Case Studies on Predictability in University Chemistry Experiment Accidents

Kenta Mizuno¹, Kaori Ueki¹ and Takashiro Akitsu¹
¹Department of Chemistry, Faculty of Science, Tokyo University of Science, Japan

ABSTRACT

In this study, we investigated prediction of fire accidents of university’s chemical experiments based on properties or data of chemicals used. By referencing hazardous compounds and their properties in the Fire Service Act in Japan, potentially dangerous operations were picked up from the textbook of General Chemistry Laboratory for undergraduate students in Department of Chemistry, Faculty of Science, Tokyo University of Science. Moreover, previous examples of fire accidents associated with such hazardous compounds and experimental operations were also searched from some databases. Comparing both facts, we concluded that most of fire accidents are predictable, and some difficult cases (i) required common sense for chemical experiments (implicit knowledge with experience) and (ii) are state-dependent properties of the hazardous compounds, e.g. very reactive nanoparticles. The results will also suggest possibility of AI-aided prediction of fire accidents in the future, the range of data required to be learnt, and remaining technical problems.

Keywords: Chemical Experiment, Hazardous Compounds, Potential Fire Risk, AI Prediction

1. INTRODUCTION

Chemistry experiments are prone to accidents such as fire. Some schools may hesitate to offer laboratory experiments out of safety concerns. Currently, the importance of ensuring laboratory safety is increasing in the school environment. In the university, it is also necessary to increase laboratory safety. Information on accidents are available in various formats. Some focus on the chemical substance to introduce accidents; others introduce examples of accidents together with commentary. There is also literature on case studies of accidents at elementary school through senior high schools [1-3]. Case studies of accidents are introduced with a particular aim or point of view. Nevertheless, it is difficult for one person to obtain and read all the published information available on accidents, and therefore, building a database of accidents is becoming necessary. To use such a database, artificial intelligence (AI) will be a useful tool in future.

Conventionally, the Safety Data Sheet (SDS) is effective for learning about reagents
used in the laboratory. The SDS is intended to provide information on physical properties, hazards and precautions for handling chemicals or mixtures when supplying or providing such chemical substances. The SDS lists information such as name and physical/chemical properties, hazards, first-aid measures upon exposure, handling, storage, and disposal methods. It is internationally standardized; many countries require by law to provide an SDS. In Japan, it has been required under the Industrial Safety and Health Act since 2000 to provide an SDS to convey information on chemical hazards and to properly manage chemicals. An SDS is easily obtained for all chemicals sold on the market [4].

The Fire Service Act in Japan categorizes hazardous substances into six categories with respect to fire hazards. The SDS contains this information; it is possible to look up substances which may cause a fire or properties such as boiling point.

At the Tokyo University of Science, chemistry majors take a total of five laboratory courses in three years: introductory chemistry laboratory, general chemistry laboratory, inorganic chemistry laboratory, organic chemistry laboratory, and physical chemistry laboratory. The general chemistry laboratory course is taken by all chemistry students in the first semester of their second year. The experiments in the course are shown in Table 1: the experiments cover organic, inorganic, and physical chemistry topics [5]. "Safety" in the Table 1 marks an experiment without Hazardous materials. The course description states, “General Chemistry Laboratory is an experimental laboratory course taken in the second year. Its main objective is for students to learn basic and general chemistry concepts and skills.” Students are not allowed to bring in the lab manual to the class. Rather, they are expected to prepare for the experiments beforehand. Students are expected to summarize the experiment’s objectives, theoretical background, properties and precautions for reagents and methods in their laboratory notebooks. During the experiment, they are only allowed to bring in their notebooks. The students have looked up potential hazards of reagents and lab methods. If an accident occurs during an experiment, then, there must be information lacking in the text.

| Experiment | Area       | Topic of theme                          |
|------------|------------|-----------------------------------------|
| 1          | Organic    | Reaction of salicylic acid (methylation)|
| 2          | Organic    | Reaction of salicylic acid (acetylation)|
| 3          | Organic    | Optical resolution of mantellic acid    |
| 4          | Organic    | Synthesis of acetanilide                |
| 5          | Physical   | Adsorption of methyl orange             |
| 6          | Inorganic  | Synthesis of coordination compounds and their physical properties |
| 7          | Inorganic  | Synthesis and analysis of metal alloys with low melting point Synthesis of alloys |
| No | Type  | Description                                                                 |
|----|-------|------------------------------------------------------------------------------|
| 8  | Inorganic | Model reaction of catalytic denitrification of waste liquid containing ammonia |
| 9  | Organic | Extraction and separation of photosynthesis pigment in chlorophyll           |
| 10 | Organic | Synthesis of macromolecular compounds                                         |

The objective of this research is to examine whether potential risk of fire hazards in university chemistry experiments are predictable automatically. This research targets fire accidents in university laboratory experiments. Reagents classified under the Fire Service Act in Japan as hazardous are selected, as well as dangerous laboratory procedures from the textbook of the General Chemistry Laboratory course manual. The materials and reagents are compared with accidents in the literature, and the differences in the results analyzed.

2. METHODS

In order to carry out the objective, we have investigated potential fire risk from the textbook of the General Chemistry Laboratory course as follows:

Step 1: Potentially dangerous operations were picked up from the textbook of General Chemistry Laboratory according to hazardous compounds and their properties in the Fire Service Act in Japan.

Step 2: By referencing hazardous compounds and their properties in the Fire Service Act in Japan, why and what risks should be noted was described. These can be regarded as basis for prediction of fire risk.

Step 3: Previous examples of fire accidents associated with such hazardous compounds and experimental operations were also searched in databases. These are actual case studies for fire risk.

Step 4: Comparing prediction with actual case study, predictable and unpredictable risk (and their characteristic features) will be discussed.

3. RESULTS

3.1 Dangerous Laboratory Procedures

All experimental procedures including hazardous compounds were cited from the General Chemistry Laboratory textbook of TUS [5]. Underlines emphasizes potentially hazardous compounds based on The Fire Service Act in Japan, which was picked up. It should be noted that the conditions (e.g. temperature, method of heating, and open/close apparatus) under which chemicals are treated are also stated.
3.1.1 Experiment 1. Reaction of Salicylic Acid (Methylation)

Keywords: flash boiling, reflux, distill

(Synthesis reaction) Take the 200 mL round-bottom flask off the reflux condenser and add 15 g salicylic acid and 35 mL methanol. While cooling the flask in a water bath, slowly add 5 mL concentrated sulfuric acid. Add a boiling chip to the flask, then attach to a reflux condenser and run for about 1 hour. During the refluxing, take care that the vapor surface does not rise over the condenser. If it rises to the top half of the condenser, take it off the heating apparatus (heating mantle) to cool the entire apparatus so that it falls to the bottom half.

(Distillation) Attach a Liebig condenser to the apparatus and distill toluene (b.p. 110.6 °C). When all the toluene is distilled, and the surface of the ester vapor rises to reach the tip of the thermometer, and the thermometer reading stops, stop heating.

3.1.2 Experiment 2. Reaction of Salicylic Acid (Acetylation)

Keywords: reaction, dehydration reaction, exothermic

Measure 30 mmol salicylic acid into a 50 mL Erlenmeyer flask and add 85 mmol acetic anhydride. (Do this step in a draft chamber). To this solution, add a few drops of concentrated sulfuric acid. When the salicylic acid has partially dissolved, set in a water bath pre-heated to 60 °C. Leave to react for about 15 minutes without stirring (The flask should be fixed with a clamp.). After the reaction has finished, take flask out of water bath and cool a little, then cool in ice bath for 5 min. While cooling in the ice bath, add cold water to the reactant solution until it becomes white and cloudy (Cold water is added while the solution is cooled because when added at room temperature, the remaining acetic anhydride is hydrolyzed and produces heat).

3.1.3 Experiment 3. Optical Resolution of Mandelic Acid

Keywords: reflux, reaction

Attach the reflux condenser to the round-bottom flask containing the suspension. Place round-bottom flask on water bath at 80-90 °C. and put on stirrer. While running some cold water into the apparatus, dissolve suspension with heat. If a large amount of crystals does not dissolve, add 2-5 mL water saturated ethyl acetate.

3.1.4 Experiment 4. Synthesis of Acetanilide

Keywords: heat

(Synthesis of acetanilide) Heat solution of aniline in hydrochloric acid to 50 °C, then add 6.2 mL acetic anhydride. Stir a little to dissolve, then immediately add aqueous solution of sodium acetate and mix well.
3.1.5 Experiment 5. Adsorption of Methyl Orange

Keywords: stirring, mixing

Preparation of methyl orange solution. Use the scale in the balance room to measure and weigh methyl orange crystals with a weighing bottle. For the aqueous solution, take 0.131 g, for the methanol solution, take 0.082 g methyl orange. The values do not need to be exact, but the weights should be recorded, and precise concentrations should be calculated. Rinse 100 mL volumetric flask with deionized water or methanol. Insert triangle funnel into flask, and wash crystals into flask with as little solvent as possible. Wash methyl orange remaining on weighing bottle, glass rod, or funnel into flask. Add solvent so contents come to about 80% of the volumetric flask, and dissolve crystals using an ultrasonic cleaner. Confirm by sight that the crystals are completely dissolved. Add solvent to the mark on the flask and close the cap. Hold the volumetric flask upside down and shake well.

3.1.6 Experiment 6. Synthesis of Coordination Compounds and Their Physical Properties

Keywords: heat bath, heating on plate, electric fire

During the synthesis of carbonatobis(ethylenediamine)cobalt(II) chloride \([Co(en)_2(CO_3)]Cl\), blow in carbonated gas so that bubbles can be observed several times per second. Put 8 mL water and 5.6 mL ethylenediamine into an Erlenmeyer flask, and blow in carbonated gas into the solution for 15 minutes while cooling. While blowing in carbonated gas, add solution of 9.8 g CoCl\(_2\)6H\(_2\)O and 9 mL water and stir well. After the reaction is complete, cool with ice as 10 mL 30% H\(_2\)O\(_2\) is added slowly using a Pasteur pipette. When added quickly, the mixture will vigorously react and heat. This step is very dangerous, so take care. Heat the solution in a heat bath at 70-75 °C for about 30 minutes. Production of trans-dichlorobis(ethylenediamine)cobalt(II) chloride trans-[Co(en)_2(CO_3)]Cl : Take 2.8 g \([Co(en)_2(CO_3)]Cl\) and drop a few mL of water and dissolve well. While cooling the solution in an ice bath, add 6-7 mL of 3 mol/L hydrogen chloride. Care should be taken, since the solution will bubble vigorously. After adding 3 mol/L hydrogen chloride, add about 5 mL of concentrated hydrogen chloride slowly, then heat and condense on a hot plate inside a fume hood until the solution solidifies into green crystals. After it solidifies, let cool, then add a small amount of cold water, then, wash with methanol. Dry well on watch glass.

3.1.7 Experiment 7. Synthesis and Analysis of Metal Alloys with Low Melting Point Synthesis of Alloys

Keywords: concentrated nitric acid and metal, exothermic, flash boiling, metal powder

Place lead in plate, put plate on wire gauze and heat with burner. Stabilize edge of plate with crucible tongs and collect lead pieces into middle of evaporating dish and melt while stirring. When the lead has melted, add bismuth and stir slowly. When all the bismuth has melted, lower heat. Add tin and let melt, lower heat further and slowly
stirs, about 1 minute so the melted metal is uniform. Collect the oxidized material on the surface of the alloy to one side of the dish, then slowly pour alloy into dry porcelain boat.

(Melting alloy reagents) The melting of the reagents should be done inside the draft chamber. Move the watch glass a little to make a gap and add a total of 7-8 mL concentrated nitric acid, 1-2 mL at a time using a 5 mL pipet. After the metals are almost dissolved, leave for about 10 min until generation of brownish gas has subsided. On a hot plate, heat for about 20 min until emission of brownish gas is completed. In this step, the lead and bismuth melt, but tin produces white stannic acid, SnO$_2$$\cdot$nH$_2$O, and precipitates. Add 20-30 mL of 1:20 nitric acid (1 part concentrated nitric acid diluted with 20 parts water). Heat for about 30 minutes, watching for flash boiling, then cool to about 40 °C. (Caution: when adding 1:20 nitric acid, lift up the conical beaker from the hot plate to add, then replace on hot plate to heat).

3.1.8 Experiment 8. Model Reaction of Catalytic Denitrification of Waste Liquid Containing Ammonia

Keywords: oxidizing solids
Prepare 100 mL sodium nitrite solution with the same nitrogen conversion factor.

3.1.9 Experiment 9. Extraction and Separation of Photosynthesis Pigment in Chlorophyll

Keywords: reaction, hydrolysis reaction, exothermic
Wash 200 g spinach leaves with water. Cut leaves into small pieces, put into mortar, add enough methanol so that the contents are covered, and grind. Extract ground ingredients several times by suction filter with methanol.

3.1.10 Experiment 10. Synthesis of Macromolecular Compounds

Keywords: contact with metal
Take 0.3 g hexamethylene diamine into 100 mL beaker and dissolve in 15 mL aqueous solution of 1% sodium hydroxide. Measure 0.3 g adipoyl chloride into another dry 100 mL beaker, add 25 mL carbon tetrachloride and dissolve. To this carbon tetrachloride solution, slowly pour in the hexamethylene diamine solution. A thin layer of 6,6-nylon will form at the interface of the two solutions. Pick up the center of the layer with tweezers and pull up, coiling the strand of nylon onto a glass rod.

3.2 Hazardous Material and Property Data in the Fire Service Act in Japan

All physical properties data, e.g. flash point, boiling point, and vapor pressure, as well as category of the Fire Service Act in Japan (Table 2) on dangerous materials were cited from the safety website of Ministry of Health, Labor and Welfare of Japan [7]. In this section, we selected the dangerous materials as we mentioned in section 2.1 and
their (physical) properties indicating what and why it may be dangerous. Properties underlined in particular provide numerical as well as situational basis for prediction of fire risk in section 3.1.

Table 2 Six categories of The Fire Service Act in Japan.

| Category | Materials                              | Examples                                      |
|----------|----------------------------------------|-----------------------------------------------|
| I        | Oxidizing solid                        | KMnO₄, K₂MnO₄, Na₂Cr₂O₇, K₂Cr₂O₇            |
| II       | Flammable solid                        | Fe, Al, Zn, Mg, P₄S₁₀, Red phosphorus (P)    |
| III      | Spontaneous combustibility, Prohibited aqueous | Li, Na, K, LiH, Yellow phosphorus (P₄) |
| IV       | Flammable liquid                       | CS₂, Hydrocarbons as organic solvents        |
| V        | Self-reactive substances               | Benzoyl peroxide, Azo-compounds              |
| VI       | Oxidizing liquid                       | H₂O₂, BrF₅, IF₅                              |

3.2.1 Toluene
The Fire Service Act in Japan: Category IV
Flash point: 4.4 °C
Vapor density: 3.1

3.2.2 Ethyl Acetate
The Fire Service Act in Japan: IV
Flash point: ~4 °C (closed cup)
Vapor pressure: 75 mmHg (20 °C)

3.2.3 Aniline
The Fire Service Act in Japan: IV
Flash point: 76 °C (closed cup)
Vapor pressure: 0.667 mmHg (25 °C)

3.2.4 Acetic Anhydride
The Fire Service Act in Japan: IV
Flash point: 49 °C (closed cup)

3.2.5 Ethylenediamine
The Fire Service Act in Japan: IV
Flash point: 34 °C
Vapor pressure: 12.1 mm Hg (25 °C)
3.2.6 Methanol

The Fire Service Act in Japan: IV
Flash point: 12 °C
Vapor pressure: 95.2 mmHg (20 °C)

3.2.7 Bismuth (Bi)

The Fire Service Act in Japan: IV
Flash point: combustible (powder)

3.2.8 Nitric Acid

The Fire Service Act in Japan: VI
Substances dangerous when mixed: hydrogen sulfate, hydrogen phosphates, carbides, hydrogen iodide, carbon dioxide, amines, hydrazines. Ignites spontaneously upon contact with organic materials such as wood chips, paper, rags. Burns with reducing agents. Corrodes some plastics.

3.2.9 Sodium Nitrite

The Fire Service Act in Japan: I
The compound is non-combustible but enhances combustion of other materials. In many reactions, it may result in fire or explosions. When heated to over 530 °C, it may explode.
Reactivity: Is a powerful oxidizing agent. Reacts with combustible compounds and reducing agents, with danger of fire and explosion.

3.2.10 Adipoyl Chloride

The Fire Service Act in Japan: III
Reactivity and chemical stability: It is decomposed by moisture in the air

3.3 Actual Accident Examples

Actual examples of accidents stating MHLW safety website were cited from the safety website of the Ministry of Health, Labor and Welfare of Japan [6]. An example of an accident that is marked as Database is quoted from Association for the Study of Failure, Failure Knowledge Database [7]. Hazardous Materials with no accident in the MHLW safety website and database were omitted. All the examples were classified into two marks: items marked ‘@’ are predictable accidents from the data of physical properties or general instruction listed in section 3.2, whereas items marked ‘#’ with underlines are impossible to expect their dangers only from the data. We judged whether the danger can be predicted only by the nature of Hazardous Materials under the Fire Service Act in Japan and SDS information.
3.3.1 Toluene

MHLW safety website
@Drying facility exploded
@Explosion during welding inside ship
@Gas burner flame ignited adhesive
@During pretreatment for incineration, fire erupts from underside of forklift
@Fuse spark from periodic repair of chemical plant ignites toluene gas, becomes covered in flames
@Injury from toluene inside pipe igniting during oxy-fuel cutting of piping in chemical plant
@Worker was injured due to fire erupted while filling reaction product from synthetic resin polymerization reaction vessel to drum.
@During production of pharmaceutical intermediates, sodium hydride ignited, and ignited toluene vapor, causing injury
@2 workers die from explosion during spray painting hold of bulk cargo ship under construction
@Explosion during loading ingredients that included toluene onto dry tank from flexible container

Database
@Toluene leakage due to detaching wrong coupling during removal of cleaning toluene
@Ignition and fire from static electricity near the ink tank of a gravure printing machine
@Earthquake caused fire in floating roof tank, and two days later, another floating roof tank catches fire, causing the first full face fire in Japan
@Ignition of printing ink due to static electricity from deterioration of static eliminator in transfer printing machine
@During step to coat paper, paper is submerged in liquid and soaked in excess toluene, causing explosion and fire
@Fire of printing ink in dryer of transfer printing machine
@Explosion of organic solvent during repacking process
@Explosion and fire from contamination of residues in alkylaluminum production apparatus
@Explosion from spark in electric grinder during repair of waste water neutralization tank
@Leak, explosion and fire of hydrogen gas from use of SUS 304 material and defective construction of hydrogenation reduction apparatus
@Explosion and fire of gas in vapor part of nitrogen sealed toluene drainage tank in hydroquinone production apparatus
@Toluidine was mistakenly added to diketene tank, causing polymerization reaction and explosion
@Explosion when stirring was resumed during sulfonylation of toluene
@Spontaneous combustion of p-toluene sulfonyl dimethyl hydrazine in temporary storage
@Sudden explosion of cleaning tank in lauroyl peroxide production plant
@Rupture of reaction tank due to water contamination in p-nitro toluene sulfonic acid reaction tank
@Explosion and fire due to use of electric sprayer during painting pontoon for floating roof tank
@Gasoline fire during draining filter in truck loading facility
@Furnace explosion due to leak in fuel gas during start up procedure of catalytic reforming apparatus
@Explosion due to static charge accumulation during toluene tank sampling
@Fire due to gas leak from dealkylation in high temperature heat exchanger in benzene production apparatus
@Leak in varnish from trench pipe in truck loading facility
@Leak and fire from suspended reaction flange in cracked gasoline hydrogenation facility

3.3.2 Ethyl Acetate
MHLW safety website
@Worker was injured due to fire erupted while filling reaction product from synthetic resin polymerization reaction vessel to drum.
@Fire during procedure to add powder ingredients to reaction vessel containing ethyl acetate
@During pretreatment for incineration, fire erupts from underside of forklift
@Explosion while paint production tank was being scrubbed with cleaning brush
@Eruption by runaway reaction due to mistake in number of reagents during acrylic resin adhesive production

3.3.3 Acetic Anhydride
Database
#Explosion and fire during synthesis of dehydroacetic acid using reagents with an inappropriate chemical formula

3.3.4 Methanol
MHLW safety website
#Explosion while scraping powder off reaction container with spatula, at facility to produce food additives from seaweed
@Explosion of drum which held methanol during cutting process
@During oxy-fuel cutting, explosive spark from used oil pit ignited due to welding sparks
@Explosion of drying facility
@Explosion of vaporized solution deriving from affixing insulating material Database
@Explosion due to polymerization reaction of benzyl chloride
@Explosion of residual methanol at organic peroxides manufacturing facility
@Breakage, explosion and fire due to elevated pressure while washing distillation container
@Breakage and leakage of reactant pipes in manufacturing equipment of methylamine
@Fire from welding sparks from methanol leaking from pipes which were mistakenly dismantled
@Explosion and fire due to accumulation of methanol peroxide in methanol refinement column of surfactant manufacturing equipment
@Explosion and fire from benzoyl peroxide
@Explosion and fire from runaway reaction at start of manufacturing adhesive
@Explosion due to delayed stirring at start of reaction of o-nitrochlorobenzene
@Decomposition reaction of tar-like waste

3.3.5 Nitric Acid
MHLW safety website
@While refining white phosphorous, runaway reaction of nitric acid solution causes explosion of reaction container
@Explosion of waste liquid treatment container at analysis room of LSI manufacturing plant
@Nitric acid from tank truck mistakenly poured into tank of triethanolamine Database
#Explosion due to reactivation of mixer during nitration reaction of 5-t-butylmetaxylene
@Rupture of triethanolamine tank due to mistakenly added nitric acid
@Explosion of waste liquid treatment container due to contamination, in analysis room of LSI manufacturing plant
@Explosion at TNT nitrification room triggered by contamination reaction
@Ignition and explosion of during nitrification completion procedure of nitrocellulose manufacturing process

3.3.6 Sodium Nitrite
Database
@Fire due to overheating of electric heater due to mis operation during periodic repair
@High pressure steam enters the molten salt side due to the opening of the steam generating thin tube of the anhydrous phthalic oxidation reactor, scattering of molten salt, fire
4. DISCUSSION

4.1 Prediction of the Risk in “General Chemistry Laboratory”

Comparing both items in sections 3.1 and 3.2, we could successfully have indicated that most of fire risks in the textbook of the General Chemistry Laboratory in section 3.1 are predictable based on the data of the Fire Service Act in Japan in section 3.2. Because it is an undergraduate student's course, the General Chemistry Laboratory deals with relatively basic and simple experiments of university chemistry. Therefore, the risk in the handling or materials used were easily understand only by the data.

In this context, all hazardous substance would not cause chemical fire accidents. However, many accidents have actually happened in real-life situations. Hence the discussion in the following sections are focused on actual examples of accidents in view of materials and situation to make the reasons clear.

4.2 Features of Predictable Accidents

Of the accidents listed in section 3.3, those predictable from properties listed in Section 3.2 are marked with “@.” Most of the accidents were predictable from properties of the hazardous substances, and many were caused by organic solvents. These accidents may be prevented by understanding the properties of hazardous substances before starting the experimental procedure [8].

Dangers common to the substances are as follows: All were inflammable liquids. Its vapors form mixtures with air and are potential source (fire or spark) of inflammation or explosion.

The relative vapor density was greater than 1, i.e. greater than that of air. Category IV hazardous substances have relative vapor density greater than 1 and their vapor remain or flow to low places. Therefore, there is danger of inflammation by a fire source in a distant location, especially in a downwind location.

The relative liquid density was less than 1, and many are insoluble in water. Many Category IV substances have relative liquid density less than 1, are lighter than water, and are insoluble in water except for some alcohols. Therefore, when such a substance leaks into water, it spreads over a large area of the water surface. When a fire erupts, it may cover a large area, with danger of spreading. When it forms a mist, its danger increases because the contact area with air is increased.

They are poor conductors of electricity. Many Category IV substances are not conductors and charge build up easily. The substance may ignite from the spark produced when the built-up static is discharged. Measures such as grounding are necessary to remove static charge from piping and hose used with these substances.

Temperature control is important for some Category IV hazardous substances with a low flash point, which may ignite upon heating even without a fire source.

For these substances, common preventive measures may be taken [8], such as: Avoid
contact with fire, sparks, hot bodies as well as heat, and avoid emission of vapor. If these cannot be avoided, adequate measures are necessary to avoid hazards.

Containers should be sealed and stored in a cool, dark place. Even substances with low flash points have increasing danger of inflammation with rising temperature; hence, containers should be stored in a cool dark place. When sealed, there should be some space between the lid and liquid surface.

When there is possibility of vapor emission, vapor in low areas should be discharged outside to an elevated location, since flammable vapor remain in low areas. Adequate ventilation should be in place as well as keeping the concentration below the lower bound of explosive limit (flammability limit).

In areas in which flammable vapor may stagnate, equipment which may produce a spark should be avoided. Electric equipment located where inflammable vapor may stagnate should have anti-explosive devices.

If there is a possibility of static charge due to flow of hazardous substances, static should be removed with grounding or other devices.

4.3 Features of Unpredictable Accidents

There were some accidents which were not predictable from only properties listed in the Fire Service Act in Japan, marked with a "#" in section 3.3. Here, four cases are discussed in detail. In Case One, Explosion while scraping powder off reaction container with spatula at facility to produce food additives from seaweed, organic solvents such as methanol and seaweed extract were in the reaction container [9]. When someone tried to scrape out the container, it exploded. This accident was caused by carelessness. Static charge had accumulated from the rotation of the container. In addition, the spatula was made of polyvinyl chloride and the blade was attached to the handle with a metal bolt, creating static discharge which ignited the vapor, causing an explosion.

In Case Two, the Fire at synthetic rubber plant due to leak caused by flange loosening from vibration, the vibration from the pump loosened the flange, causing the hexane to leak and igniting the spark from static. This accident was also caused by carelessness [10]. If the production facility was operating properly, there would not have been a problem.

In Case Three, Explosion and fire during synthesis of dehydroacetic acid using reagents with an inappropriate chemical formula the explosion occurred because of an abnormal reaction caused by impurities in the ingredients [11]. The accident is considered to be caused by complex factors. A mid-sized production experiment of dehydroacetic acid was conducted, resulting in an abnormal reaction, which led to an exothermic explosion. There were two main causes of the accident. The first was the purity of the ingredients. The container which held acetic anhydride was reused as a reaction vessel. In addition, the diketone and acetic anhydride were derived from the drain of the factory production process and used without purification. Therefore, the substances contained impurities, which are thought to have caused the abnormal
reaction. The second cause was the reaction scale. This experiment took place in a chemical factory, at a stage of scaling up from laboratory scale. The inadequacy of research on scale-up was a causal factor.

Case Four is the Explosion and fire during the pulverization of aluminum at a metal powder factory. The powdered aluminum resulted in a dust explosion. This case is another example of carelessness. Metal in bulk form is not a fire hazard in general; however, it is known that the danger of a fire increases with decreasing particle size [13,14].

In this way, accidents which were not predictable from just the properties in the Fire Service Act in Japan can be categorized as follows: One, the accidents are due to human error. The source of fire was unintentionally created due to carelessness. Substances that caused such accidents were Category IV inflammable liquids. To conduct experiments safely with these substances, it is necessary to maintain a distance from a fire source.

Secondly, the accidents are due to a lack of understanding about the properties of the hazardous substances. Several patterns were observed. One is carelessness with respect to purity or impurities of the reagents, or dangers associated with number of reagents or experimental scale. It is necessary to know the purity of the reagents as well as scaling up an experiment with care. When handling solid metals, it should be noted that particle size is related to its safety. In recent years, use of nanoscale materials are increasingly common; the form of the metal, its surface state and particle size should be considered.

4.4 Issues Surrounding AI in Future

Artificial intelligence (AI) can handle much more data compared with humans. There are two main advantages to using AI. One is that it can handle and process very large amounts of data. When humans process data, there were time limitations as well as amount of data that could be handled. However, since AI can handle much more data at high speeds, it is possibly more accurate. The second is that AI may bring to light new information that humans may overlook. Therefore, it will become necessary to use AI in database of accidents. One method of using artificial intelligence is text mining. Text mining analyzes sentences and processes statistics. Text mining also makes it possible to discover the relationship between words and new relevance that cannot be found by humans. Therefore, it is expected to find the dangers and elements of hazardous materials that human beings are unaware of. Specifically, there is an example of analyzing occupational accidents in the steel industry using text mining and performing a risk assessment [15].

Although AI has advantages, it also has disadvantages. In particular, AI cannot read between the lines. When humans read text, they can make inferences and think about what is unwritten. AI, on the other hand, can mine text; however, there are reports that it is unable to understand the meaning of text [16]. AI can only do searches and statistical processing. Taking this weakness into consideration, data input format must be considered when building a database of laboratory accidents for use with AI.
There are some issues that may arise when using AI. When doing a search, names of hazardous substances and laboratory manuals are referenced. When analyzing the cause of accidents, is it possible to predict a hazard from just names of reagents, hazardous substances, or laboratory procedures? It is necessary to explore whether the text of the manual is sufficient to pinpoint the cause of accidents such as those caused by human error.

5. CONCLUSION

In summary, this study picked out chemicals which may cause fire accidents and dangerous laboratory operations, to evaluate their dangers according to properties of hazardous substances. Furthermore, by comparing them with actual accidents, omissions were enumerated. It was found that for most of the hazardous chemicals used in the General Chemistry Laboratory, it was possible to predict fire accidents from the information in the Fire Service Act in Japan or SDS. Nevertheless, some accidents were not predictable from only the textbook, the Fire Service Act in Japan, or an SDS. There were examples of accidents caused by external factors, properties of laboratory equipment, or unexpected mistakes. We also found that most of fire accidents are predictable, and some difficult cases may (i) require common sense for chemical experiments and (ii) are state-dependent properties of the hazardous compounds beyond expected situation.

When using AI in the future, it should be noted that some accidents cannot be prevented from only the textbook nor properties of reagents. It is also important to input the experimental environment, experimental scale, and common sense. For future AI use, it is necessary to clarify elements such as human error and complex factors for its judgement to approach that of humans.

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