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Development of a hazardous material selection procedure for the chemical accident response manual

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Abstract−After the accidental hydrogen-fluoride leak in Gu-mi city, Korea, the Korean government revised its laws on chemical management. The hazardous chemical management laws were strengthened to meet the legal standards, and now the selection of Accident Precaution Chemicals (APCs) is required. This study introduces a novel hazardous material selection procedure for industrial chemical management. The proposed method consists of screening, scoring, rating, and selection procedures. Among the 4,994 hazardous chemicals in the database, 1,362 chemicals were selected through the screening process. The selected chemicals were classified as flammable, explosive/reactive, and toxic materials, and in the final step, flash point, heat of combustion, and toxicity of these chemicals were considered in chemical ratings. According to the ratings, 100 toxic materials were selected and used to modify the safety management manual development software, currently used in Korean companies that deal with hazardous chemicals. The developed algorithm and software are expected to greatly aid plants that deal with hazardous materials.

Keywords: Chemical Management Manual, Chemical Classification, Hazardous Material Management, Accident Precaution, Accident Response

INTRODUCTION

The risk of an accident in the chemical industry grows with an increase in the number of chemical plants. Especially, due to the nature of a chemical plant, one accident can cause terrible damage. Therefore, the importance of risk management in chemical plants is very significant. In terms of risk management, there are many approaches to take into consideration the role between human and non-human factors [1], or contribute to the collection and management of existing quantitative data [2]. Although measures to reduce damage from chemical accidents include prevention, preparation, response, and recovery, it is best to prevent accidents in advance.

Accident prevention initiatives continue to be made not only in Korea but around the world. In China, among four categories, which are particularly serious accident (PSA), major accident (MA), serious accident (SA), and ordinary accident (OA), efforts for prevention of PSA and MA are reported [3]. Due to ongoing research and regulation, China's PSA and MA are decreasing. Life cycle approach is also used for accident prevention [4]. This method considers process design lifecycle, which leads to hazard identification and determines accident contributors. Based on this approach, design and operational errors could be identified earlier and appropriate control at sources actions could be taken as accident prevention measures. In Korea, recent efforts have been made to reorganize the government, enact relevant legislation, and to change the corporate culture to better respond to chemical accidents [5-7]. In particular, efforts have been made to thoroughly regulate chemical substances at the management stage.

In the USA, OSHA's Process Safety Management (PSM) standard and EPA's Risk Management Plan (RMP) regulation is widely used [8,9]. PSM sets requirements for facilities which handle hazardous chemicals and aim to protect workers. It is designed to help prevent unexpected accidents like toxic chemical release, reactive and flammable liquids or gasses. The PSM standard mainly applies to manufacturing industries like chemical, transportation equipment, and fabricated metal products. The key provision of PSM is process hazard analysis (PHA). Employers must identify hazardous chemicals in their process and develop prevention plan for releases of hazardous chemicals. PSM has 13 other elements besides PHA, and they must be integrated into both planning and operations at a facility; 14 elements are shown in Table 1.

RMP is intended to protect the environment and the community from accidents. RMP regulation requires facilities that use haz-

Table 1. PHA elements

1. Process safety information	8. Management of change
2. Process hazard analysis	9. Incident investigation
3. Operating procedures	10. Compliance audits
4. Training	11. Trade secrets
5. Contractors	12. Employee participation
6. Mechanical integrity	13. Pre-startup safety review
7. Hot work	14. Emergency planning and response

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ardous chemicals to develop an RMP plan. The plan identifies the potential effects of a chemical accident, steps the facility is taking to prevent an accident, and spells out emergency response procedures should an accident occur. Facilities that have more than the limit of regulated substances in the process must comply with EPA's risk management program regulations. This requirement requires the owner or operator of the facility to implement a risk management program and submit an RMP to the EPA. The program should include hazard assessment, prevention program, and emergency response program. RMP rule is broken into three programs based on the threat posed to the community and environment. Many requirements of the RMP program are the same as those of the PSM. The coverage between the two standards is overlapping, but not complete. In the Unites states, guidelines are in place to ensure RMP and PSM programs in different environments.

The Seveso directives are the main EU legislation dealing specifically with the control of on-shore major accident hazards involving dangerous substances. The Seveso III directive came into force on 1 June 2015, replacing the Seveso II directive. They control major accident hazards involving dangerous substances [10]. Current European and UK chemical classification is set out in the dangerous substances directive and dangerous preparations directive. These directives are implemented in UK by the Chemicals Hazard Information and Packaging for supplying regulations (CHIP). CHIP is well known to chemical suppliers, and many chemical users and consumers are accustomed to the orange and black hazard symbols that have appeared in chemical products for many years.

As shown above, many other countries are trying to prevent chemical accidents with a risk management program. It helps to prevent chemical accidents and improves risk management in a facility. Since there are various types of accidents in the chemical industry, it is important to develop a detailed management system. Accidents in the chemical industry can be classified into fires, explosions, and leaks. Fires are the most common accidents, followed by explosions. In the case of toxic substance leakage, there are characteristics that can lead to secondary damage [11]. Once a chemical leakage accident takes place, it causes enormous human and material damage. It also affects the health, environment and society of residents depending on the severity level [12]. Flixborough, Bhopal, and Seveso disaster began with a chemical leakage accident. Hydrogen fluoride leakage accident in Gu-mi is a representative case of a chemical leakage accident in Korea [5]. Such leakage accidents cause enormous damage to human life and also cause secondary damage like fire and explosion, so chemical leakage risk management is very important.

As there are numerous types of chemical substances, it is impossible to control all chemical substances. Therefore, the control substance selection process must be preceded by a management system, which is a necessary process to improve the management efficiency and to preferentially select substances that need management. The first consideration while setting up a controlled substance is the environment in which it should be handled. The type and amount of substances handled by different countries or regions as well as the rules governing them are different. Therefore, substance selection must be carried out according to the regulations and laws of the relevant countries.

There are many ways to select the materials, and substance selections for management are actively carried out not only on chemical substances but also in environmental pollution related fields [13]. A data prioritization method by sample analysis is provided in advance [14]. In general, the substance classification method depends on the physical properties of a given substance [15]. After appropriate criteria for each purpose are set, each item should be rated. Then, the calculated scores can be added together to prioritize the scores in ascending order so that the relative impacts can be compared [13,16].

The Globally Harmonized System of Classification and Labelling of Chemicals (GHS) is a system developed by the UN for standardizing and harmonizing the classification and labelling of chemicals globally [17,18]. It is known as the UN GHS purple book, and defines physical, health and environmental hazards of chemicals and harmonized classification criteria. The GHS purple book is updated frequently, and the latest edition was revised in 2017 [19]. This system has been developed to unify international trade and information delivery by unifying the worldwide MSDS technology method, which was different from each other in terms of notation. There are 17 classes of physical hazards, 10 classes of health hazards, and 2 classes of environmental hazards [19]. The GHS classification criteria are used for many studies which deal with chemicals. The positive effect of its implication is studied in South Africa [20]. It is used for the selection of the reference chemicals for hazard identification of eye irritating chemicals [21]. Chemical hazardous liquid waste classification method is also suggested based on lower heating value and on both water and pollutant content of the residues [22]. Hazard study in unconventional oil and gas operation is also based on GHS classification [23].

Previous studies suggested numerous classification methods and classified cases for chemicals, and these methods help manage hazardous chemicals well. In Korea, a web-based chemical management system was developed in 2011 [24], which deals with hazardous chemicals. However, maintenance has not been done well since the management system was developed. Therefore, the system needs to be updated, and new chemicals need to be selected. This study aims to construct additional data for efficient hazardous chemical management to add to the existing management substances. We propose three material selection stages and set the selection criteria using these stages. Materials selected by the suggested procedure are used to update the chemical accident response manual (CARM) development software.

HAZARDOUS MATERIALS AND METHODS

1. Accident Precaution Chemicals (APCs) Background

Chemicals are used not only in industry but also in various fields such as agriculture and manufacturing [25]. In the case of chemical industrial complexes, it is likely to lead to a series of accidents because they handle various materials and are concentrated [26]. Chemical management is important owing to the increasing demand for domestic chemicals, which has gradually increased the scale of potential damage. As the chemical industry develops, efforts should be made in terms of its management [27]. In many countries, management substances are selected and managed ac-

Table 2. Accident Precaution Chemicals (APCs)

ID	Chemical name	ID	Chemical name
1	Formaldehyde	50	Hydrogen sulfide
2	Methyl hydrazine	51	Arsine
3	Formic acid	52	Chlorosulfonic acid
4	Methanol	53	Phosphine
5	Benzene	54	Phosphorus oxychloride
6	Methyl chloride	55	Chlorine dioxide
7	Methylamine	56	Diborane
8	Hydrogen cyanide	57	Nitric oxide
9	Vinyl chloride	58	Nitromethane
10	Carbon disulfide	59	Ammonium nitrate
11	Ethylene oxide	60	Hexamine
12	Phosgene	61	Hydrogen peroxide
13	Trimethylamine	62	Potassium chlorate
14	Propylene oxide	63	Potassium nitrate
15	Methyl ethyl ketone	64	Potassium perchlorate
16	Methyl vinyl ketone	65	Potassium permanganate
17	Acrylic acid	66	Sodium chlorate
18	Methyl acrylate	67	Sodium nitrate
19	Nitrobenzene	68	O-Isopropyl methyl phosphonofiuoridate
20	4-Nitrotoluene	69	Cyanogen chloride
21	Benzyl chloride	70	Nickel carbonyl
22	Acrolein	71	Germane
23	Allyl chloride	72	Tetrafluoroethylene
24	Acrylonitrile	73	Trifluoroborane
25	Ethylenediamine	74	Boron trichloride
26	Allyl alcohol	75	Hexafluoro-1,3-butadiene
27	m-Cresol	76	Bromine
28	Toluene	77	Hydrogen selenide
29	Phenol	78	Isoprene
30	n-Butylamine	79	1,1-Dichloroethylene
31	Triethylamine	80	Hexamethyl disiloxane
32	Ethyl acetate	81	Pentacarbonyl iron
33	Sodium cyanide	82	Bromine pentafluoride
34	Ethylenimine	83	Thionyl chloride
35	Toluene-2,4-diisocyanate (TDI)	84	Titanium tetrachloride
36	Carbon monoxide	85	Chloropicrin
37	Acrylyl chloride	86	Vinyl ethyl ether
38	Zinc phosphide	87	Silane
39	Methyl ethyl ketone peroxide	88	Disilane
40	Isophorone diisocyanate	89	Dichlorosilane
41	Sodium	90	Trichlorosilane
42	Hydrogen chloride	91	Methyldichlorosilane
43	Hydrogen fluoride	92	Methyltrichlorosilane
44	Ammonia	93	Trichlorovinylsilane
45	Sulfuric acid	94	Trichloroethylsilane
46	Nitric acid	95	Tetramethylsilane
47	Phosphorus trichloride	96	Silicon Tetrachloride
48	Fluorine	97	Silicon tetrafluoride
49	Chlorine		

cording to the management regulations of each country [28,29]. In this social atmosphere, materials with the potential to cause great damage during an accident are designated and managed in Korea. The controlled substances are referred to as "APCs", which are defined as follows:

- APCs: Chemical substances that are likely to cause serious damage due to strong acute toxicity or explosion risk or are likely to cause an accident if an accident occurs ['Chemical Control Act' Chapter 5 Section 1 Article 39].

Currently, 69 types of APCs are registered in the 'Chemical Control Act,' shown in Table 2. However, in reality, there are more than 69 chemical species, and thus additional designation of controlled substances is required [24].

2. Candidates for Additional APC Designation

2-1. Definition of Property

Chemicals are classified according to their characteristics. Chemicals have characteristics that are specific to each substance and must be managed accordingly [30]. Therefore, chemical management should proceed from the point of use and storage, and its characteristics must be understood correctly [31,32]. The chemical properties considered in the text, as well as their definitions, are summarized as follows.

(1) Explosive substance:

Solids, liquids or mixtures that produce gases (from their own chemical reactions), and can damage the surrounding environment by their temperatures, pressures, and speeds.

(2) Flammable substance:

Gases with a flammable range when mixed with air at a standard pressure of 101.3 kPa at 20 °C and liquids that have a <60 °C flash point at a 101.3 kPa standard pressure.

(3) Self-reactive substance:

Substances that are easy to decompose exothermically to a thermally unstable state without the supply of liquid oxygen and solid material pyrophoric substance.

(4) Pyrophoric material:

Liquids and solids that can ignite in less than 5 minutes in air.

(5) Water-reactive substance:

Substances or mixtures that react with water to release flammable gases.

(6) Organic peroxide:

Hydrogen peroxide derivatives in which one or two hydrogen atoms have a bivalent **-O-O-** structure and are replaced by organic radicals.

2-2. Classification Criteria of Additional APC Designations

The substances designated as APCs are physically and chemically hazardous and have risks, such as flammability, explosion, reactivity, and leakage. They are also acutely toxic when orally ingested, inhaled or exposed to the skin. These substances have a high probability of accidental exposure due to a large domestic distribution. Other considered substances require special care due to high accident risk [33].

The initial research subjects were 4,994 species, including Design Institute for Physical Properties (DIPPR) (1,700 species), hazardous material (2,527 species), and toxicological (767 species of Risk Management Plan (RMP and COMMA) data. We proposed a three-step substance selection procedure to select additional APCs, which

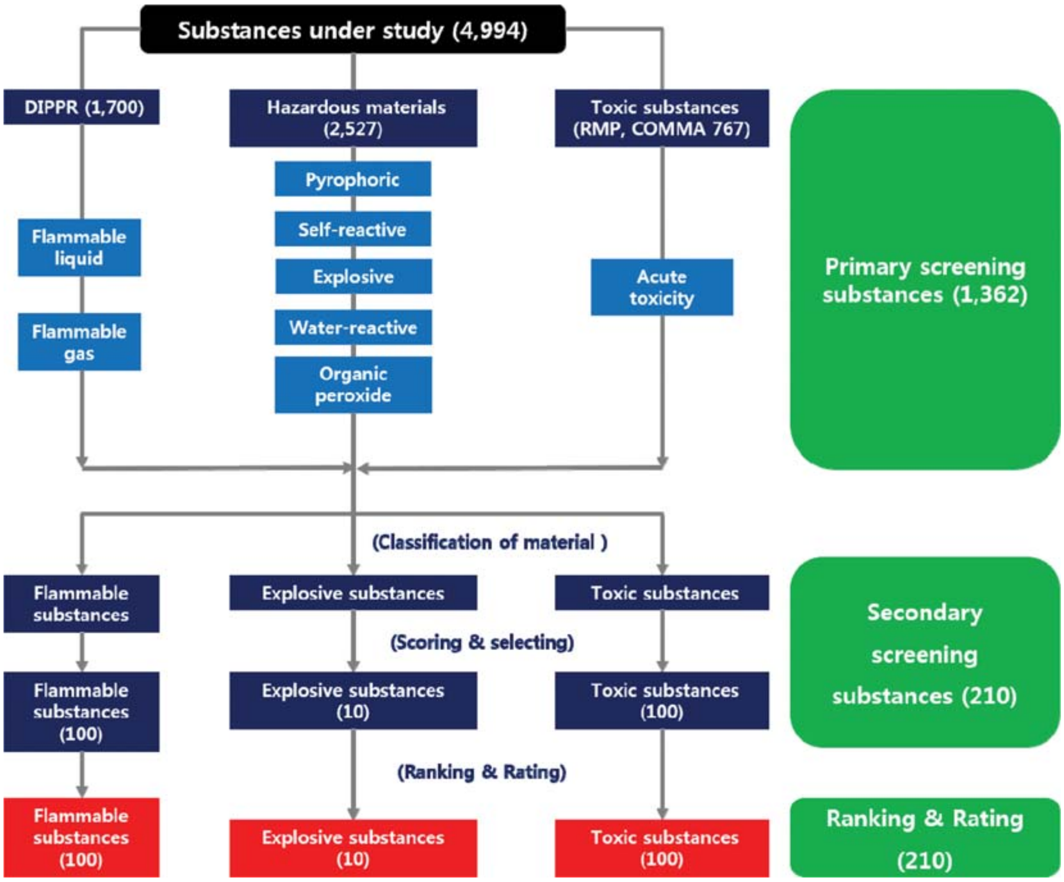

Fig. 1. APC addition procedures schematic.

includes screening, scoring, rating, and selection. During the screening process, 1,362 species were selected, and 210 species were selected through the rating process (Fig. 1).

ADDITIONAL APC SELECTION

The expansion of management materials is necessary as the scale of handling facilities and materials is diversified, as shown above. Additional APCs were selected by considering the handled amount and the substance risk, except for the substances which overlapped with the APCs. To select additional APCs, the substances were classified into substances with high physicochemical hazards, such as flammability, explosion, and reactivity, substances with high acute toxicity, and substances with high accident exposure due to the high domestic distribution. In addition, workplaces that are based in industrial complexes or near residential areas will suffer more damage during accidents, and thus the chemicals used were identified by classifying the plants according to their estimated scale of damage. The screening, scoring, and rating phases were used to identify the additional candidate substances for accident assignment. The next step was to select substances to add to the accidental substance, including 100 flammable, 100 toxic, and 10 explosive substances.

1. Procedures for Classifying Hazardous Materials

The procedures of classification and selection are applied differently depending on the application. The selection and classification of substances is mainly applied in the process of selecting specific substances in the environmental and medical fields, and most of them are evaluated through experiments and sample analysis [34-37]. In this study, the evaluation based on the physical properties of the chemicals was carried out. In this process, each rating criterion refers to domestic and global regulations and is re-set as needed to facilitate evaluation and interpretation [38].

1-1. Screening Procedure

Through the selection process, 1362 out of 4994 substances were selected by several criteria that are summarized in Table 3. Materials were first selected to conform with the regulations by applying different criteria according to the data type. We selected 1700 DIPPR substances, which included 646 flammable liquids and 60 flammable gases. Additionally, 2527 kinds of hazardous materials were selected, which included 17 pyrophoric substances, 2 self-reactive substances, 2 explosive substances, 24 water-reactive substances, and 7 organic peroxides. Furthermore, 767 kinds of toxic chemicals were screened as 604 acute toxicity species.

1-2. Scoring and Selection Procedures

Prior to substance screening, primary sorting materials were classified as flammable, explosive/reactive, and toxic. Explosive reactive substances that cause the largest damage in case of an accident were prioritized. As a result of secondary screening, 210 kinds of substances were selected, including 100 kinds of flammable sub-

Table 3. Screening criteria and number of selected species for each data type

Data type (Number of species)	Screening criteria		The number of selected species
DIPPR (1,700)	Flammable liquid	Flash point below 60 °C (GHS Categories 1, 2, and 3)	646
	Flammable gas	Explosion limit 13% or lower, explosion upper/lower limit difference of 12% or more (GHS Category 1)	60
Hazardous materials (2,527)	Pyrophoric substances	GHS Category 1	17
	Self-reactive substances	GHS Types A and B	2
	Explosive substances	GHS Class 1.1	2
	Water-reactive substances	GHS Category 1	24
	Organic peroxides	GHS Types A and B	7
Toxic chemicals (767)	Acute toxicity	GHS criteria oral, dermal, inhalation categories 1, 2, 3, and 4	604
		Total	1362

Table 4. Flammable substance rating criteria

	Risk characteristic (1)	Risk characteristic (2)	Risk characteristic (3)	Leakage diffusion characteristic (1)	Leakage diffusion characteristic (2)
Score	1-5	1-5	1-3	1-4	1-3
Flammable liquid	Flash point (Step 5)	Explosion risk (Step 5)	Heat of combustion (TNT combustion heat ratio) (Step 3)	Diffusion potential index (Step 4)	Vapor pressure (25 °C) (Step 3)
Flammable gas	Lower explosion limit (Step 5)	Explosion risk (Step 5)			

Table 5. Rating section and value for each characteristic

Score	1	2	3	4	5
Flash point (°C) (Flammable liquid)	X>50	25<X≤50	0<X≤25	−30<X≤0	X≤−30
Lower explosion limit (%) (Flammable gas)	X>8.4	4.3<X≤8.4	1.8<X≤4.3	1.6<X≤1.8	X≤1.6
Explosion risk	X≤3.5	3.5<X≤5	5<X≤6.7	6.7<X≤9	X>9
TNT combustion heat ratio	X≤2	2<X≤3	X>3	-	-
Diffusion potential index	X≤8	8<X≤10	10<X≤12	X>12	-
Vapor pressure (mm Hg)	X≤10	10<X≤125	X>125, gas (25 °C)	-	-

stances, 10 kinds of explosive/reactive substances, and 100 kinds of toxic substances.

1-3. Ranking and Rating Procedures

An indicator was created according to the substance characteristics to set priorities for each substance type. Then, these substances were ranked according to their indicators.

1-3-1. Ranking and Rating of Flammable Substances

Physical hazards, such as flash point and heat of combustion, were evaluated by considering the distribution of substance characteristics and referring to the DIPPR data from the American Chemical Society. As summarized in Table 4, the risk index (out of 20 points) is calculated by summing the risk characteristics (Section 3) and the leakage/diffusion characteristics (Section 2). Explosive substances (Class 1.1), self-reactive substances (Types A and B), and pyrophoric solids (Category 1) were prioritized. Higher values were obtained by comparing the leakage/diffusion characteristic scores (7 points total) and the basic scores (5 points total) for pyrophoric liquids (Category 1), water-reactive substances (Category 1), and organic peroxides (Types A and B).

- TNT Combustion Heat Ratio

$$= \frac{\text{(Combustion Heat of the Material)}}{\text{(Combustion Heat of the Combustion (Explosive))}}$$

- Explosion risk

$$= \frac{\text{(Explosion upper limit} - \text{Lower explosion limit)}}{\text{(Lower explosion limit)}}$$

- Diffusion potential number (V) $= \frac{(1.6 \times M^{(0.67)})}{(T+273)\times 100}$

where M is molecular weight and T is boiling point (°C).

The scores were divided by the score of each characteristic, described in Table 5.

Through the secondary screening, 100 flammable substances and 10 explosive/reactive substances were selected, as summarized in Table 6, 7 and 8.

Table 6. Ranks of the 84 selected flammable liquids

Rank	CHEM_NAME	CAS_NO	Score	Rank	CHEM_NAME	CAS_NO	Score
1	VINYLTRICHLOROSILANE	75945	15	43	cis-2-OCTENE	7642048	12
2	4-METHYL-cis-2-PENTENE	691383	15	44	TRICHLOROACETALDEHYDE	75876	12
3	2-CYCLOHEXYL CYCLOHEXANONE	90426	14	45	TRIPROPYLAMINE	102692	12
4	1,1-DICHLOROETHANE	75343	14	46	2,2,5-TRIMETHYLHEXANE	3522949	12
5	n-HEPTYLAMINE	111682	13	47	n-PENTYL ACETATE	628637	12
6	ETHYL ISOPROPYL KETONE	565695	13	48	1,2-DICHLOROBUTANE	616217	12
7	DI-n-BUTYLAMINE	111922	13	49	DIETHYL CARBONATE	105588	12
8	GLYOXAL	107222	13	50	sec-BUTYL MERCAPTAN	513531	12
9	1-ISOPROPOXY-2-PROPANOL	3944363	13	51	n-BUTYL ACETATE	123864	12
10	cis-2-HEPTENE	6443921	13	52	2,2-DIMETHYLBUTANE	75832	12
11	n-PENTYLAMINE	110587	13	53	5-METHYL-1-HEXENE	3524730	11
12	ISOBUTYL ISOBUTYRATE	97858	13	54	1-HEPTENE	592767	11
13	3,3,5-TRIMETHYLHEPTANE	7154805	13	55	CYCLOHEPTENE	628922	11
14	ETHYL METHACRYLATE	97632	13	56	2,2,3-TRIMETHYLPENTANE	564023	11
15	2-ETHYLHEXANAL	123057	13	57	trans-CROTONALDEHYDE	123739	11
16	1-DECYNE	764932	13	58	TETRAMETHYLETHYLENEDIAMINE	110189	11
17	4-METHYLOCTANE	2216344	13	59	METHYL ISOBUTYRATE	547637	11
18	cis-1,2-DIMETHYLCYCLOHEXANE	2207014	13	60	7-METHYL-1-OCTENE	13151069	11
19	cis-3-OCTENE	14850227	13	61	n-BUTYL MERCAPTAN	109795	11
20	2,2,5,5-TETRAMETHYLHEXANE	1071814	13	62	tert-BUTYL ACETATE	540885	11
21	CYCLOPENTENE	142290	12	63	4-METHYLHEPTANE	589537	11
22	2,3-DIMETHYL-1-HEXENE	16746864	12	64	METHYL n-PROPYL SULFIDE	3877154	11
23	1-NITROPROPANE	108032	12	65	DIETHYLAMINE	109897	11
24	ETHYLCHLOROACETATE	105395	12	66	1-PENTENE-3-YNE	646059	11
25	trans-1,2-DIMETHYLCYCLOHEXANE	6876239	12	67	INDANE	496117	11
26	n-BUTYL IODIDE	542698	12	68	ISOBUTYL ACETATE	110190	11
27	BENZOTRIFLUORIDE	98088	12	69	BROMOETHANE	74964	11
28	CYCLOHEPTANE	291645	12	70	DICYCLOPENTADIENE	77736	11
29	N-HEXANE	110543	12	71	2-PENTANONE	107879	11
30	1,3-DICHLORO-trans-2-BUTENE	10075384	12	72	2,3-DIHYDROFURAN	1191997	11
31	n-PENTYL FORMATE	638493	12	73	METHACRYLONITRILE	126987	11
32	1-HEXANAL	66251	12	74	3-METHYL-3-ETHYLPENTANE	1067089	11
33	DIISOPROPYL KETONE	565800	12	75	MONOCHLOROBENZENE	108907	11
34	1,1-DIBROMOETHANE	557915	12	76	n-PROPYL ACETATE	109604	11
35	2-METHYLHEXANE	591764	12	77	2,5-DIMETHYLOCTANE	15869893	11
36	trans-2-HEPTENE	14686136	12	78	5-ETHYLIDENE-2-NORBORNENE	16219753	11
37	p-XYLENE	106423	12	79	p-CHLOROTOLUENE	106434	11
38	4-METHYL-1-PENTENE	691372	12	80	METHYLCYCLOPENTADIENE	26519915	11
39	3,4-DICHLORO-1-BUTENE	760236	12	81	ISOPROPYL ISOBUTYL ETHER	78448336	11
40	5-METHYL-2-HEXANONE	110123	12	82	2-METHYL-1-NONENE	2980714	11
41	CUMENE	98828	12	83	3-METHYLCYCLOPENTENE	1120623	11
42	BUTYL VINYL ETHER	111342	12	84	METHYL n-BUTYL ETHER	628284	11

1-3-2. Ranking and Rating of Toxic Substances

The toxic substances were rated based on US EPA (138 species), UK COMMA (50 species), ERPG-2 values, and toxicological data. The scores were given in the order of inhalation, transdermal, and oral toxicities, as summarized in Table 9.

Different scores were assigned according to the toxicity and risk characteristic classifications, and the respective rating values are summarized in Tables 10 and 11.

In addition, acute toxicity classification criteria (limit values) for substances are as shown in Table 11 [E].

1-3-3. Rating of Common Characteristics

In addition, flammable and toxic substances have common leakage and diffusion characteristics, and for these characteristics, the number of diffusion potentials was applied on the same standard. The rating criteria shown in Tables 12 and 13 for vapor pressure were applied to gases.

Table 7. Ranks of the 16 selected flammable gases

Rank	CHEM_NAME	CAS_NO	Score	Rank	CHEM_NAME	CAS_NO	Score
1	HYDROGEN	1333740	12	9	cis-2-BUTENE	590181	8
2	DEUTERIUM	7782390	12	10	CYCLOBUTANE	287230	8
3	ETHYLACETYLENE	107006	10	11	HYDROGEN SULFIDE	7783064	8
4	DICHLOROSILANE	4109960	10	12	VINYL FLUORIDE	75025	8
5	VINYLACETYLENE	689974	10	13	PROPADIENE	463490	4
6	ETHYLENE	74851	10	14	N-BUTANE	106978	2
7	METHYL VINYL ETHER	107255	9	15	1-BUTENE	106989	2
8	3-METHYL-1-BUTENE	563451	8	16	NEOPENTANE	463821	2

Table 8. Ranks of the 10 selected explosive substances

Rank	CHEM_NAME	CAS_NO	Score	Rank	CHEM_NAME	CAS_NO	Score
1	DIBORANE	19287457	10	6	DIMETHYL CARBONATE	616386	8
2	ETHYL ISOPROPYL ETHER	625547	10	7	ISOPROPYL CHLORIDE	75296	7
3	METHYLACETYLENE	74997	9	8	ETHYLENE OXIDE	75218	7
4	ACETYLENE	74862	9	9	2-METHYL-1-BUTENE-3-YNE	78808	6
5	DIMETHYL SILANE	1111746	9	10	2,4-DIMETHYLOCTANE	4032944	6

Table 9. Toxic substance rating criteria

	Risk characteristic (1)	Risk characteristic (2)	Risk characteristic (3)	Leakage diffusion characteristic (1)	Leakage diffusion characteristic (2)
Score	0 to 8	0 to 3	0 to 3	1 to 4	1 to 3
Toxic category	Inhalation toxicity categories 1, 2, 3, and 4	Dermal toxicity classifications 1, 2, 3, and 4	Oral toxicity category 1, 2, 3, and 4	Diffusion potential index (Step 4)	Vapor pressure (25 °C) (Step 3)

Table 10. Inhalation toxicity sets the risk characteristic score by category

	Inhalation toxicity category 1	Inhalation toxicity category 2	Inhalation toxicity category 3	Inhalation toxicity category 4	Inhalation toxicity No classification
Risk characteristic score	8 to 13	4 to 9	2 to 7	1 to 3	0 to 2

Table 11. Acute toxicity classification criteria for substance (limit value)

	Acute toxicity value by route of exposure				
	Oral	Percutaneous	Inhalation (LC50, 4 hours)		
	(LD50, mg/kg)	(LD50, mg/kg)	Gas (ppm)	Vapor (mg/L)	Dust/Mist (mg/L)
1	5	5	100	0.5	0.05
2	50	200	500	2.0	0.5
3	300	1000	2500	10	1.0
4	2000	2000	20000	20	5

Table 12. Rating section and diffusion potential value

Score	1	2	3	4
Diffusion potential index	X≤8	8<X≤10	10<X≤12	X>12

- The diffusion potential index (X)

$$=(1.6*(M^{0.67}))*\left(\frac{1}{(273+T)*100}\right),$$

Table 13. Rating section and value for vapor pressure

Score	1	2	3
Vapor pressure (mm Hg)	X≤10	10<X≤125	X>125, gas (25 °C)

where M is molecular weight and T is boiling point (°C).

The risk index is calculated by summing up the risk character-

Table 14. Ranks of the 100 selected toxic substances

Rank	CHEM_NAME	CAS_NO	Score	Rank	CHEM_NAME	CAS_NO	Score
1	Dimefox	115264	13	51	Dimethyl phenol	1300716	8
2	1,4-Benzenediamine	106503	12	52	Phorate	298022	8
3	Toluidinium chloride	540238	12	53	2-Chloroethanol	107073	8
4	1,3-Phenylenediamine hydrochloride	541695	12	54	Hexachlorocyclohexanes	608731	8
5	Fluvalinate	69409945	12	55	Pirimicarb	23103982	8
6	4-Methyl-1,3-benzenediamine	95807	11	56	Tetramethyl lead	75741	8
7	Tetramethylammonium hydrogen phthalate	79723027	11	57	Disulfoton	298044	8
8	1,3-Bis[(acrylamidomethoxy) methyl]urea	30417379	11	58	Dimethyl sulfate	77781	7
9	Phenylhydrazine	100630	11	59	1-Chloro-2-nitropropane	2425663	7
10	4-Bromo-2-(4-chlorophenyl)-5-(trifluoromethyl)-1H-pyrrole-3-carbonitrile	122454299	11	60	Thiofanox	39196184	7
11	Tebupirimfos	96182535	11	61	Difenacoum	56073075	7
12	Lead alkyls	NA	11	62	Metaldehyde	108623	6
13	Nickel dinitriate	13138459	10	63	2-Chloropyridine	109091	6
14	Difenoconazole	119446683	10	64	Di-n-butylamine	111922	6
15	1,3-Benzenediamine	108452	10	65	Disodium hexafluorosilicate	16893859	6
16	Trichloroacetonitrile	545062	10	66	Malathion	121755	6
17	Tetramethylammonium chloride; N,N,N-Trimethyl methanaminium chloride	75570	10	67	4-Bromo-2-(4-chlorophenyl)-1-(ethoxymethyl)-5-(trifluoromethyl)pyrrole-3-carbonitrile	122453730	6
18	Methomyl	16752775	10	68	Inorganic antimony compounds	NA	6
19	2-Vinylpyridine	100696	10	69	Inorganic tin, salts	NA	6
20	Trialkyltin hydroxide, salts	NA	10	70	p-Aminoazobenzene	60093	6
21	Dicrotophos	141662	10	71	Malononitrile	109773	6
22	Osmium tetroxide	20816120	10	72	Chlorphonium chloride	115786	6
23	Chlorthiophos	21923239	10	73	2,6-Dimethylphenol	576261	6
24	Methiocarb	2032657	10	74	MNFA	5903139	6
25	Aphidan	5827054	10	75	Butocarboxim	34681102	6
26	Coumatetralyl	5836293	10	76	Indoxacarb	173584446	6
27	Endrin	72208	10	77	Chlormephos	24934916	6
28	Epichlorohydrin	106898	9	78	Strychnine	57249	6
29	o-Toluidine	95534	9	79	Sodium fluoroacetate	62748	6
30	2-Furanmethanol	98000	9	80	Pentachlorophenol	87865	6
31	Furfural	98011	9	81	Coumafuryl	117522	6
32	3,5-Dimethylphenol	108689	9	82	Thionazin	297972	6
33	Zeta cypermethrin	52315078	9	83	Maleimide	541593	6
34	Nickel carbonyl	13463393	9	84	Dimetilan	644644	6
35	Diafenthiuron	80060099	9	85	Triamiphos	1031476	6
36	Inorganic silver,salts	NA	9	86	Dinoterb	1420071	6
37	Toluenediamine, salts	NA	9	87	Mecarbam	2595542	6
38	Diamidafos	1754581	9	88	Promecarb	2631370	6
39	Ammonium hexafluorosilicate	16919190	9	89	Chlorophacinone	3691358	6
40	1,1-(p-Tolylimino) dipropan-2-ol	38668483	9	90	3,3,4,4-Tetrachlorotetra-hydrothiophene 1,1- dioxide	3737415	6
41	Cyfluthrin	68359375	9	91	Phosphamidon	13171216	6

Table 14. Continued

Rank	CHEM_NAME	CAS_NO	Score	Rank	CHEM_NAME	CAS_NO	Score
42	O,O-Diethyl O-1-phenyl-3-trifluoromethylpyrazol-5-ylphosphorothioate	122431247	9	92	Demeton-S-methylsulfone	17040196	6
43	4,4′-Methylenebis (2-chloroaniline)	101144	8	93	Isobutylamine	78819	6
44	3,3′-Dimethoxy-[1,1′-biphenyl]-4,4′-diamine	119904	8	94	Edifenphos	17109498	6
45	Triphenylphosphine	603350	8	95	Pindone	83261	6
46	Trichloroethylene	79016	8	96	Methyl isothiocyanate	556616	6
47	Cadmium oxide	1306190	8	97	Triphenyltin compounds	NA	6
48	Chlorobenzilate	510156	8	98	Ebivit	67970	6
49	N,N′-Bis(3-aminopropyl)-1,2-ethanediamine	10563265	8	99	Parathion	56382	6
50	Reaction products of phosphoryl trichloride, o-phenylphenol and phenol	NA	8	100	Fensulfothion	115902	6

istics (total of 20 points; Section 3) and the leakage/diffusion characteristics (Section 2), as summarized in Table 14.

APPLICATION OF HAZARDOUS MATERIAL INFORMATION

A web-based emergency response plan system that provides safety management systems to each facility was developed in 2011 [24], so the program needs to be updated. The information from 100 toxic materials, selected by the developed algorithm in this study, was added to the existing web-based CARM development system. The management system provides management and analyzation capabilities and makes the emergency plan convenient. In this section, the management system is described in detail.

1. User Registration and Login Module

To develop CARM, user registration and login information are needed. Basic company information, such as name, registration number, address, representative, contact information, and password, is required for registration. The login and registration screens are shown in Fig. 2.

2. Hazardous Material Safety Information Module

This module provides important safety information for each material. The material safety database sheet (MSDS) information provided by the Korea Occupational Safety and Health Agency was used to develop this module.

Fig. 3 shows the material search and safety information screens.

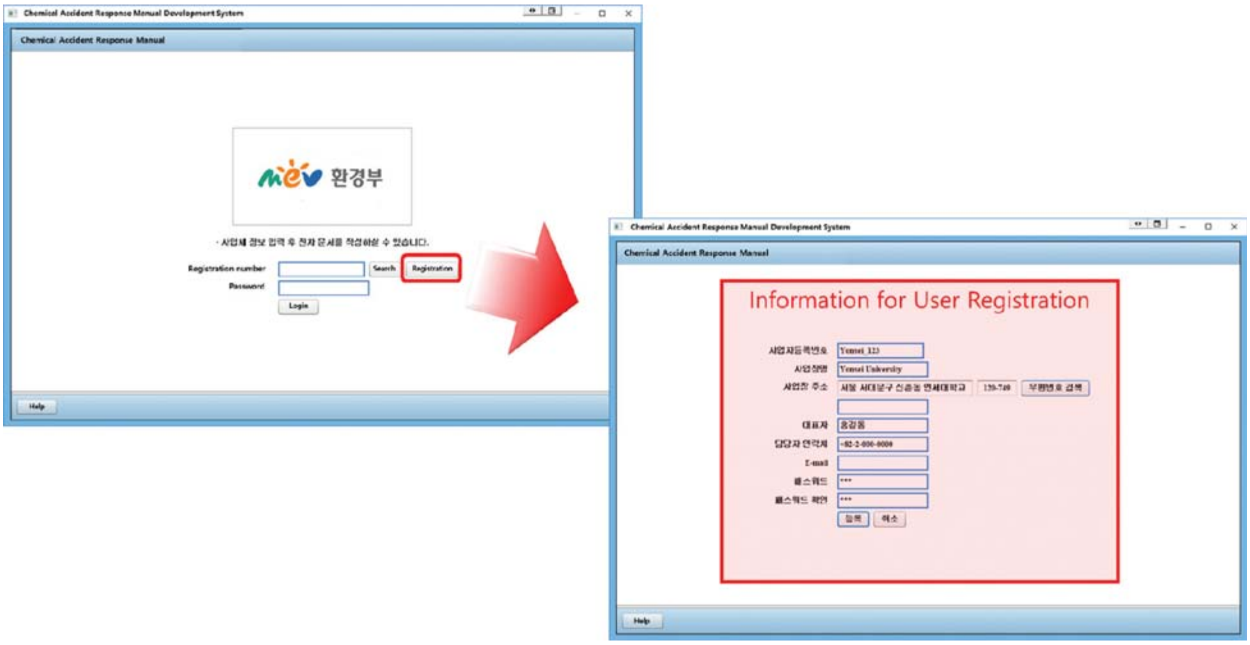

Fig. 2. CARM user registration and login screen.

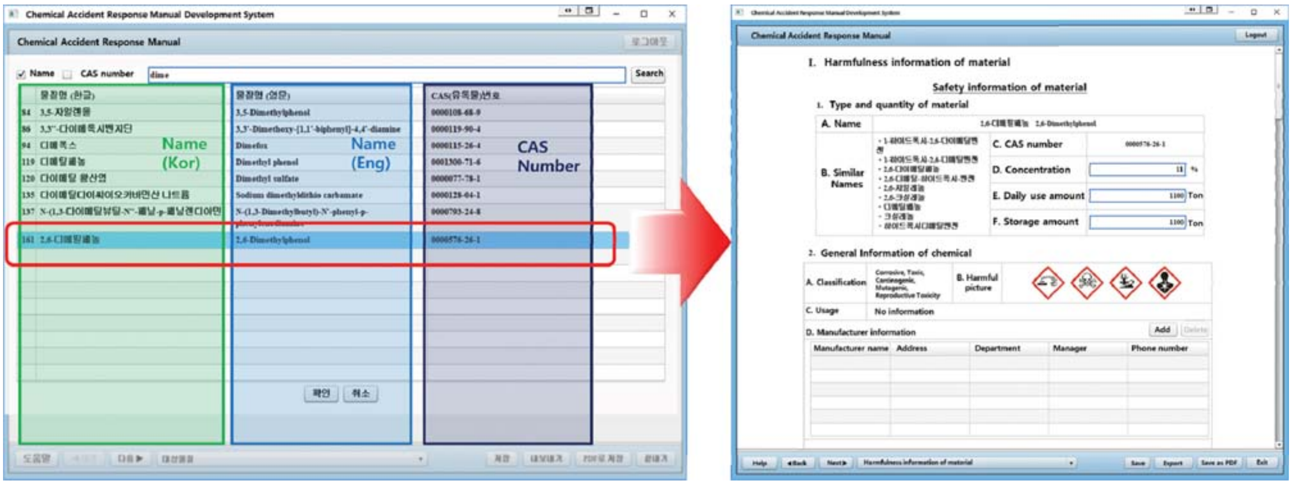

Fig. 3. Material search and safety information screen.

Fig. 4. Facility floor plan and equipment status screen.

When a user selects a target material, its MSDS information is automatically generated on the system start-up screen. The user can also input material information, such as the concentration, daily amount used, and average storage amount.

3. Status of the Chemical Accident Control Facilities and Equipment Module

This module describes the status of the chemical accident control facilities and equipment. Fig. 4 shows an example of a control facility diagram. Users can easily draft a floor plan of their plant using the line, square, triangle, and circle icons.

The CARM development system also supports the direct insertion of a plant floor plan in image formats. After doing so, users can input the status and location of each piece of equipment by dragging and dropping. The system supports a variety of safety equipment icons, including for wastewater treatment, fire suppression, and human body and respiratory protection.

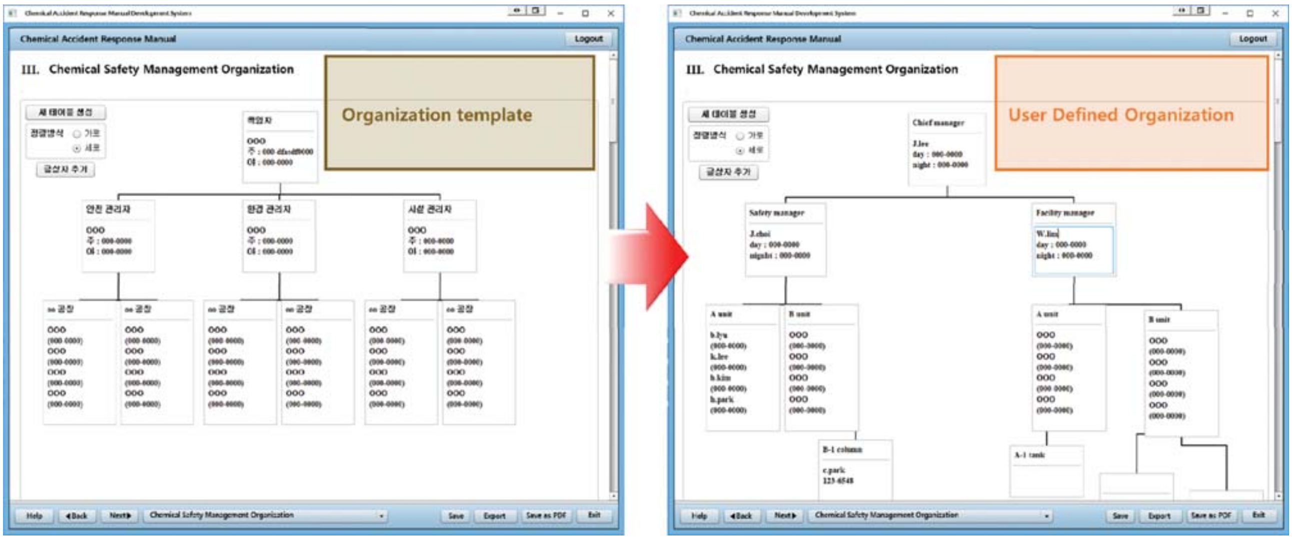

Fig. 5. Organization of the safety management screen.

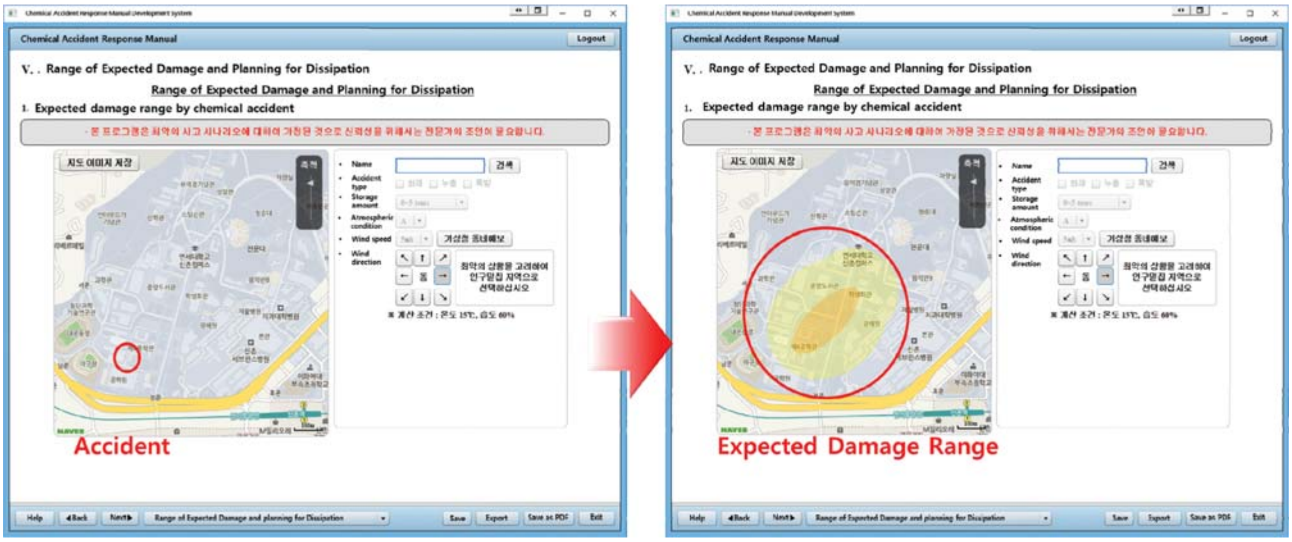

Fig. 6. Expected damage range screen.

4. Safety Management Organization and Emergency Response System Module

The safety management organization chart is created in this module.

Fig. 5 shows the template of the organization module. The user can input the name and contact information of the safety, environmental, and facility managers. The software supports organization chart templates as well as the division of works when an emergency occurs. Additionally, emergency measures for an accident situation are drafted. A basic emergency measure template is provided for users, who can subsequently modify it according to their environment and needs. The module also supports emergency contacts with relevant agencies, such as the ward office and fire department.

5. Range of Expected Damage and Planning for Dissipation

This module supports expected damage ranges and considers various conditions to establish a resident evacuation plan. For user convenience, the CARM development system sets the default value of input parameters to facilitate use of the risk assessment system. The risk assessment program may perform less reliably if the input parameters are over-simplified. Therefore, to increase the reliability, US Environmental Protection Agency (EPA)'s ALOHA simulation results are loaded into the expected damage range module. Fig. 6 shows the parameter input screen. Here the user can input the chemical name, type of accident, storage amount, atmospheric conditions, and wind information. Following input, the system outputs the expected damage range, shown in Fig. 6.

CONCLUSION

As the chemical industry has changed dramatically, it has become necessary to select additional substances for systematic management. In Korea, there has been a policy revision in the chemical management guidelines in the wake of the recent hydrogen-fluoride leak accident in Gu-mi. Certain criteria and screening steps are essential for selecting the most important substances out of the many different chemicals used. In this study, criteria were established for substance selection, and a three step procedure was proposed. A total of 210 kinds of flammable materials, 10 explosive substances, and 100 toxic substances were selected from 4,994 target substances in two screening stages. Priorities of the classified substances were determined by applying a rating method. At each step, substance selection criteria are needed. Therefore, appropriate criteria were prepared and applied according to a given material's characteristics. For toxic substances, the information of the selected 100 toxic substances was added to the existing web-based CARM system. This system includes modules for hazardous material information, accident management facility and installation, emergency response, accident scope, and dissipation planning. Managers will become more comfortable owing to the ease in managing the greater number of materials. Thus, the developed hazardous substance information system will improve chemical safety management in the workplace. Moreover, it is expected that this system will contribute to safer work environments in terms of chemical substance management.

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