

# **Development of Chemical Reactivity Matrix Databases for Industrial Applications**

By

Muhammad Syuwari bin Mohd Hussain (8891)

Dissertation submitted in partial fulfillment of  
The requirements for the  
Bachelor of Engineering (Hons)  
(Chemical Engineering)

JULY 2010

Supervisor's Name: Dr. Mohanad El-Harbawi

Universiti Teknologi PETRONAS  
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# **CERTIFICATION OF APPROVAL**

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## **CERTIFICATION OF ORIGINALITY**

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken by unspecified sources or persons.

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MUHAMMAD SYUWARI BIN MOHD HUSSAIN

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## ABSTRACT

The major hazard with which the chemical industry is concerned is misidentifying chemical reactivity and hazards. The impacts of misidentifying chemical hazards in the process industries may be predicted by the application of chemical reactivity matrix. However, the applications of these models require competency in computer programming. Therefore, the objective of this project is to develop an application which is able to study the chemical reactivity and hazards. The application is developed using JAVA programming language and MySQL database. The application is helpful to know the chemical descriptions, chemical hazards, safety issues of chemicals and predict the new hazards when these chemicals are mixed with each others.

The methodology of the project includes; search relevant information and chemical data that are related to the project. The development of the software has been divided into five stages, which are: planning the application, building the database, building the Graphical User Interface (GUI), writing the computer program, software validation and verification.

This application required chemical name, Chemical Abstracts Service (CAS) number or United Nation/North American (UN/NA) number as inputs for and the outputs of the software can be displayed as results. The users able to know regarding to the description of the chemical which are chemical properties. Furthermore, the users can mix the chemicals as an input then predict the hazards of the mixing chemical as an output. The software is able to present the hazard of mixing two chemicals.

The chemical reactivity matrix application is useful and feasible due to its user friendlies and ability to function as a stand alone application and it is compatible with all windows operating system. Furthermore, the cost of developing the software is cheap and the application can be updated by user. The software has been tested with few case studies and the results shows a good agreement with the other results from different softwares.

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# CHAPTER 1

## INTRODUCTION

### 1.1 Background of Study

One of the most important parts in chemical process plant is safety of the plant. All operations and processes must be carried out under safe condition in order to protect the human health and environment. Misidentifying chemical hazards are among the commonly occurring major accidents in chemical process plants. Consequences of not identifying chemicals correctly are obvious and include fires, explosions, and injury to workers.

The use of computers for rapidly and easily identifying chemical hazards has been done tremendously lately. There are a lot of software has been developed and available in identifying chemical hazards. Usually, we use Material Safety Data Sheet (MSDS) to identify the chemical hazards but sometimes MSDS can be too hard for identifying chemical hazards. Furthermore, some MSDS are sometimes not available for free. Thus, many people, company and organization have developed software to overcome these issues. Therefore, Chemical Reactivity Matrix database can be used to predict the chemicals hazards easily.

Basically, Chemical Reactivity Matrix database obtained the chemicals data from MSDS. They consist of physical and chemical properties. The properties such as physical state, molecular weight, boiling point, freezing point, specific gravity, latent heat of vaporization and others. In the MSDS also provided the hazards of each chemicals and possible chemical that will come out after react with each other. It also provided the first aid measures, fire and explosion data, accidental release measures, handling and storage, exposure control, personal protection, stability and reactive data, toxicological information, ecological information, disposal considerations, transport information and other regulatory information. All of these data are hard to be found

manually by using the MSDS because there are more than 5,000,000 of chemicals exist. By using Chemical Reactivity Matrix Database, the identification of chemicals hazard can be more easily to identify.

Since the evolution of computer software, it has become a useful tool in investigating the consequences of chemical hazards. Some of the software provides powerful tools for identifying chemical reactivity matrix. Hence, with the necessary databases and expert systems, within a common and interactive graphical user interface would provide a more powerful and user-friendly risk information systems.

## **1.2 Problem Statement**

Hazard identification in the area of chemical safety is so burdensome and because people with a wide variety of training are called upon to perform this work, tools is required to aid in chemical hazard identification. Many tools have been developed. Unfortunately, many of these tools are not seen as the limited resource that they are and are used inappropriately.

The most common of these tools is the Material Safety Data Sheet (MSDS). MSDS are valuable tools to use in the hazard identification process, but these MSDS have their limitations. Other sources that people use to determine chemical reactivity are reference materials such as books and Websites. These reference materials tend to provide more in-depth information, but have drawbacks of their own. Websites can be difficult to find, navigate within, and typically contain only MSDS-type information. Books can be expensive and not always available. Furthermore, these references don't always agree with each other and vary in the amount of information provided.

Numerous chemical reactivity worksheets have been developed in an effort to overcome the above listed shortcomings of various data resources and to simplify

chemical reactivity hazard identification. Chemical reactivity worksheets provide good information, they are, many times, misused or misapplied. It is important to understand the intent of these worksheets, their limitations, and how they can be properly used if they are to be incorporated into a chemical hazard identification process.

However, these spreadsheets pose too many restrictions upon the act of chemical hazard identification so attempts have been made to produce very large matrices that address specific chemical interactions with other specific chemicals. Because these chemical specific matrices can become quite large, they are usually built around a parsing function that allows one to call up chemicals of specific interest.

### **1.3 Objectives of Study**

The main objectives of this study are:

- i) To develop a stand-alone user-friendly Chemical Reactivity Matrix using JAVA Eclipse application to predict the chemical's basic hazards (such as flammability, explosiveness, or polymerizability).
- ii) To study the potential hazardous of chemical materials using the developed application.
- iii) To determine the compatibility hazards (such as heat generation, gas generation, or water-soluble toxic product formation) that might occur while mixing any two materials together.
- iv) To verify and validate the results with other established softwares.

## **1.4 Scope of Study**

This study is mainly to develop a software call using JAVA programming language. The software is able to identify the hazard of the chemicals. The data of the chemicals were used in this project are obtained from the MSDS (Material Safety Data Sheet). The software is developed by using the linking technique in the JAVA Eclipse application.

The database of the chemical properties has been built using MySQL which include the physical and chemical properties, hazard identification, first aid measures, fire and explosion data, accidental release measures, handling and storage, exposure control, personal protection, stability and reactive data, toxicological information, ecological information, disposal considerations, transport information and other regulatory information. It is also to identify the reactivity when the chemicals react with each other.

## **CHAPTER 2**

### **LITERATURE REVIEW**

#### **2.1 Introduction**

Numerous chemical substances are distributed in normal commerce and many new ones are introduced every year. Some of these substances have the potential to cause environmental problems, affect health adversely, or to cause fires or explosions. These chemicals are regulated as hazardous materials and are handled with appropriate care to minimize accident (Yaws, 1999).

Chemical substances are materials which can be produced or used in chemical processes. Chemical processes include such reactions as combustion. Since the rise of the modern chemical industry in the nineteenth century, numerous chemical substances have been developed and created include acids, bases, fertilizers, ceramics, catalysts, dyestuffs, fabrics, explosives, paints, plastics, petrochemicals, pharmaceuticals, agricultural chemicals, specialty chemicals, automotive materials, and home and commercial electronics components (Yoshida et al., 1994).

Chemical substances which may cause adverse effects to human health, endanger people's lives or damage the environment are called hazardous materials. In Japan, hazardous chemicals are distinguished by two general legal definitions; namely, hazardous chemicals in a narrow sense and hazardous materials in a broad sense. Hazardous chemicals in a narrow sense are those substances having ignitability and flammability as specified in the Japanese Fire Services Law; these materials are listed in the Exhibit of the Law (Cheremisinoff, 1999).

The category "hazardous materials" includes a group of chemical substances called "reactive chemicals". A reactive chemical initiates a group of chemical substances called "reactive chemicals". A reactive chemical initiates reaction by itself or with other

substances. These reactions are often exothermic (heat releasing) or produce flammable gases or explosive materials, which may in turn trigger accidents (Davletshina et al., 1998).

## **2.2 Physical and Chemical Properties**

Physical and thermodynamic property data for organic and inorganic chemicals are of special value to engineers in the chemical processing and petroleum refining industries. The engineering design of process equipment often requires knowledge of such properties as heat capacity, enthalpy, density, viscosity, thermal conductivity and others. Usually, misidentification of these properties can produce a huge accident in chemical plant. That is why all of these properties are important even it is a small value can make a huge impact to the plant (Crowl et al., 2002).

The properties such as physical state basically is measures at 15°C and 1 atm and is defined as the statement indicates whether the chemical is a solid, liquid, or gas after it has reached equilibrium with its surroundings at “ordinary” conditions of temperature and pressure (Mcleod, 2009).

Molecular weight is defined as the value is the weight of a molecule of the chemical relative to a value of 12 for one atom of carbon. The molecular weight is useful in converting from molecular units to weight units, and in calculating pressures, volumes and temperatures relationships for gaseous materials. The ratio of the densities of any two gases is approximately equal to the ratio of their molecular weights. The molecular weights of mixtures can be calculated if both the identify and quantity of each component of the mixture are known (Yoshida et al., 1994).

The other properties of chemicals are boiling point and freezing point. Boiling point at 1 atm is defined as the value is the temperature of a liquid when its vapour

pressure is 1 atm. For example, when water is heated to 100°C, its vapor pressure rises to 1 atm and the liquid boils. The boiling point at 1 atm indicates whether a liquid will boil and become a gas at any particular temperature and sea-level atmospheric pressure. Freezing point is the temperature at which a liquid changes to a solid. For example, liquid water changes to a solid ice at 0°C. Some liquids solidify very slowly even when cooled below their freezing point. When liquids are not pure (for example, salt water) their freezing points are lowered slightly (Tweeddale, 2003).

The specific gravity of a chemical is the ratio of the weight of the solid or liquid to the weight of an equal volume of water at 4°C (or at some other specified temperature). If the specific gravity is less than 1.0 (or less than 1.03 in seawater) the chemical will float; if higher, it will sink. For vapour phase, the value is the ratio of the weight of vapour to the weight of an equal volume of dry air at the same conditions of temperature and pressure. Buoyant vapours have a vapour specific gravity less than one. The value may be approximated by the ratio  $M/29$ , where  $M$  is the molecular weight of the chemical. In some cases the vapour may be at a temperature different from that of the surrounding air. For example, the vapour from a container of boiling methane at -113.33°C sinks in warm air, even though the vapour specific gravity of methane at 15.55°F is about 0.6 (Knight et al., 2003).

Latent heat of vaporization is also the properties that need to be considered. The latent heat of vaporization is defined as the value is the heat that must be added to the specific weight of a liquid before it can change to vapour (gas). It varies with temperature; the value given is that at the boiling point at 1 atm. The units used are Btu per pound, calories per gram, and joules per kilogram. No value is given for chemicals with very high boiling points at 1 atm, because such substances are considered essentially non-volatile (Reynolds et al., 2002).

Heat of combustion is also taken as consideration for chemical properties. Heat of combustion is defined as the value is the amount of heat liberated when the specified

weight is burned in oxygen at 25°C. The products of combustion, including water, are assumed to remain as gases; the value given is usually referred to as the ‘lower heat value’. A negative sign before the value indicates that heat is given off when the chemical burns. The units typically used are Btu per pound, calories per gram, and joules per kilogram (Blackman, 2001).

Heat of decomposition is the amount of heat liberated when the specific weight decomposes to more stable substances. Most chemicals are stable and do not decompose under the conditions of temperature and pressure encountered during shipment. A negative sign before the value simply indicates that heat is given off during the decomposition. The value does not include heat given off when the chemical burns. The units typically used are Btu per pound, calories per gram, and joules per kilogram (Cheremisinoff, 1999).

Heat of solution is the value represents the heat liberated when the specified weight of chemical is dissolved in a relatively large amount of water at 25°C (“infinite dilution”). A negative sign before the value indicates that heat is given off, causing a rise in temperature. A few chemicals absorb heat when they dissolve, causing the temperature to fall. The units used are Btu per pound, calories per gram, and joules per kilogram. In those few cases where the chemical reacts with water and the reaction products dissolve, the heat given off during the reaction is included in the heat of solution (Fingas, 2001).

Heat of polymerization is the value that the heat liberated when the specified weight of the compound (usually called the monomer) polymerizes to form the polymer. In some cases the heat liberated is so great that the temperature rises significantly, and the material may burst its container or catch fire. The negative sign before the value indicates that the heat is given off during the polymerization reaction. The units used are Btu per pound, calories per gram, and joules per kilogram (Florczak et al., 2001).



Liquid heat capacity is the heat (in Btu) required raising the temperature of one pound of the liquid one degree Fahrenheit at constant pressure. For example, it requires almost 1 Btu to raise the temperature of 1 pound of water from 20°C to 20.5°C. The value is useful in calculating the increase in temperature of a liquid when it is heated, as in a fire. The value increases slightly with an increase in temperature (Davletshina et al., 1998).

Liquid viscosity is the value (in centipoises) that is a measure of the ability of a liquid to flow through a pipe or a hole; higher values indicate that the liquid flows less readily under a fixed pressure head. For example, heavy oils have higher viscosities (i.e. are more viscous) than gasoline. Liquid viscosities decrease rapidly with an increase in temperature. A basic law of fluid mechanics states that the force per unit area needed to shear a fluid is proportional to the velocity gradient. The constant of proportionality is the viscosity (Houghton, 2008).

The properties of solubility in water are also taken in the consideration because water is the universal solution. The value represents the pounds of a chemical that will dissolve in 100 pounds of pure water. Solubility usually increases when the temperature increases. The following terms are used when numerical data are either unavailable or not applicable: The term “Miscible” means that the chemical mixes with water in all proportions. The term “Reacts” means that the substance reacts chemically with water; thus, its solubility has no real meaning. “Insoluble” usually means that one pound of the chemical does not dissolve entirely in 100 pounds of water. However, weak solutions of “Insoluble” materials may still be hazardous to humans, fishes, and waterfowl (Yoshida et al., 1995).

## 2.3 Chemical Reactivity

There are a lot of reaction exists between chemicals but the reactivity also can be classified into some classes which are reactivity with water, reactivity with common materials, stability during transport, neutralizing agents for acids and caustics, polymerization and inhibitor of polymerization.

For the reactivity with water, the term “No Reaction” means that no hazard results when the chemical reacts or mixes with water. When there are hazard does result, it is described for specific chemicals .The reactivity with common materials is limited to hazardous reactions with the fuels and with common materials of construction such as metal, wood, plastics, cement, and glass. The nature of the hazard, such as severe corrosion or formation of a flammable gas, is described for specific chemicals (Cheremisinoff, 1999).

For the stability during transport, the term “stable” means that the chemical will not decompose in a hazardous manner under the conditions of temperature, pressure, and mechanical shock that are normally encountered during shipment; the term does not apply to fire situation. For neutralizing agents for acids and caustics, in all cases involving accidental discharge, dilution with water may be followed by use of the agent specified, particularly if the material cannot be flushed away; the agent specified need not necessarily be used (Houghton, 2008).

There are also a few chemicals can undergo rapid polymerization to form stickly, resinous materials, with the liberation of much heat. Under these conditions the chemical’s containers may explode due to internal pressure build up. The chemical names and concentrations of inhibitors added by the manufacturer to prevent polymerization are given where appropriate (Patnaik, 2007).

## **2.4 Hazards**

### **2.4.1 Health Hazards**

Personal Protective Equipment is the items that recommended by manufacturers, either in technical bulletins or in Material Safety Data Sheets, the Manufacturing Chemists Association, or the National Safety Council, for use by personnel while responding to fire or accidental discharge of the chemical. They are intended to protect the lungs, eyes and skin (Kutz, 2009).

For the toxicity by inhalation, the threshold limit value (TLV) is usually expressed in units of parts per million (ppm). For example, the parts of vapor (gas) per million parts of contaminated air by volume at 25°C and atmospheric pressure. For a chemical that forms a fine mist or dust, the concentration is given in milligrams per cubic meter (mg/m<sup>3</sup>). The TLV is defined as the concentration of the substance in air that can be breathed for five consecutive eight hour workdays (40-hour work week) by most people without adverse effect (ACGIH, 1972). As some people become ill after exposure to concentrations lower than the TLV, this value cannot be used to define exactly what is a "safe" or "dangerous" concentration (Davletshina et al., 1998).

In the Short-Term Inhalation Limits, the parts of vapor (gas per million parts of contaminated air by volume at 25°C and atmospheric pressure is given. The limits are normally given in milligrams per cubic meter for chemicals that can form a fine mist or dust. The values given are the maximum permissible average exposures for the time periods specified. The term Short Term Exposure Limit (STEL) is also used and is considered interchangeable with Short - Term Inhalation Limit. The STEL designation is derived from OSH standards. In some instances the values disagree, or the short-term limits overlap the TLV. These are not errors; the values were supplied by several laboratories, each of which used its own experimental techniques and methods of calculation (Santoleri, 2000).

For toxicity by ingestion, the term LD<sub>50</sub> (meaning "lethal dose at the 50th percentile population") signifies that about 50% of the animals given the specified dose by mouth will die. Thus, for a chemical whose LD<sub>50</sub> is below 50 mg/kg, the toxic dose for 50% of animals weighing 70 kg (150 lb) is  $70 \times 50 = 3500$  mg = 3.5 g, or less than one teaspoonful; it might be as little as a few drops. For a chemical with an LD<sub>50</sub> of between 5 to 15g/kg, the LD<sub>50</sub> would be between a pint and a quart for a 150 lb man. All LD<sub>50</sub> values have been obtained using small laboratory animals such as rodents, cats, and dogs. The substantial risks taken in using these values for estimating human toxicity are the same as those taken when new drugs are administered to humans for the first time (Yoshida et al., 1994).

For the late toxicity, where there is evidence that the chemical can cause cancer, mutagenic effects, teratogenic effects, or a delayed injury to vital organs such as the liver or kidney, a qualitative description of the effect is often given on a material safety data sheet. The term can be interpreted as implying long term or chronic effects due to exposure to the chemical. In this respect, a distinction must be made between acute and chronic effects. An acute effect is one in which there is a short term or immediate response, usually due to exposure of the chemical at a high concentration. A chronic effect implies a long term exposure to small doses, with symptoms sometimes taking years to materialize (Maczulak, 2009).

For vapor (gas) irritant characteristics since MSDS often provide non-qualifying statements, the most appropriate of five statements listed below is given (NASCHM, 1970).

- i) Vapors are non-irritating to eyes and throat.
- ii) Vapors cause a slight smarting of the eyes or respiratory system if present in high concentrations. The effect is temporary.
- iii) Vapors cause moderate irritation such that personnel will find high concentrations unpleasant. The effect is temporary.

- iv) Vapors are moderately irritating such that personnel will not usually tolerate moderate or high concentrations.
- v) Vapors cause severe irritation of eyes and throat and can cause eye and lung injury. They cannot be tolerated even at low concentrations.

#### **2.4.2 Fire Hazards**

Flash Point is defined as the lowest temperature at which vapors above a volatile combustible substance will ignite in air when exposed to a flame. Depending on the test method used, the values given are either Tag Closed Cup (C.C.) (ASTM D56) or Cleveland Open Cup (O.C.) (ASTM 093). The values, along with those given below, provide an indication of the relative flammability of the chemical. In general, the open cup value is about -12.2°C to -9.4°C higher than the closed cup value (Yoshida et al., 1994).

For the Flammable Limits in Air the percent concentration in air (by volume) is given for the lower (LFL) and upper (UFL) limit. The values, along with those for flash point and ignition temperature, give an indication of the relative flammability of the chemical. The limits are sometimes referred to as "lower explosive limit" (LEL) and "upper explosive limit" (UEL) (Crowl et al., 2002).

Flammability Range defined as the difference between the UFL and LFL. This difference provides an indication of how wide the flammability limits of a chemical are. Generally, the wider the range, the more hazardous the chemical may be considered from a fire standpoint (Blackman, 2001).

For special hazards of combustion products some chemicals decompose or burn to give off toxic and irritating gases. Such gases may also be given off by chemicals that vaporize in the heat of a fire without either decomposing or burning. If no entry appears

with a chemical, the combustion products are thought to be similar to those formed by the burning of oil, gasoline, or alcohol; they include carbon monoxide (poisonous), carbon dioxide, and water vapor. The specific combustion products are usually not well known over the wide variety of conditions existing in fires; some may be hazardous (Florczak, 2001).

Ignition Temperature is the minimum temperature at which the material will ignite without a spark or flame being present. Along with the values of flash point and flammable limits in air, it gives an indication of the relative flammability of the chemical. It is sometimes called the "auto ignition temperature" (Gallant, 2006).

## 2.5 Response to Discharge

In every case of a discharge or leak, it is obvious that an effort should be made to reduce, stop, or contain the flow of material at its source if this can be done safely. The purpose of the terms used in this section is to describe in a general way the cautionary and corrective responses that are well recognized by trained emergency response personnel (Davletshina et al., 1998).

- i) **Issue warning** is used when the chemical is a poison, has a high flammability, is a water contaminant, is an air contaminant (so as to be hazardous to life), is an oxidizing material, or is corrosive. This type of response warning is most often applied for cautionary purposes to restrict ignition, and to restrict contaminated water for human use, farm use, and industrial use.
- ii) **Restrict access** is used only for those chemicals that are unusually and immediately hazardous to personnel unless they are protected properly by respirators, eye goggles, protective clothing, etc. This type of cautionary response is sometimes used

in a broader sense to ensure exclusion of spectators and others who might ignite flammable compounds.

- iii) **Evacuate area** is used primarily for unusually poisonous chemicals or those that ignite easily. The same expression can be used for a cautionary response.
- iv) **Mechanical containment** is used for water-insoluble chemicals that float and do not evaporate readily. The corresponding corrective response is "Contain".
- v) **Should be removed** is used for chemicals that cannot be allowed to disperse because of their harmful effect on humans or on the ecological system in general. The term is not used unless there is a reasonable chance of preventing dispersal, after a discharge or leak, by chemical and physical treatment.
- vi) **Chemical and physical treatment** is recommended for chemicals that can be removed by skimming, pumping, dredging, burning, neutralization, absorption, coagulation, or precipitation. The corrective response may also include the use of dispersing agents, sinking agents, and biological treatment.
- vii) **Disperse and flush** is used for chemicals that can be made non-hazardous to humans by simple dilution with water. In a few cases the response is indicated even when the compound reacts with water because, when proper care is taken, dilution is still the most effective way of removing the primary hazard.

## 2.6 Hazard Classification

Table 2.1 shows the hazard classification for most chemical. This classification basically is the common classification that we use today in most of the places that contain several chemicals. The hazard class specified in the Code of Federal Regulations which is chemicals not specifically listed within have been classified as “Flammable” if their flash point (closed cup) is below 37.78°C (Crowl et al., 2002).

There are also classes and divisions in hazard. According to UN Hazard Classes and Divisions, the hazard class of a material is indicated either by its class (or division) number, or its class name. For a placard corresponding to the primary hazard class of a material, the hazard class or division number must be displayed in the lower corner of the placard (Fingas, 2001).

## 2.7 Summary of Other Reactivity Software

There are some of the companies and organizations have developed the similar function software for the Chemical Reactivity Matrix. There is some software that has been used by the people to overcome the problem when it comes to the Chemical Process Safety. The examples of the software are Chemical Reactivity Worksheet (CRW2) and Chemistry Database (ChemDB).

Basically, CRW2 is use to find out a chemical's intrinsic hazards (such as flammability, explosiveness, or polymerizability) by looking at the chemical datasheets. The CRW database contains hazard information for over 5,000 common materials. The user can add chemicals to the Reactivity Worksheet to determine the compatibility hazards (such as heat generation, gas generation, or water-soluble toxic product formation) that might occur while mixing any two materials together (CRW2 User Guide). This software has been developed by U.S Environmental Protection Agency and



Emergency Response Division of National Oceanic and Atmospheric Administration with collaboration of Center for Chemical Process Safety. The software can be downloaded from the following websites: <http://software.informer.com/>

Chemistry Database (ChemDB) provides the useful information such as material information, safety information of the chemical, reactivity of the chemical, emergency response and others. This software has been quite useful tool as it has been use by most of the people to predict the chemical hazards. This software has been developed by the ATSOFT organization. The software can be downloaded from the following website: <http://www.softpedia.com/>

Table 2.1: Hazard Classification of the materials (Cheremisinoff, 1999).

Classification	Definition				
	Health Hazard (Blue)	Flammability (Red)	Reactivity (Yellow)	Other (White)	
4	Materials which on very short exposure could cause death or major residual injury even though prompt medical treatments were given.	Materials which will rapidly or completely vaporize at atmospheric pressure and normal ambient temperature, or which are readily dispersed in air and which will burn readily.	Materials which in themselves are readily capable of detonation or of explosive decomposition or reaction at normal temperatures and pressures.	ALK	Alkaline
3	Materials which on short exposure could cause serious temporary or residual injury even though prompt medical treatments were given.	Liquids and solids that can be ignited under almost all ambient temperature conditions.	Materials which in themselves are capable of detonation or explosive reaction but require a strong initiating source or which must be heated under confinement before initiation or which react explosively with water.	ACID	Acidic
2	Materials which on intense or continued exposure could cause temporary	Materials that must be moderately heated or exposed to relatively high ambient	Materials which in themselves are normally unstable and readily undergo violent	COR	Corrosive

	incapacitation or possible residual injury unless prompt medical treatment is given.	temperatures before ignition can occur.	chemical change but do not detonate. Also materials which may react violently with water or which may form potentially explosive mixtures with water.		
1	Materials which on exposure would cause irritation but only minor residual injury even if no treatment is given.	Materials that must be preheated before ignition can occur.	Materials which in themselves are normally stable, but which can become unstable at elevated temperatures and pressures or which may react with water with some release of energy but not violently.	OX	Oxidizing
0	Materials which on exposure under fire conditions would offer no hazard beyond that of ordinary combustible material.	Materials that will not burn	Materials which in themselves are normally stable, even under fire exposure conditions, and which are not reactive with water.	<del>W</del>	Material that react violently. Similar to Reactivity Classification

Table 2.1 shows hazard classification for the chemicals. Basically, this information is useful when it comes to the work in laboratory and plant. Every laboratory required this kind of information to ensure the safety of the laboratory. Also for the plant work, Health, Safety and Environment (HSE) department in every chemical company is responsible to put this information to ensure the safety of the plant.

## **CHAPTER 3**

### **METHODOLOGY**

#### **3.1 Project Workflow**

The methodology will describe the development steps of the application called Chemical Reactivity Matrix (ChReM), which enables the users to obtain the data of chemicals including chemical and physical properties, hazard identification, first aid measures, fire and explosion data, accidental release measures, handling and storage, exposure control, personal protection, stability and reactive data, toxicological information, ecological information, disposal considerations, transport information and other regulatory information. As it is difficult to gather the data of chemicals from MSDS (Material Safety Data Sheet), stand-alone user-friendly software has been developed using JAVA to allow users to obtain the chemical data in an easy and accurate way. The tool will enable the users to understand the chemical reactivity when each of the chemical reacts with each other. Figure 3.1 shows the methodology of this project.

The data that have been collected to develop the software are: chemical and physical properties of the chemicals, hazard identification, first aid measures, handling and storage, exposure control, personal protection, stability and reactivity data, toxicology information, ecological Information, disposal consideration, transport information and other regulatory information

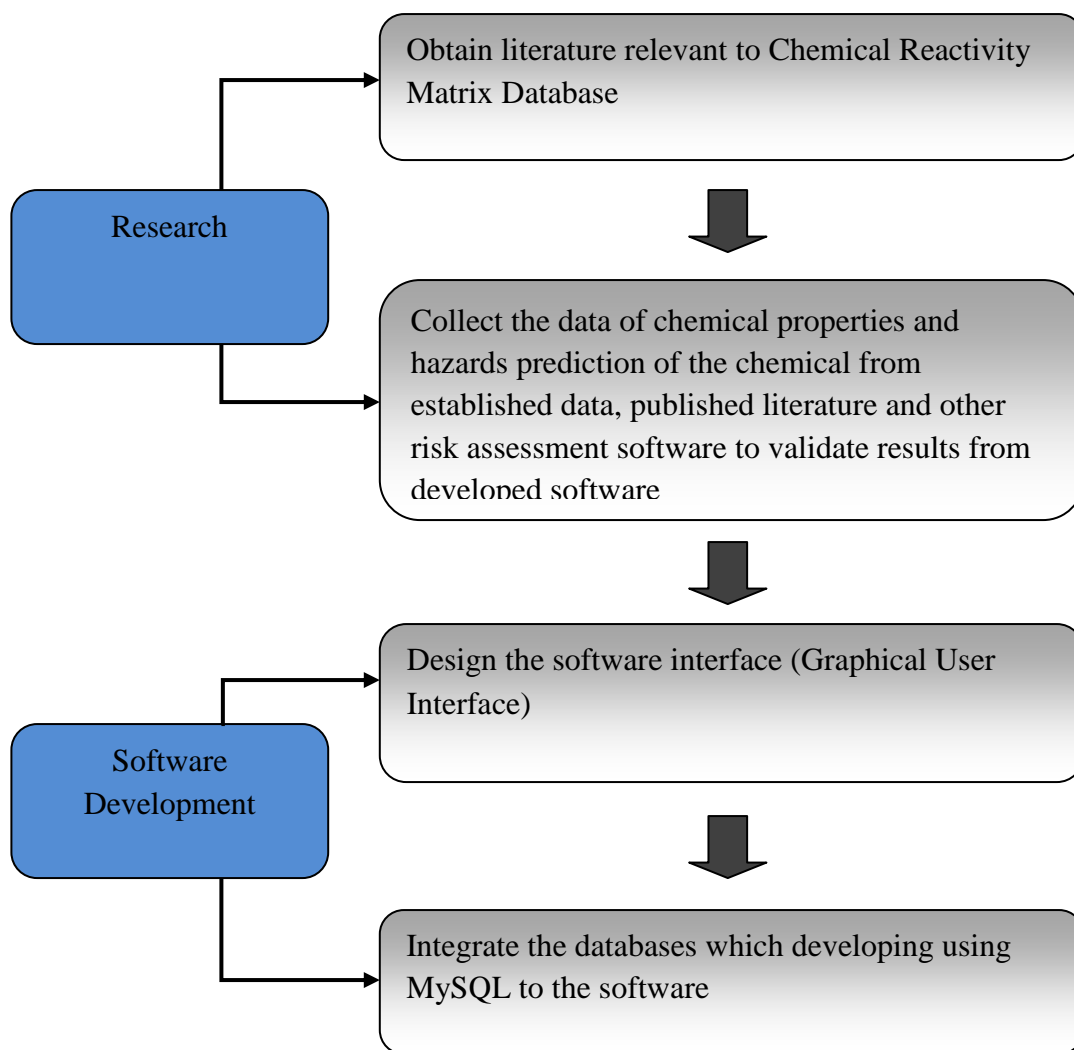


Figure 3.1: Methodology of the project.

### 3.2 Project Activities

There are 3 main activities in this project which are research, data collection and software development. In the research part, the author has done the research about the topic, Chemical Reactivity Matrix, which is the objective, is to predict the hazards when the chemicals react with each other. The database of this software has been built by gathering relevant information and data from different sources.

The data basically about the chemical and physical properties of chemicals, hazard identification and safety issues that related to the chemicals. This data usually is used by the people that handled the chemicals and it is important to know about all this information to make sure there are no accidents happen while working with the chemicals.

The first step in the software development is to design the software interface. After that, the interfaces will be linked with each other using programming language and can function by clicks on few buttons. The final step is to key-in the collected data into the database.

### **3.3 Software Development Stages**

The application used in developing the Chemical Reactivity Matrix is JAVA Eclipse programming. JAVA is relatively simple to learn and use programming language due to its graphical development features.

Basically, JAVA is a programming language originally developed by James Gosling at Sun Microsystems (which is now a subsidiary of Oracle Corporation) and released in 1995 as a core component of Sun Microsystems' JAVA platform. The language derives much of its syntax from C and C++ but has a simpler object model and fewer low-level facilities. JAVA applications are typically compiled to byte code (class file) that can run on any JAVA Virtual Machine (JVM) regardless of computer architecture. JAVA is a general-purpose, concurrent, class-based, object-oriented language that is specifically designed to have as few implementation dependencies as possible. It is intended to let application developers "write once, run anywhere". JAVA is currently one of the most popular programming languages in use, and is widely used from application software to web applications (JAVA User Guide, 2008).

Chemical Reactivity Matrix is a software package for estimating the impacts of chemicals in the process industries. The codings for Chemical Reactivity Matrix are built using JAVA programming language, which consists of a graphic user interface (GUI). The results of using the codes can be presented in tabulated or graphical forms, can be saved and exported to the Microsoft Word for hazards presentation.

The development of this software has been divided into five different stages, which are:

- Planning the application
- Building the databases
- Building the graphical user interface (GUI)
- Writing the computer program
- Integrating the results to WORD application
- Software validation and verification

Figure 3.2 shows the flowchart of the software which describe how the software works. By running the application which is the first step of the process, the user need to do the chemical selection by entering whether chemical name, CAS number, and UN/NA number.

After the search results appear, user can make the choice whether to search for new chemical or see further about the chemical which is chemical description. The user also can add the chemical to the worksheet as the preparation to predict the new hazards when the chemical mix with other chemical. Furthermore, the user can save, export or print the results for the future references.



### **3.3.1 Planning the Application**

The first step in application planning is identifying the various tasks that the application needs to perform. The second step is to determine how these tasks are logically related and to identify objects to which each task will be assigned. The following step is to classify the events needed to trigger an object into executing its assigned tasks. Lastly, a sketch of the graphical user interface is prepared. The application should be able to identify the hazard identification of the chemicals.

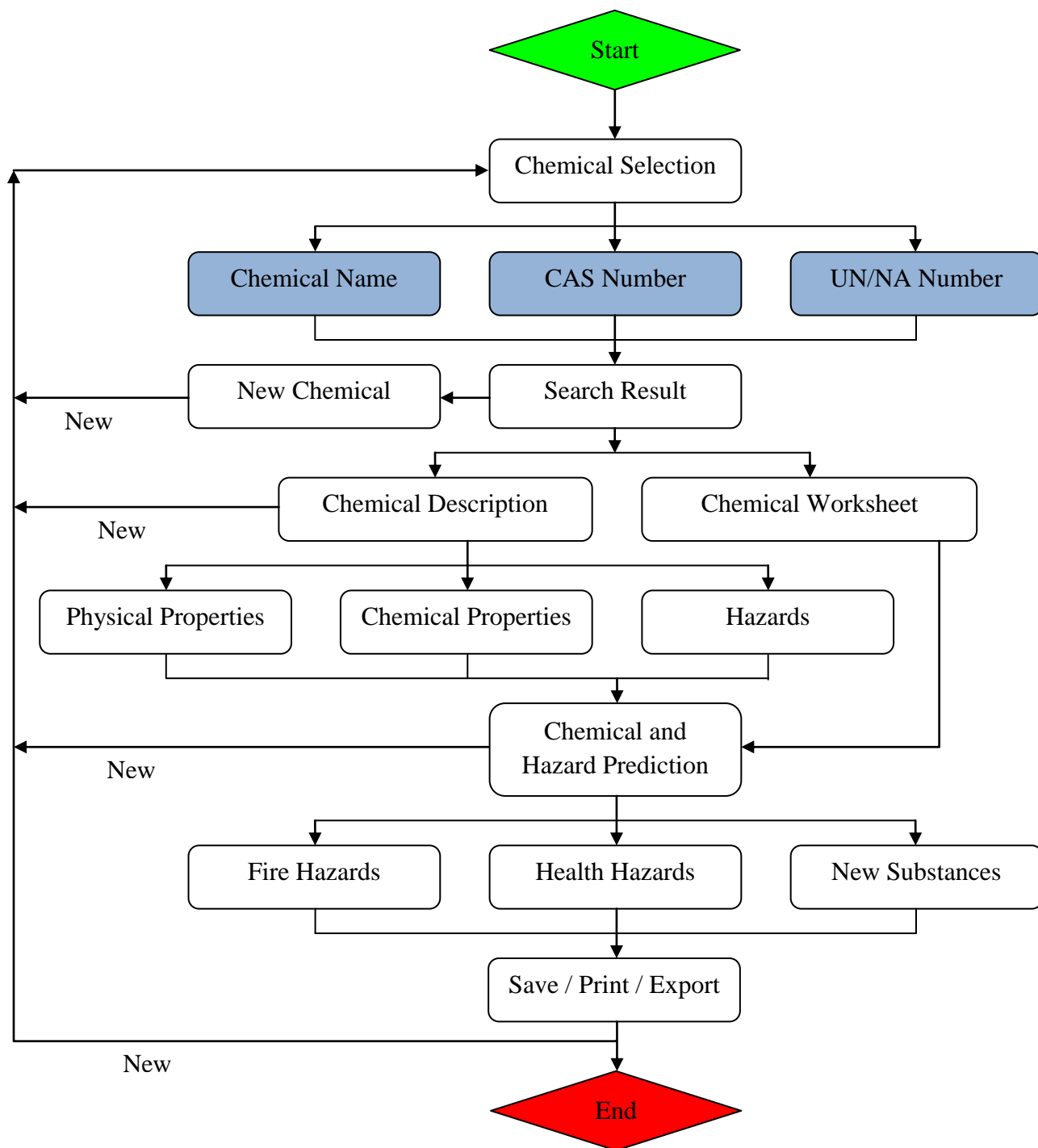


Figure 3.2: Flowchart of the software (ChReM).

### 3.3.2 Building the graphical user interface (GUI)

Basically, the software is working by searching option. The desire chemicals using either three identical features for the chemical which are chemical name, Chemical Abstracts System (CAS) number and United Nation/North America (UN/NA) number. Figure 3.3 shows chemical search interface.

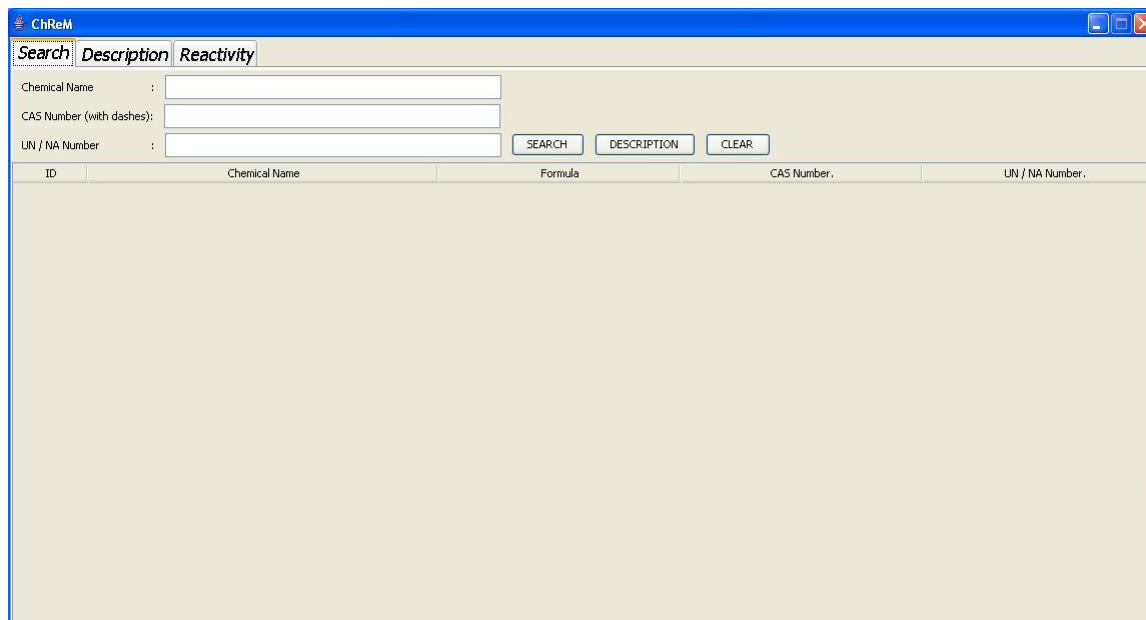


Figure 3.3: Chemical Search and Result Interface.

The result of the search will be presented as a result box which the users required to choose their desire chemical. Then, the users can choose whether they want to see the chemical description or transfer the desire chemical into the worksheet. Figure 3.3 also shows the result from the search box. There are several chemicals that have similar names. Therefore, this interface designed to allow the users to find required chemicals.

In the chemical description, there will be four part of descriptions which are general description, physical and chemical data, general properties and reactivity. Figure 3.4 shows the chemical descriptions. The general information such as chemical name, chemical formula, CAS number, UN/NA number, USCG Chris Code, DOT Hazard

Class, Reactive group numbers, DOT Hazard Label and special hazards can be view in general description part. The data such as boiling point, freezing point, molecular weight and specific gravity can be view in physical and chemical data part. The chemical hazard can be view in the general properties part and reactivity with air and water can be view in reactivity part.

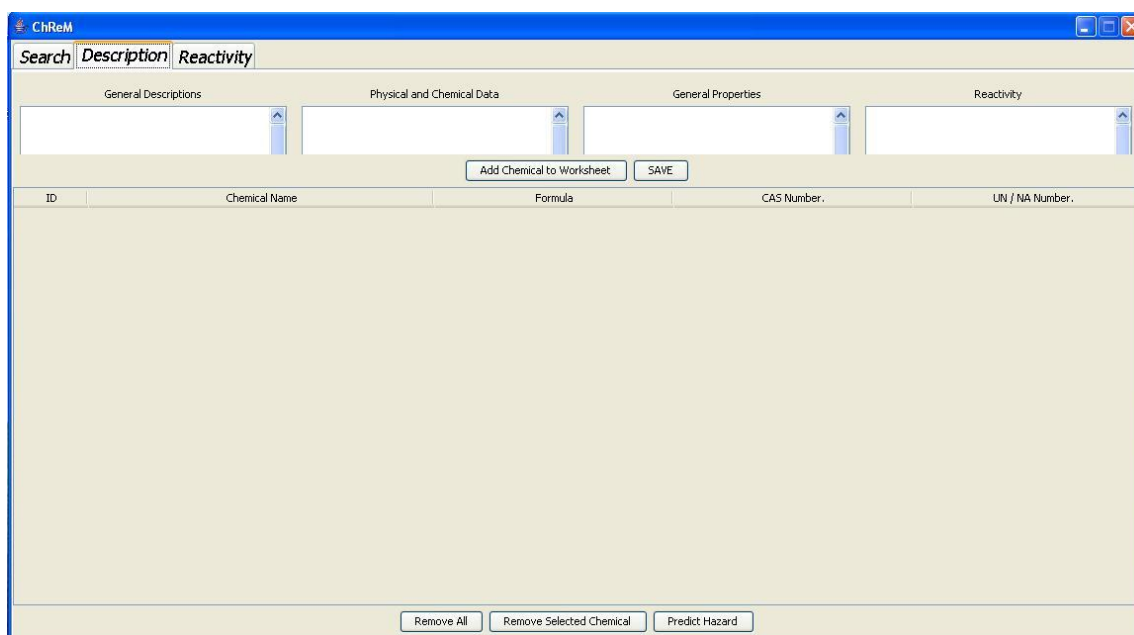


Figure 3.4: Chemical Description and Worksheet Interface.

Figure 3.4 also shows the worksheet of this application. Users can add the chemical into the worksheet in as the first step to react the chemical with other chemical. Figure 3.5 shows the chemical hazard prediction after two chemicals react with each other.

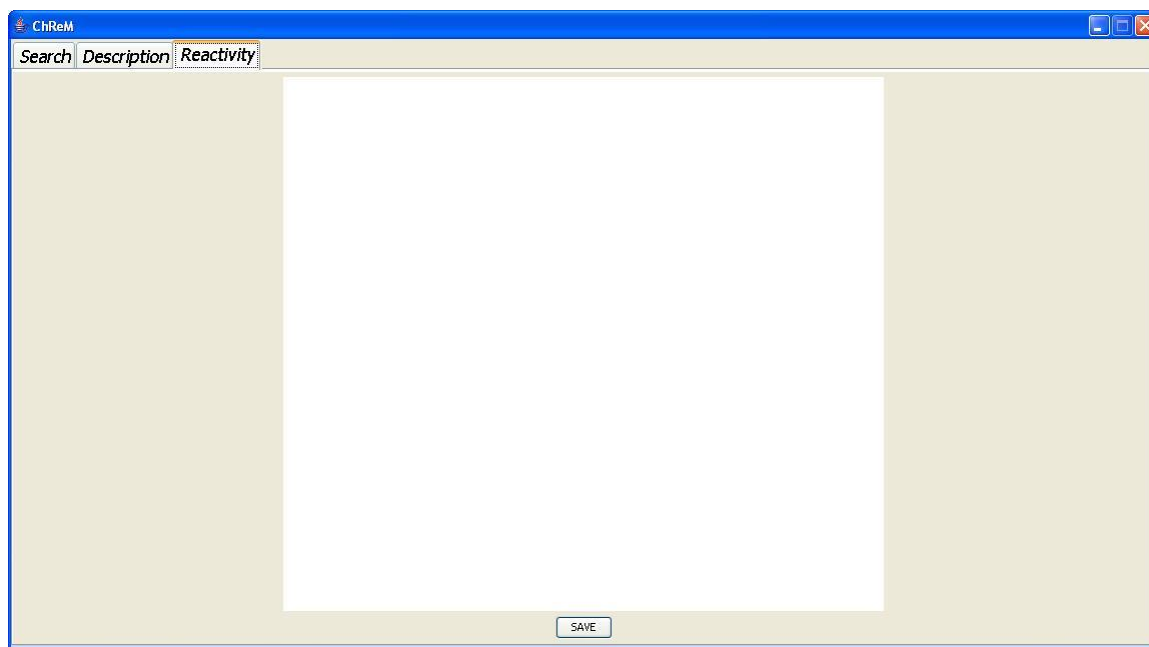


Figure 3.5: Chemical Reactivity Hazard Prediction Interface.

### 3.3.3 Writing the Computer Programme

The application is written in standard JAVA eclipse application and distributed in object format with the source code. After the interface of ChReM application has been developed, it is necessary to write the code that defines the applications behaviour. JAVA is used to develop the application and predict the reactivity of chemicals and hazard identification. Figure 3.6 shows some of the coding part in the JAVA eclipse program.

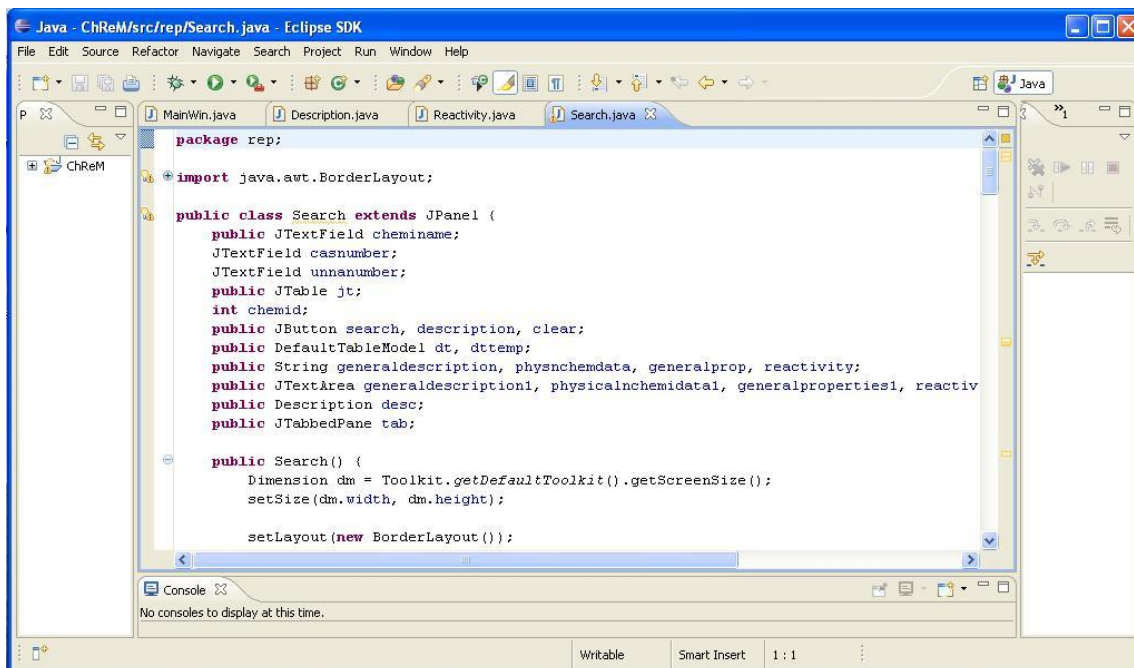


Figure 3.6: JAVA Eclipse programming code.

### 3.3.4 Building the databases

The databases are written in standard MySQL and integrated to the application interfaces. The databases consist of several chemicals and developed in flexible way to allow users to add a new chemical when it's required. Figure 3.7 shows some part of the chemical databases using MySQL.

The screenshot shows a MySQL database window titled "[Table] chemical @chrem (localhost)". The table contains the following data:

ID	cheminame	casnumber	formula	generaldescription	physnchemdata	gen
7	Diethylene Glycol	111-46-6	C4H10O3	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	
1	Ethylene	74-85-1	C2H4	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	
6	Ethylene Oxide	75-21-8	C2H4O	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	
3	Hydrogen	1333-74-0	H2	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	
5	Nitrogen	7727-37-9	N2	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	
4	Oxygen	7782-44-7	O2	GENERAL DESCRIPTION	PHYSICAL AND CHEMICAL DA1 GEN	

The status bar at the bottom of the window displays the SQL query: "SELECT \* FROM `chemical` ORDER BY `cheminame` LIMIT 0,1000" and indicates "Record 1 of 6 in Page 1".

Figure 3.7: Databases using MySQL.

### 3.3.5 ChReM Validation and Verification

Verification and validation of software is the most important step to build confidence and quantify results. Verification is a process to ensure that the software that is made matches with the original design. It checks whether the software is made according to the criteria and specification described in the requirement documents.

The validation process confirms that a correct system is being made (i.e., the system requirements are correct, complete, consistent, operationally and technically feasible, and verifiable). The verification process ensures that the design solution has met the systems requirement and that the system is ready for use in the operational environment for which it is intended.

ChReM application has been validate and verify by compare the functions of the software by using another similar software. By comparing the functions with other software, ChReM shows more detail in chemical description and it is more easy and

friendly-user compared to other software. ChReM also provided more useful information than other software which are general properties, physical and chemical data, general description and reactivity. In general properties part, it included chemical name, CAS number, UN/NA number, chemical formula, USCG Chris Code, DOT Hazard Class and DOT Hazard Label. There are more physical data provided in physical and chemical data as well as chemical data.



### 3.4 Gantt Chart

Table 3.1: The gantt chart of the project

No	Detail/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20		
1	Project Work	█	█	█	█	█	█	Mid-Semester Break		█	█	█	█	█	█								
2	Submission Progress Report 1					█																	
3	Submission of Progress Report 2											█											
4	Poster/Pre-EDX											█											
5	EDX												█										
6	Submission of Final Report (CD & Softbound)															█							
7	Final Oral Presentation																			█	█		
8	Submission of Hardbound Copies																						█

# CHAPTER 4

## RESULT AND DISCUSSION

### 4.1 ChReM application

By clicking on the run button, the software will be initiated and the search box will be appeared. The user required to enter the desire chemical name. Figure 4.1 shows the example on how to search the chemical. In this case, Ethylene will be used as an example to show the steps of using this application.

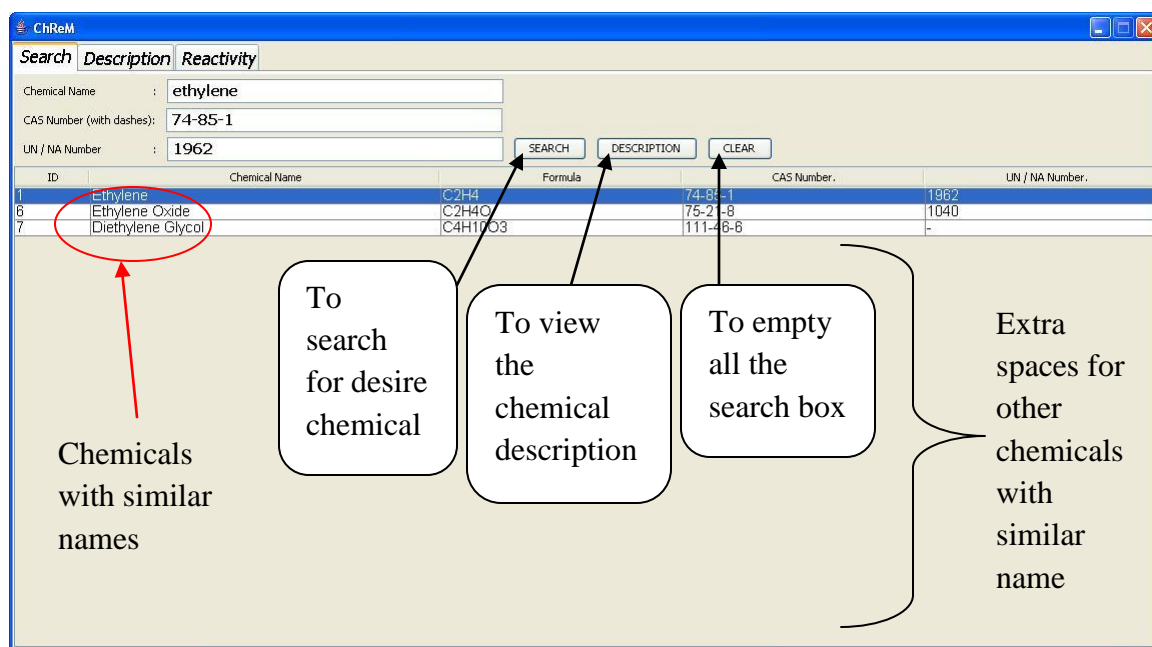


Figure 4.1: Chemical Search and Result.

The users can use either chemical name, CAS number and UN/NA number of desired chemical to start the search. Figure 4.1 shows the buttons which are search, description and clear. The function of the search button is to start the search after the users insert the chemical name into the search box. For the description button, the function is to view the description of the chemical. Clear button is to empty entire search box if the users want to make the new search for chemicals. Then, the result for the

chemical will be appeared below the search box. The table is designed to have extra empty space to enable similar chemical name to be listed. For example, if we search for Ethylene, the following names will be appeared such as Ethylene Oxide, Diethylene Glycol and others.

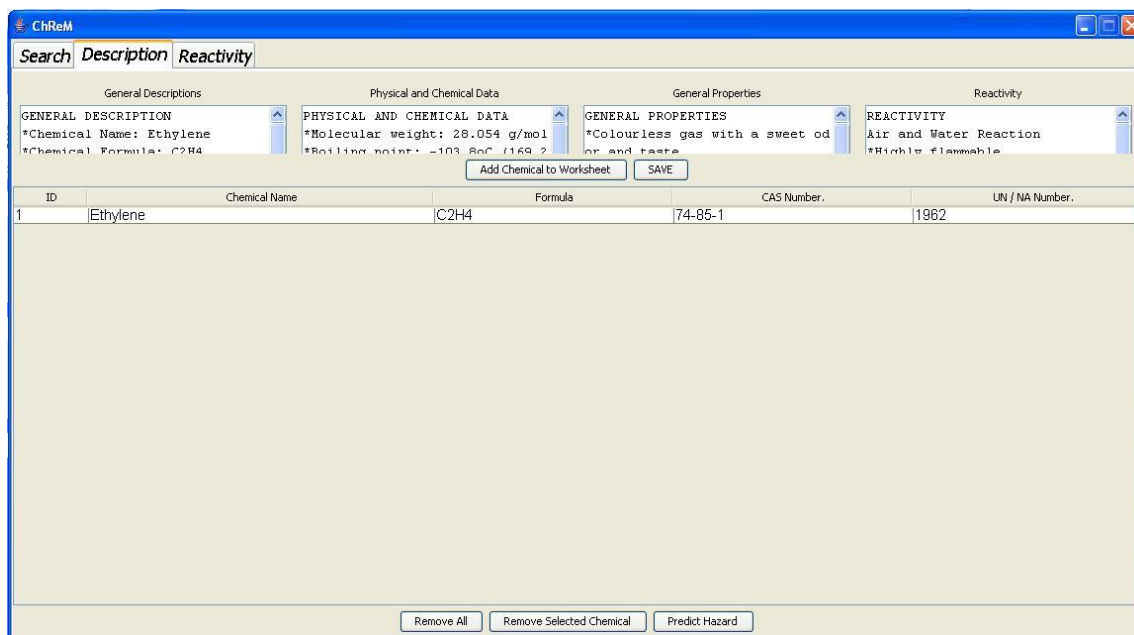


Figure 4.2: Descriptions of the Chemical.

Figure 4.2 shows the descriptions of chemical and worksheet. There are five function buttons in this interface. First button is ‘add chemical to worksheet’ button. The function of this button is to add the chemical to the worksheet after the users found the desire chemical. Next button is ‘save’ button which is to integrate the chemical description into the word document. ‘Remove all’ button is to clear all the chemicals in the worksheet part. ‘Remove selected chemical’ is to remove the chemical which is selected by users. The function of ‘Predict Hazard’ button is to predict the hazard after two chemicals react with each other. After clicking ‘Predict Hazard’ button, the reactivity part will be appeared also.

The description of the chemical (Ethylene) can be save into the word document. Basically, users are tending to save the chemical description as references to use the

information for the works (e.g. laboratory works, plant works or others). This is a useful tool as this application provide the save button to save the chemical description into the word document and it is easy for the users to refer back about the chemical that they are handling on that time.

After users save the chemical description into the word document, they can read the description properly to verify the information and to confirm that they did not misidentifying the chemical hazards. Figure 4.3 shows the example of the save word document. This application also provides the simple and understanding of the chemical description in the word document.

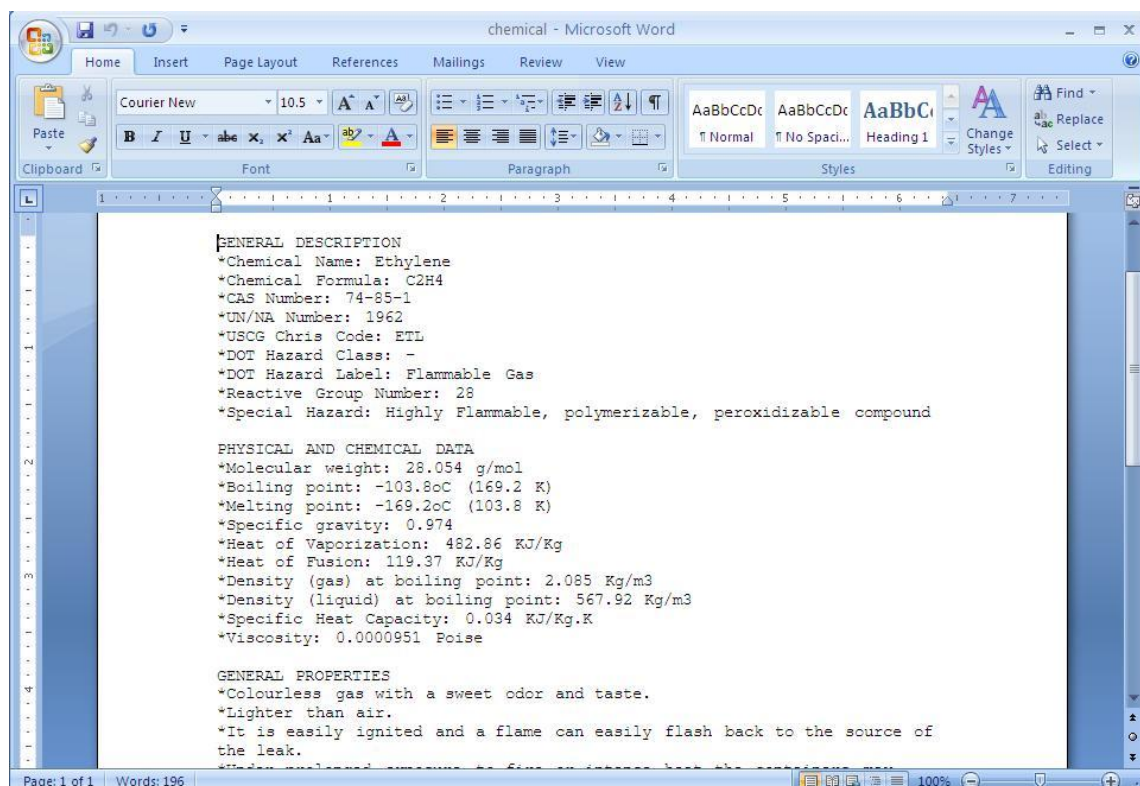


Figure 4.3: The example of the chemical description in word document format.

## 4.2 Case Study

The development of ChReM application has been verified and validated with other reactivity software which are CRW2 and ChemDB. Both of these software have their uniqueness but some of the features in this software are quite hard to handle. Both of these software are categorized in the reactivity software which can show the description of chemical and safety precautions of hazards. Basically, CRW2 has been developed by National Oceanic Atmospheric Administration (NOAA) and ChemDB is developed by ATSOFT Company which is Software Development Company.

Table 4.1 shows the case study of the ChReM application. This case study has been validated with the other chemical reactivity software which are Chemical Reactivity Worksheet 2 (CRW2) and Chemistry Database (ChemDB). This case study shows the differences between ChReM application, ChemDB and CRW2 application.

Table 4.1: Case study of Chemical

BENZENE				
PROPERTIES	VALUE	ChReM	CRW2	ChemDB
Chemical Formula	C <sub>6</sub> H <sub>6</sub>	Yes	Yes	Yes
CAS number	71-43-2	Yes	Yes	Yes
UN/NA number	1114	Yes	Yes	Yes
USCG Chris Code	BNZ	Yes	Yes	Yes
DOT Hazard Label	Flammable Liquid	Yes	Yes	Yes
DOT Hazard Class	Flammable	Yes	Yes	Yes
Reactive Group number	16	Yes	Yes	Yes
Special Hazards	Highly Flammable	Yes	Yes	Yes
Molecular Weight	78.11 g/mol	Yes	No	No
Boiling point	80.1°C (353.1 K)	Yes	No	No
Freezing point	5.5°C (278.5 K)	Yes	No	No
Specific Gravity	0.882 - 0.886	Yes	No	No
Heat of Vaporization	30.72 KJ/mol	Yes	No	No
Heat of Fusion	10.0 KJ/mol	Yes	No	No
Density	0.88 g/mol	Yes	No	No
Specific Heat Capacity	1.74 J/g.K	Yes	No	No

The case study of this project is to differentiate between this software (ChReM) with CRW2 application. The results presented in Table 4.1 shows that ChReM can provide more information than CRW2 and ChemDB. This case study shows the improvement of this software from the other software to ensure the users get the information required. ChReM application is user-friendly which is easy to learn and use by the users.

For the hazard prediction, ChReM application provides useful information which the other software also provides but the information is not enough for the users to make as references. Figure 4.4 shows the hazard prediction of chemicals when it mixes with each other.

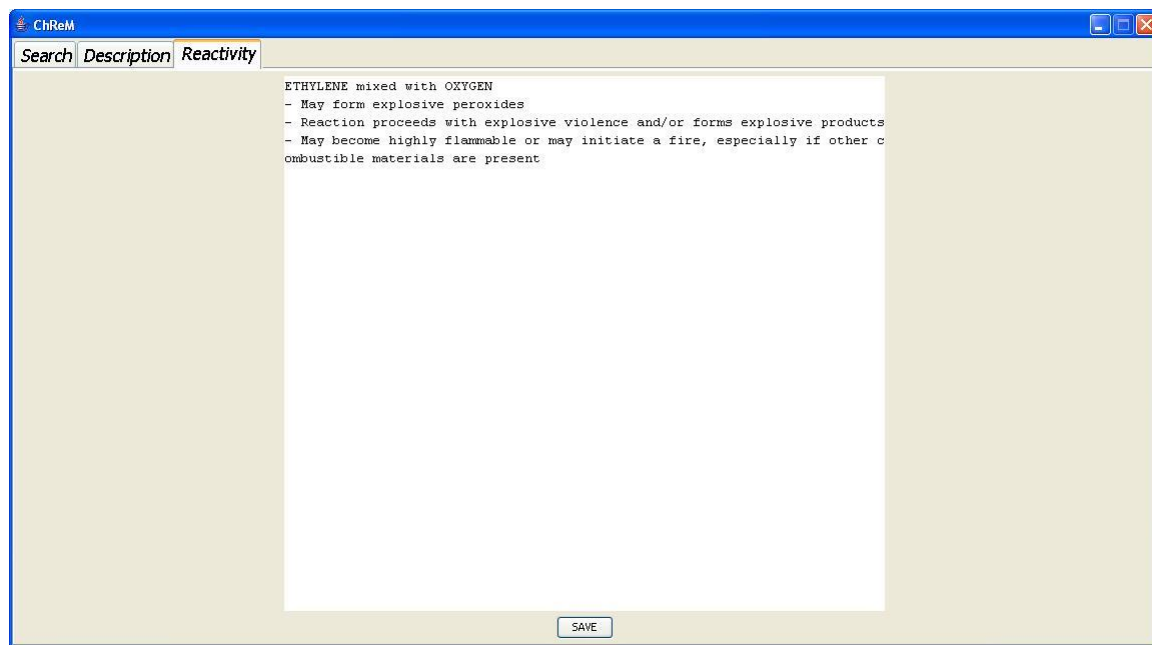


Figure 4.4: Hazard Prediction when Ethylene reacts with Oxygen.

In Figure 4.4, it shows the prediction of hazards after chemicals mixes with each other. For example, if Ethylene and Oxygen react with each other, then it will show the hazards prediction and possible gases that will appear. For the comparison with other

software, ChemDB not provides the hazard prediction for the chemical reactivity but CRW2 provides the hazards prediction information but the result from CRW2 is quite hard to read compared with ChReM which is more easy to read. But the result of hazard prediction in the CRW2 cannot be saving by the users, so it is difficult to the users to make the references for future work.

The result from the CRW2 application contains all the information including the unused information which can confuse the users to select the important information but the result of ChReM application is only for more useful and important information that the users required.

## **CHAPTER 5**

### **CONCLUSION**

ChReM application has been developed using JAVA Eclipse programming application with the database using MySQL. Chemical Reactivity Matrix is important to ensure that safety for the environment. ChReM application provides useful tools to obtain the general properties of the chemicals which are important to differentiate between hazardous and non-hazardous material. Generally, this information is important for the work that involve with chemical (e.g. experimental work, plant work or others) because we need to know the properties of the chemicals or substances before we handled it. This is to prevent any accident to happen and harm peoples and environment. The class of hazards also has been provided in the ChReM application to ensure that we follow the rules when handling the chemicals or substances.

Misidentifying chemical hazards and properties also happen and generally lead to accident such as fires, explosions, injuries and deaths. ChReM application provides more authentic information of the chemicals to prevent the users from misidentifying the chemicals hazards. ChReM application also provides the hazards prediction when the chemicals mix with each other.



## **CHAPTER 6**

### **RECOMMENDATION**

This ChReM application can be improved time to time in order to satisfy the users need. One of the things that can be improved is the databases. The users can find descriptions of more chemicals using the ChReM application if the databases are bigger which contain millions of chemical databases.

ChReM application also can be improved by create more reactivity combination which is in the hazard prediction. The users can react chemical with two or more chemicals to make the hazard prediction. By improved on this feature, ChReM application can be more useful tool of reactivity software.

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