

CHAPTER 4

RESULTS AND DISCUSSIONS

This chapter explains and discusses the results obtained from the current research in the context with the findings of earlier studies. The CRHS software has been successfully developed and implemented in an interactive Visual Basic (VB) environment. The software is designed to be user-friendly to simulate chemical reactivity hazard. It is developed using VB language with database at the back end (source code). The result of the chemical reaction gives the specific hazard code.

4.1 Software Introduction Interface

After accessing the software, the interface shown below (Figure 4.1) would appear on the screen and is visible for about 5 seconds before proceeding automatically to the main general interface (Figure 4.2).

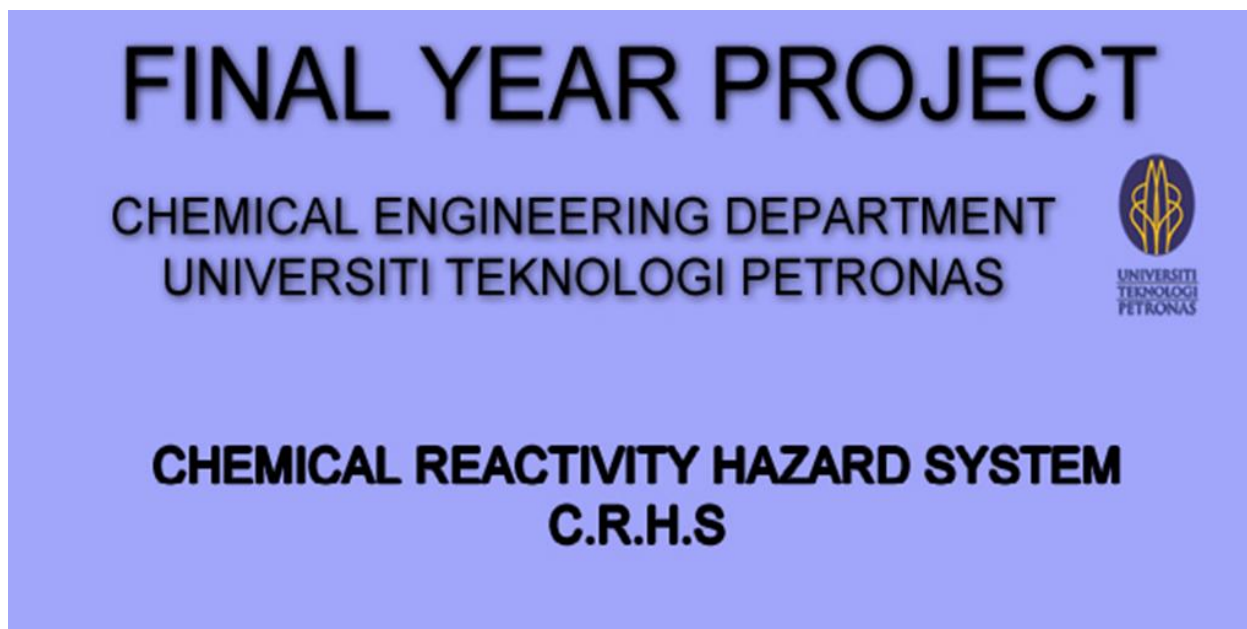


Figure 4.1: CRHS introduction interface

4.2 General Interface

The main general interface will provide the users several options. Figure 4.2 represents the main general interface of the software.

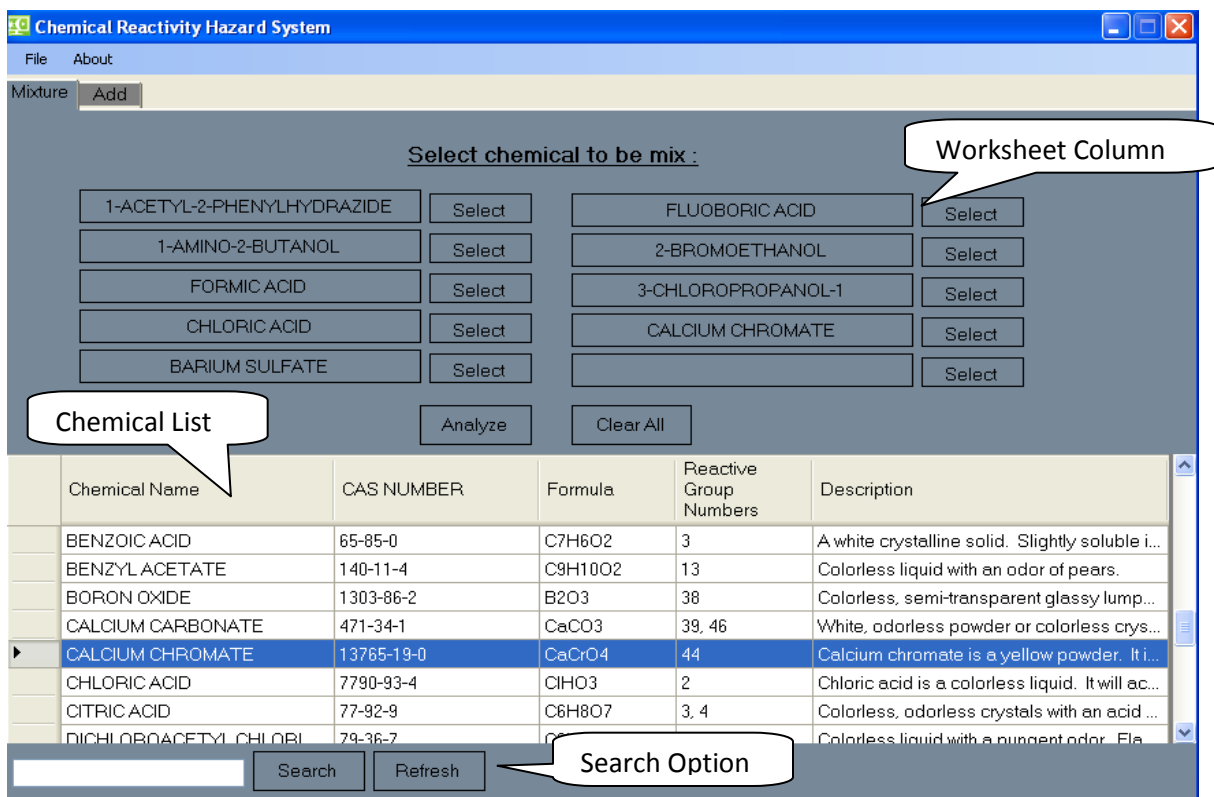


Figure 4.2: CRHS main general interface

The users can select the required chemical from the chemical list that was placed below the worksheet column. The chemical from the chemical list is select by clicking the select button beside the respective worksheet column. The chemical from the chemical list will show the users the chemical name, CAS number, chemical formula, reactive group number and also the chemical description. As we can see in Figure 4.2, the users can select up to ten different chemicals for the analysis. The users must select at least two chemicals to be analyze and if the users click the analyze button without doing so, an error message will be generated by CHRS as shown in Figure 4.3.

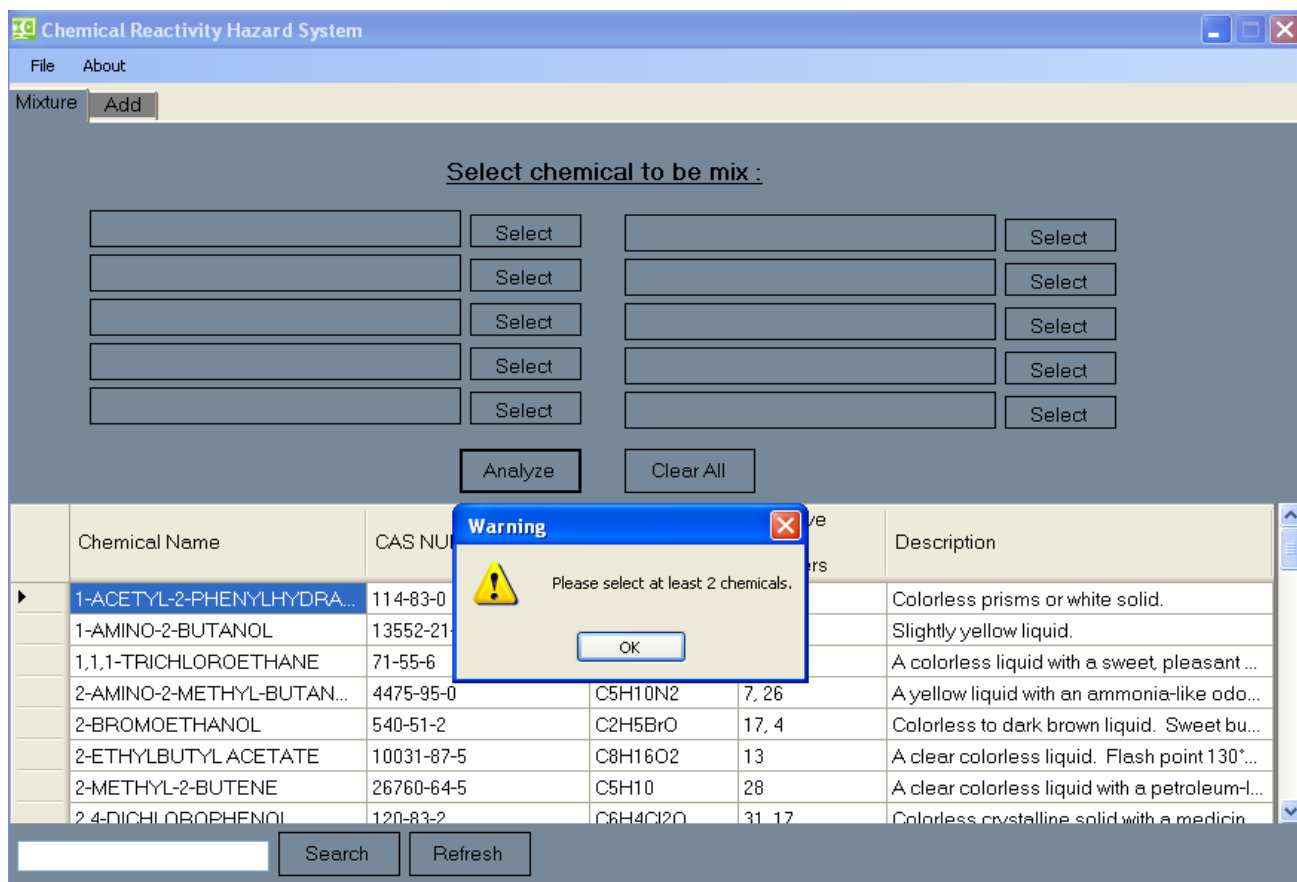


Figure 4.3: Error message generated for general interface

4.2.1 Search Option Interface

In the search option interface, the users will find the column search, the search button and the refresh button as shown in Figure 4.3. The users can search for desired chemical by using the search option interface rather than search it in the chemical list. The users just have to enter the desired chemical name into the search column and click the search button.

	Chemical Name	CAS NUMBER	Formula	Reactive Group Numbers	Description
	ETHYLENE CYANOHYDRIN	109-78-4	C3H5NO	4, 26	Colorless to yellow-brown liquid with a w...
	EUGENOL	97-53-0	C10H12O2	28, 31	Clear colorless pale yellow or amber-col...
▶	FERRIC NITRATE	10421-48-4	Fe(NO3)3	44	A violet crystalline solid. Noncombustibl...
	FLUOBORIC ACID	16872-11-0	HBF4	1	A colorless odorless poisonous liquid. B...
	FOLIC ACID	59-30-3	C19H19N7O6	3, 6	Odorless orange-yellow needles or plat...
	FORMIC ACID	64-18-6	CH2O2	3	A colorless liquid with a pungent odor. FL...
	Search Column	54-31-9	C12H11ClN2...	3, 6, 7, 14, 16, ...	Odorless white to slightly yellow crystallin...

ferric nitrate Search Refresh

Figure 4.4: Search Option Interface for CRHS software

The desired chemical will automatically be highlighted in the chemical list as shown in the example in Figure 4.3. The refresh button allows the users to clear the search column for the users to find different chemical.

4.3 Add Chemical Interface

As the CRHS software wants to be user-friendly and flexible application, the add chemical interface is developed to help the users in adding new chemical into the database of the software. This interface allows the users to add chemical by key in the information regarding the chemical. The information that have to be key in are the chemical name, CAS number, chemical formula, reactive group number and the chemical description. Figure 4.4 shows the example of adding a chemical into the data base using the add chemical interface.

Chemical Reactivity Hazard System

File About

Mixture Add

Info Column

Chemical Name: BORIC ACID
 Cas Number: 11113-50-1
 Formula: BH3O3
 Reactive Group No.: 1

Description: Odorless white solid.

Add
Clear
Refresh

Chemical Name	CAS NUMBER	Formula	Reactive Group Numbers	Description
DICHLOROACETYL C...	79-36-7	C2HCl3O	40, 17	Colorless liquid with a pungent odor. Flash point 151°.
DIETHYL CARBONATE	105-58-8	C5H10O3	13	A colorless liquid with a mild pleasant odor. It is slight.
DIETHYL ETHYLPHOS...	78-38-6	C6H15O3P	32	Colorless liquid with a mild odor.
DIMETHYL PHOSPHA...	813-78-5	C2H7O4P	32	Syrupy pale yellow liquid.
DIMETHYL SULFATE	77-78-1	C2H6O4S	13	Dimethyl sulfate is a colorless oily liquid, odorless to ...
ETHYL BROMOACETA...	105-36-2	C4H7BrO2	13, 17	A clear, colorless liquid (b.p. 318°F). Flash point 47°C...
ETHYL CHLOROACET...	105-39-5	C4H7ClO2	13, 17	A clear colorless liquid with a pungent odor. Flash po...
ETHYL LACTATE	97-64-3	C5H10O3	13	A clear colorless liquid with a mild odor. Flash point 1...
ETHYLENE CYANOHY...	109-78-4	C3H5NO	4, 26	Colorless to yellow-brown liquid with a weak odor. Sin...
EUGENOL	97-53-0	C10H12O2	28, 31	Clear colorless pale yellow or amber-colored liquid. ...
FERRIC NITRATE	10421-48-4	Fe(NO3)3	44	A violet crystalline solid. Noncombustible but it will ac...
FLUOBORIC ACID	16872-11-0	HF4	1	A colorless odorless poisonous liquid. Boiling point 1...
FOLIC ACID	59-30-3	C19H19N7O6	3, 6	Odorless orange-yellow needles or platelets. Darke...
FORMIC ACID	64-18-6	CH2O2	3	A colorless liquid with a pungent odor. Flash point 156...
FUROSEMIDE	54-31-9	C12H11ClN2...	3, 6, 7, 14, 16, ...	Odorless white to slightly yellow crystalline powder. A...
BORIC ACID	11113-50-1	BH3O3	1	Odorless white solid.

Figure 4.5: Add Chemical Interface in CRHS software

The users must key in all the data in the information column in order to add the chemical into the data base. If the users fail to key in all the necessary information on that chemical, an error message will be generated by CRHS as shown in Figure 4.6. The clear button will clear all data in the information column to allow the users to continue adding new chemical into the data base of the software.

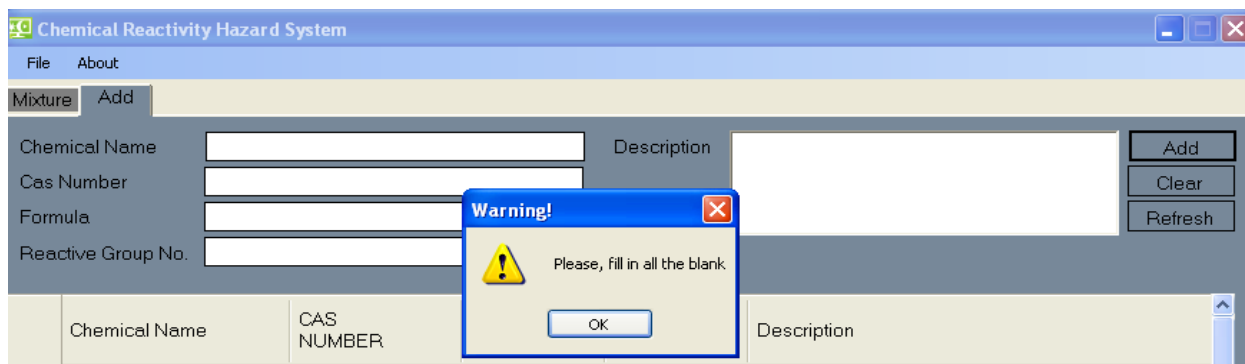


Figure 4.6: Error message generated for add chemical interface

4.4 Result Interface

When the users click the analyze button in the main general interface, the result interface will appear with the respective chemical mixture and their hazard codes. The CRHS application predicts the reactivity between two chemical at a time. Figure 4.7 shows the predicted hazard code with it respective chemical mixture.

Mixture Column	Hazards Code Column
1-ACETYL-2-PHENYLHYDRAZIDE + 1-AMINO-2-BUTANOL =	B6 C
1-ACETYL-2-PHENYLHYDRAZIDE + FORMIC ACID =	CD6
1-ACETYL-2-PHENYLHYDRAZIDE + CHLORIC ACID =	A6 A9 B1 B4 B6 CD6
1-ACETYL-2-PHENYLHYDRAZIDE + BARIUM SULFATE =	A3 A6 A9 B4 B6 CD3 D4
1-ACETYL-2-PHENYLHYDRAZIDE + FLUOBORIC ACID =	CD3 D6 G
1-ACETYL-2-PHENYLHYDRAZIDE + 2-BROMOETHANOL =	CD3 G
1-ACETYL-2-PHENYLHYDRAZIDE + 3-CHLOROPROPANOL-1 =	CD3 G
1-ACETYL-2-PHENYLHYDRAZIDE + CALCIUM CHROMATE =	A3 A6 A9 B4 B6 CD3 D4
1-ACETYL-2-PHENYLHYDRAZIDE + FERRIC NITRATE =	A3 A6 A9 B4 B6 CD3 D4
1-AMINO-2-BUTANOL + FORMIC ACID =	CD6 G
1-AMINO-2-BUTANOL + CHLORIC ACID =	A6 A9 B1 B4 B6 CD6
1-AMINO-2-BUTANOL + BARIUM SULFATE =	A3 A6 A9 B4 B6 CD3
1-AMINO-2-BUTANOL + FLUOBORIC ACID =	CD6 G
1-AMINO-2-BUTANOL + 2-BROMOETHANOL =	CD3
1-AMINO-2-BUTANOL + 3-CHLOROPROPANOL-1 =	CD3

Figure 4.7: Result interface for CRHS software

The users can click to the respective hazard code column to get the hazard description of the mixture. Figure 4.8 shows an example of the hazards description for one of the mixture.

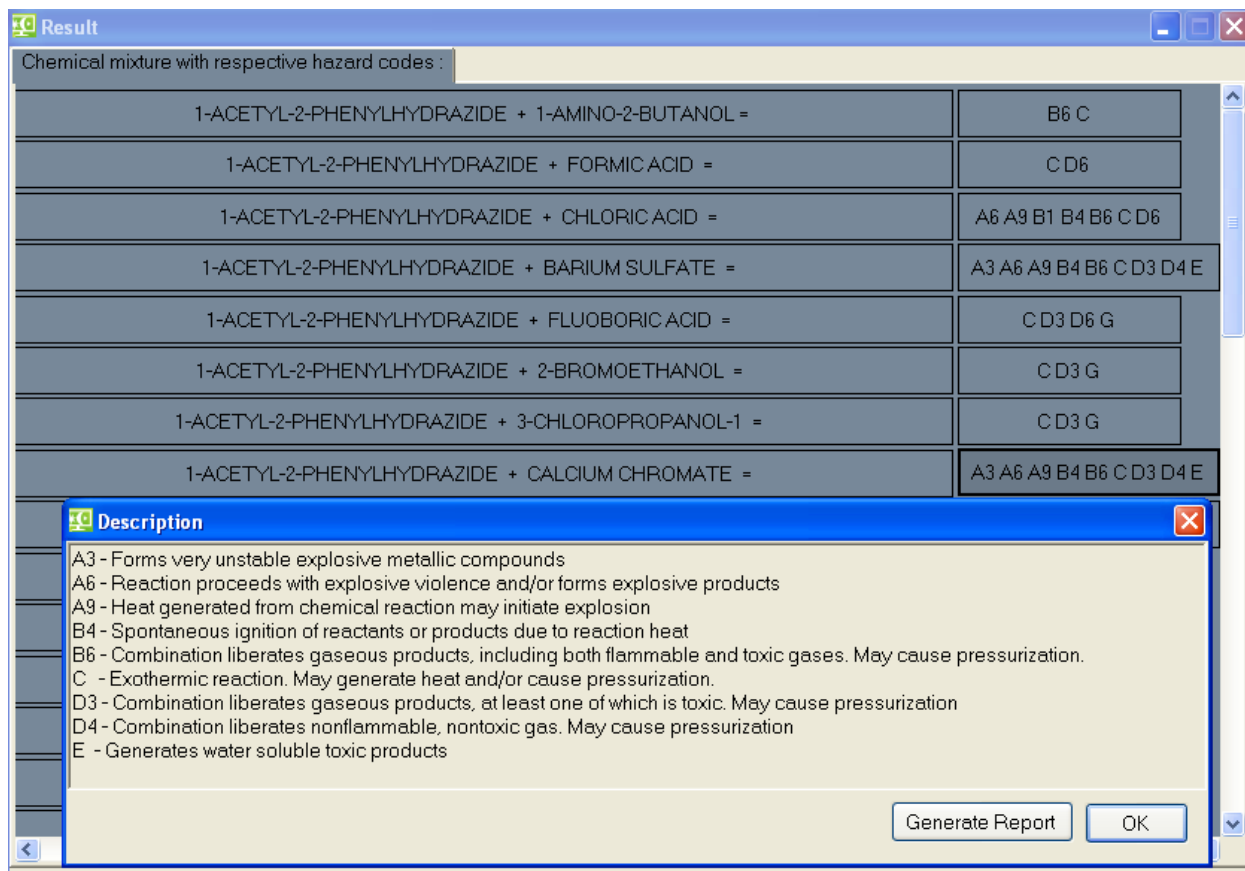


Figure 4.8: Hazards description generated by CRHS

The descriptions of the hazards are based on a particular mixture and this will help the user to specified and select the required information. The representation of the data is in order and individual so that the users will not have any problem to understand and gather information. In the description interface, there is option to generate report. When the users click the generate report button, the CHRS automatically generate the report based on the particular mixture that have been selected by the users. Figure 4.9 shows an example report that has been generated report by CRHS.

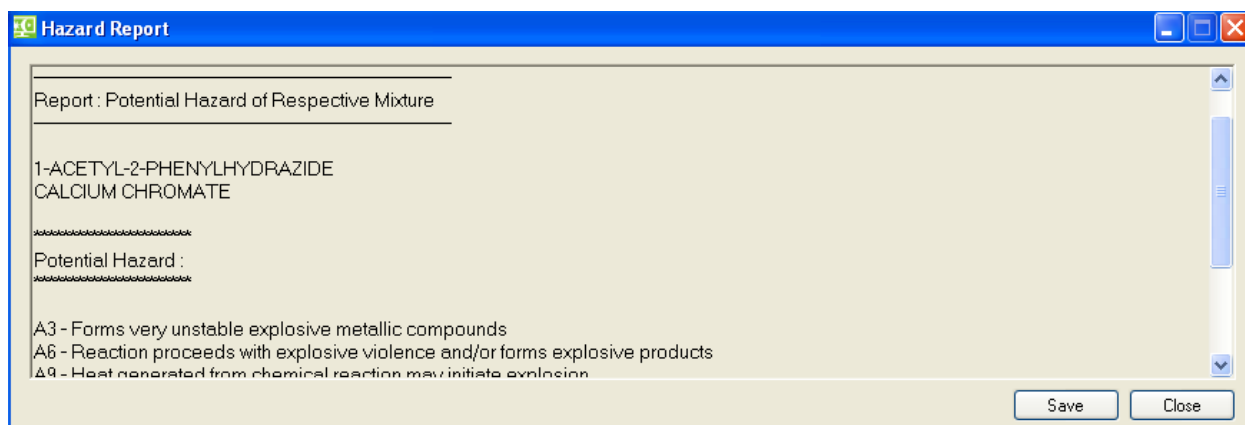


Figure 4.9: Hazard Report generated by CRHS software

The hazard report consists of information that is the two chemical names, the respective hazard codes and the hazards description. In the hazard report interface, there are save button to allow the user to save the report that has been generated. When the users click at the save button, the CRHS will automatically save the report in the user's desktop. An icon will be generated in the desktop to show that the report has been saved (Figure 4.10). Figure 4.11 shows an example of the save report in text format.



Figure 4.10: Icon for the Hazard Report in the desktop generated by CRHS


```
ReportCRHS.txt - Notepad
File Edit Format View Help
CHEMICAL REACTIVITY HAZARD SYSTEM
-----
Report : Potential Hazard of Respective Mixture
-----
1-ACETYL-2-PHENYLHYDRAZIDE
CALCIUM CHROMATE
*****
Potential Hazard :
*****
A3 - Forms very unstable explosive metallic compounds
A6 - Reaction proceeds with explosive violence and/or forms explosive products
A9 - Heat generated from chemical reaction may initiate explosion
B4 - Spontaneous ignition of reactants or products due to reaction heat
B6 - Combination liberates gaseous products, including both flammable and toxic gases. May cause pressurization.
C - Exothermic reaction. May generate heat and/or cause pressurization.
D3 - Combination liberates gaseous products, at least one of which is toxic. May cause pressurization
D4 - Combination liberates nonflammable, nontoxic gas. May cause pressurization
E - Generates water soluble toxic products
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Figure 4.11: Hazard Report in text format form

4.5 Case Study

4.5.1 Validation of the Software

The development of CRHS application has been verified and validated with other reactivity software and some published literatures. For the validation process, we take two chemicals that are arsenic and calcium chromate as our desired chemical for the reactivity study. We want to use CRHS application to predict the hazard of this mixture. Arsenic is a grayish metallic solid that turns black upon exposure to air, insoluble in water and toxic by ingestion (Henke, 2009). For calcium chromate, it is a yellow powder and it is slightly soluble in water. It is an inorganic oxidizing agent and the primary hazard is the threat to the environment (Pohanish and Greene, 2009). Figure 4.12 shows the respective hazards codes generated by CRHS application on the mixture of arsenic and calcium chromate.

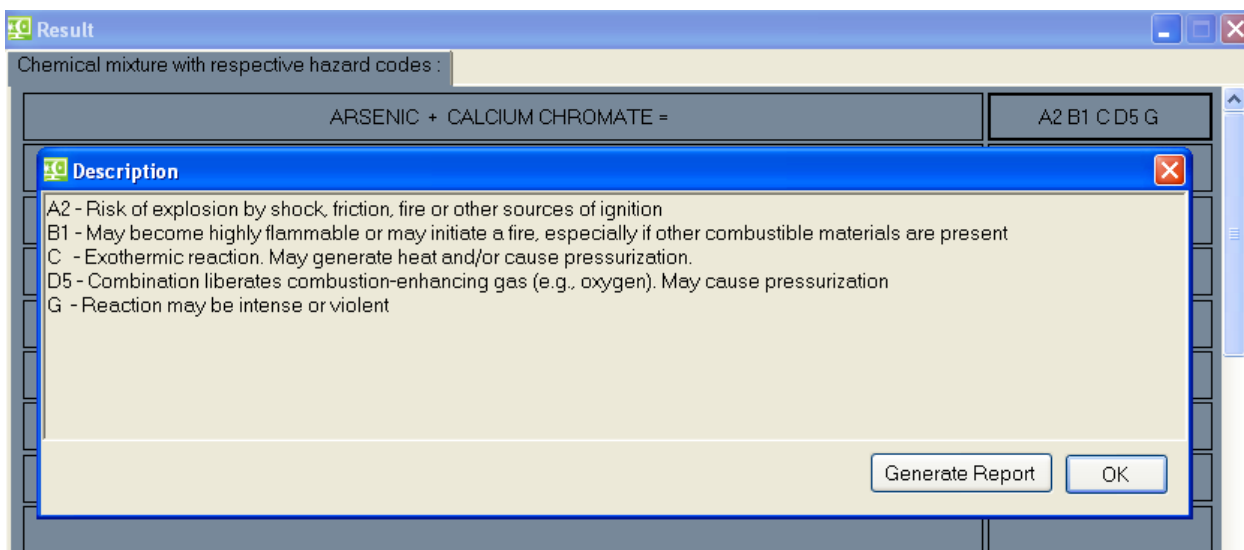


Figure 4.12: Hazards descriptions on mixture

The CRHS application predicted that the mixture of arsenic and calcium chromate will produce the above hazards. This is consistent with Bretherik (1995) that stated that silver, copper, and lead (metal) react violently and may ignite on contact with chlorine trifluoride (ClF₃) an oxidizing agent. Pohanish and Greene (2009) also discussed reactivity between metal group and oxidizing groups by stating that silver can cause explosive decomposition of ozonides. Furthermore, Mellor (1941) stated that copper forms explosive mixtures with chlorate or iodate salts; the mixtures are sensitive to shock, heating, or friction and also mercury (metal) forms a shock-sensitive explosive mixture with chlorine dioxide (ClO₂) an oxidizing agent.

These published literatures prove that the predicted hazards that are generated by CRHS application are accurate and consistent with the chemical reactivity studies.

4.5.2 Verification of the Software

For the verification part, the CRHS software is being compared with other reactivity software that is available in the market. There are few reactivity software available and one of it is Chemical Reactivity Worksheet 2 (CRW2). CRW2 software has its uniqueness but some of

the features in this software are quite hard to handle. CRW2 has been developed by National Oceanic and Atmospheric Administration (NOAA). We take also arsenic and calcium chromate as our example for this verification process. Figure 4.13 shows the result generated from CRW2 software.

The screenshot shows the CRW2 software interface. At the top, there is a menu bar with 'File', 'Edit', 'Scripts', and 'Help'. Below the menu bar is a toolbar with buttons for 'Worksheet', 'New Search', 'Search Results', 'Export to Excel', 'Print Chart', and 'Help'. The main area contains a 'Reactivity Compatibility Chart' table. The table has columns for 'ARSENIC' and 'CALCIUM CHROMATE'. The first row is labeled 'Reactivity Compatibility Chart'. The second row shows 'ARSENIC' in the first column and 'A2, B1, C, D5, G' in the second column. The third row shows 'CALCIUM CHROMATE' in the first column and 'A2, B1, C, D5, G' in the second column. Below the table is a large empty space. At the bottom, there is a 'Hazard Summary' section with tabs for 'Hazard Summary', 'Potential Gases', 'Pot. Gases Documentation', and 'General Documentation'. The 'Hazard Summary' tab is selected. It shows 'Selected Chemical Combination' as 'CALCIUM CHROMATE' and 'ARSENIC'. Below this, there is a list of hazard codes and their descriptions: A2 - Risk of explosion by shock, friction, fire or other sources of ignition; B1 - May become highly flammable or may initiate a fire, especially if other combustible materials are present; C - Exothermic reaction. May generate heat and/or cause pressurization; D5 - Combination liberates combustion-enhancing gas (e.g., oxygen). May cause pressurization; G - Reaction may be intense or violent.

Worksheet	New Search	Search Results	Export to Excel	Print Chart	Help
Reactivity Compatibility Chart	ARSENIC	CALCIUM CHROMATE			
ARSENIC		A2, B1, C, D5, G			
CALCIUM CHROMATE	A2, B1, C, D5, G				

Hazard Summary | Potential Gases | Pot. Gases Documentation | General Documentation

Selected Chemical Combination + CALCIUM CHROMATE
 ARSENIC

A2 - Risk of explosion by shock, friction, fire or other sources of ignition
 B1 - May become highly flammable or may initiate a fire, especially if other combustible materials are present
 C - Exothermic reaction. May generate heat and/or cause pressurization
 D5 - Combination liberates combustion-enhancing gas (e.g., oxygen). May cause pressurization
 G - Reaction may be intense or violent

Figure 4.13: Result from CRW2 Software

Figure 4.13 shows the hazards codes and description as generated by CRHS software. This shows that the CRHS software is producing the same result as the available software in the same field (chemical reactivity). The case studies of this project also want to differentiate between this software (CRHS) with CRW2 software. This case study shows the improvement of this software from the other software to ensure the users get the information required. CRHS software is user-friendly which is easy to learn and use by the users.

The result from the CRW2 software contains all the information including the unused information which can confuse the users to select the important information but the result of CRHS software is only for more useful and important information that the users required. Furthermore, the result of hazard prediction in CRW2 software cannot be save by the users as shown in Figure 4.13, so it is difficult for the users to make the references for future work. Other than that, the CRW2 software cannot generate hazard report as CRHS software, this is one of the improvement that are being integrated in CRHS software to be more efficient.

CHAPTER 5

CONCLUSION

Chemical reactivity hazards pose great danger to humans, environments and properties. There are urgent needs in the industry chemical and process industries to developed mitigation method to prevent incident from occurring. History has reminded us about the devastating effect these hazards can pose such as Seveso in 1976, Bhopal in 1984 and also Toulouse in 2001. This incident not only affects the people back then but the affect can be seen until now.

The objective of developing Chemical Reactivity Hazard System (CRHS) application is to mitigate and prevent such incidents from happening. This application has been develop using Visual Basic programming language with the data base is stored in Microsoft Office Database file. CRHS application provides useful tool to obtain general information of the chemical 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 CRHS application to ensure that we follow the rules when handling the chemicals or substances.

CRHS application also provides the hazards prediction when the chemicals mix with each other. This hazards prediction is important to prevent the users from misidentifying the chemicals hazards.