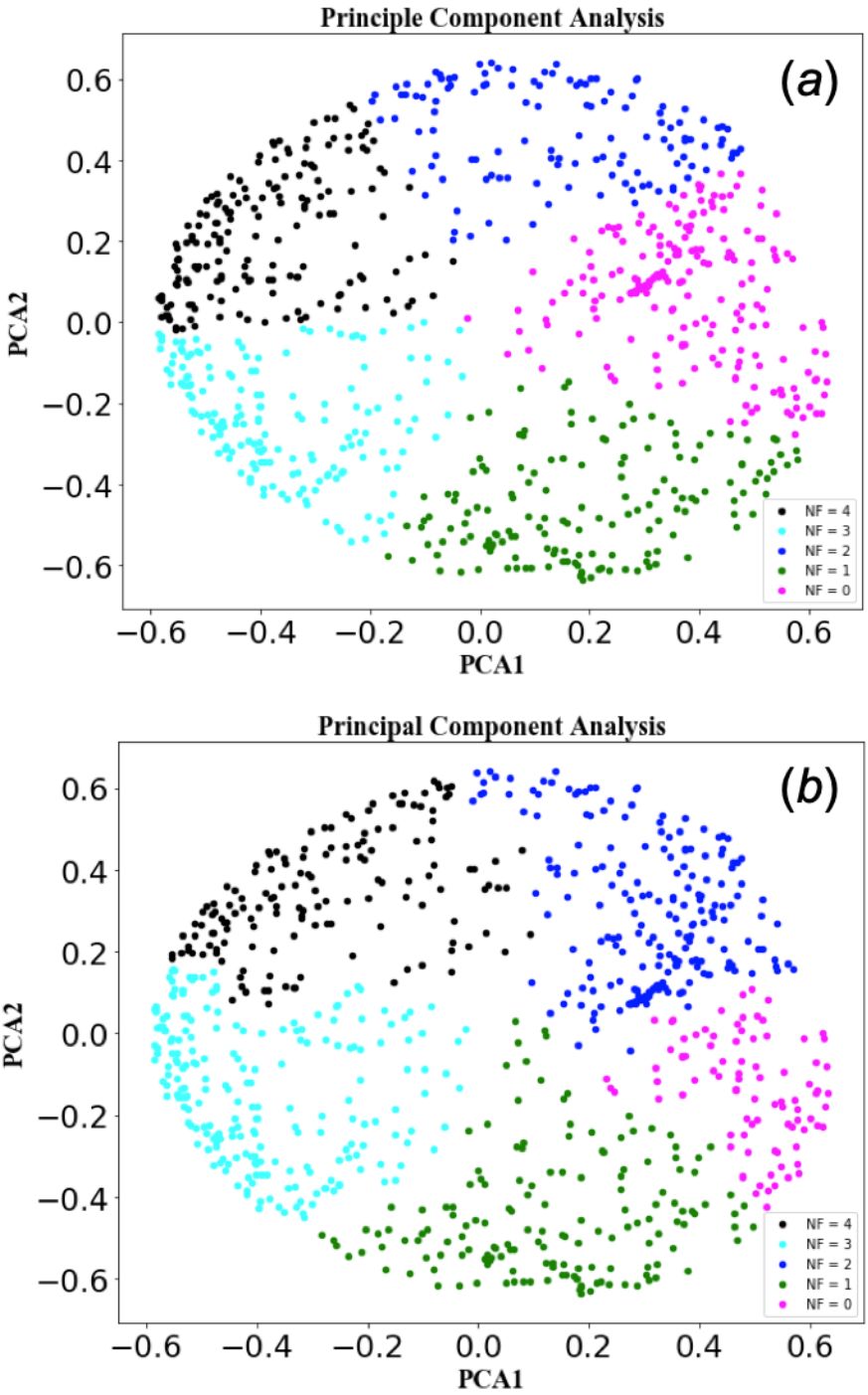

Figure 8. Principal component (PCA1 and PCA2) clusters using (a) KC algorithm (b) HC algorithm.

4. Case study

4.1 Data collection

Houston Chronicle has published a series of articles [21], aiming at exploring fatal mistakes that could have the largest consequences and probes that put the citizen in jeopardy. Houston Chronicle has collected 2581 facilities and over 18000 chemical records in the greater Houston area. The raw data is in EPA Tier II standard and shared with MKOPSC. After data cleaning, at least 33 warehouses that have more than 400 records and over 170 kinds of hazardous chemicals will be used in this research. The raw database includes company information, location information, chemical information, and storage quantity.

4.2 Sample calculation

Table 6 is the sample hazard review for 2-Butoxyethanol from DIPPR 801, DOE's PAC, and NFPA database.

Table 6. Hazard review: 2-Butoxyethanol

Parameter	Data
CAS No.	111-76-2
NFPA NR	0
NFPA NH	2
PAC-3	3400 mg/m^3
NFPA NF	2
Flash point	334.15 K
Autoignition temperature	511.15 K
LFL/UFL	1.1% / 12.7%
Viscosity	2.9 cP at 25°C
Surface tension	26.1 mN/m at 25 °C

Based on the data above, the SHF should be:

1. The original NFPA NR rating is 0, in our calculation, keep the original value.
2. The original NFPA NH rating is 2, and the PAC-3 value is 3400 mg/m^3. Based on the previous discusstion, the modified NH value is still 2.
3. The original NFPA NF rating is 2, the flash point is 334.15 K, autoignition temperature is 511.15 K, LFL / UFL are 1.1% / 12.7%, viscosity is 2.9 cP, and surface tension is 26.1 mN/m. The result of the machine learning method using KC algorithm is 3, but the result become 4 when using HC algorithm. As we discussed in the previous section, result with KC algorithm is more reasonable. So the modified NF value is 3.
4. $SHF = 2^3 + 2^0 + 2^2 = 13$

With the chemical information, we can get the SHF value using the method discussed above. Then the storage quantity information allowed us to convert it into units in pounds. Finally, the location

information will help us extract information about population density and distance to FS. Continue the 2-Butoxyethanol example and calculate the LWHI. (Table 7)

Table 7. Tier II information for 2-Butoxyethanol in facility #33

Parameter	Data
CAS No.	111-76-2
SHF	13
Quantity	4 (original code)
Population density	4154 (in a radius of two miles)
Distance to FS	1.62 miles

Based on the data above, the LWHI should be:

1. SHF for 2-Butoxyethanol is 13, based on the calculation from last example.
2. For facility #33, the quantity indicator of 2-Butoxyethanol is 4, which means in (1000,5000) pounds range, and the penalty value is 1.6 based on Table 3.
3. For facility #33, the population density in a radius of two miles is 4154, and the penalty value is also 1.6 based on Table 4.
4. For facility #33, the distance to the nearest fire station is 1.62 miles, and the penalty value is 1.4 based on Table 5.
5. Therefore, the LWHI for 2-Butoxyethanol in facility #33 is: $13 \times 1.6 \times 1.6 \times 1.4 = 46.592$.

5. Conclusions

In this thesis, a hazard index for the hazard identification of chemical logistic warehouses was created and named LWHI. The aim of this index is to numerically calculate the potential hazards in a logistic facility. And the manager or the emergency reponder can use those results to develop their hazard chemicals management plan.

To reach the goal mentioned above, the SHF was introduced to the index. First, two machine learning based methods for liquid flammability rating with the consideration of aerosolization have been proposed. The first method applies KC and HC algorithms in machine learning to chemical classification. The 823 organic compounds in DIPPR 801 are clustered into 5 groups based on their flash point and autoignition temperature. Then the 5 groups regarding liquid flammability are rated from 0 to 4 based on 4 is the most hazardous rating. The advantage of the KC and HC clustering method is its high interpretability. With the analysis mention in previous, the KC algorithm has a more reasonable rating on liquid flammability clustering.

The second method presented uses PCA to reduce the four features (i.e., flash point, autoignition temperature, viscosity, and surface tension) into two principal components (PCA1 and PCA2). The advantage of the PCA rating method is that the weight of contribution of the four features is automatically considered. Admittedly, the lack of interpretability is a disadvantage of the PCA method as the principal components do not have physical significance but only statistical significance. However, compared with traditional flammability classification methods which only

rely on flash point and boiling point, the two proposed methods have shown a statistical correlation with liquid flammability. Additionally, one obvious disadvantage of traditional flammability classification methods is the threshold values are determined by humans, which invariably has bias. While machine learning based methods partly eliminate this bias. Also, the boundary of traditional flammability classification methods is linear. But the boundary of the proposed machine learning based methods can be nonlinear to eliminate some misclassification cause by the linear boundary.

After the modified classification metheds and the SHF was developed, LWHI can be calculated with the proposed equation. In chapter 5, we applied real-time data from Houston Chronicle to test and verify LWHI. The results shows high level of reliability, and the distribution of LWHI is left-skewed normal distribution. With this reliable result, the LWHI can serves as a simple and effective hazard identification method that can be included in the overall PHA (Process Hazard Analysis) process of the facility.

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