Analytica Lab (Version 1.0.0.0 - Qualitative Analysis) Model Summary

Qualitative analysis of cations determines the existence of particular cations of an unknown sample. Being one of the two major branches of chemical analysis, it is included in high school and first year university syllabuses where students gain principles of qualitative analysis and practically apply them. However in the case of practical applications, students are given the opportunity of carrying out experiments only related to more common metal ions in the laboratory. This is due to the limited resources and time available for practical classes. Moreover, the experiments release a large amount of various chemicals in to the environment. Despite these limitations, the students must be given an opportunity to apply theoretical principles in practical problems as the practice makes the theory more understandable. Therefore, it is essential to find a solution which lines up with both above mentioned difficulties and students' need.

Analytica Lab is a software solution which allows students to carry out cation analysis experiments as if they were carried out in a real laboratory. The program provides a virtual sample of several unknown cations, reagents and instruments in a virtual environment. Students can add reagents and perform operations on the sample. Upon these actions, the program simulates the changes of physical properties of the sample (eg. color of the sample, changes in the physical state of the sample and etc.). The students can observe the changes and understand the underlying mechanisms/reactions, hence identify the cations presenting in the sample.

The unknown samples of Analytica Lab may contain a mixture of the following cations.

Ag^{+}, Hg_2^{2+}, Pb^{2+}, Hg^{2+}, Bi^{3+}, Cu^{2+}, Sn^{2+}, Sn^{4+}, Zn^{2+},Fe^{2+}, Fe^{3+}, Ni^{2+}, Cr^{3+}, Al^{3+}, Ca^{2+}, Sr^{2+}, Ba^{2+}

The work bench contains following reagents.

- Aqueous ammonia ($NH_{3(aq)}$)
- Sodium hydroxide (NaOH)
- Hydrochloric acid (HCl)
- Hydrogen sulfide (H_2S)
- Water (H_2O)
- Sulfuric acid (H_2SO_4)
- Ammonium carbonate (NH_4CO_3)
- Potassium chromate (K_2CrO_4)
- Sodium oxalate (NaC_2O_4)
- Hydrogen peroxide (H_2O_2)
- Ammonium thiocyanate (NH_4CN)
- Potassium ferrocyanide ($K_4[Fe(CN)_6]$)
- Potassium ferricyanide ($K_3[Fe(CN)_6]$)
- Potassium thiocyanate (KSCN)

- Sodium monohydrogen phosphate (Na_2HPO_4)
- Magnesium hydroxide ($Mg(OH)_2$)
- Dimethylglyoxime ($CH_3CNOH)_2$

The work bench also contains a centrifuge machine, bunson burner and all the other equipments on a regular work bench in a laboratory.

Technical summary of the program

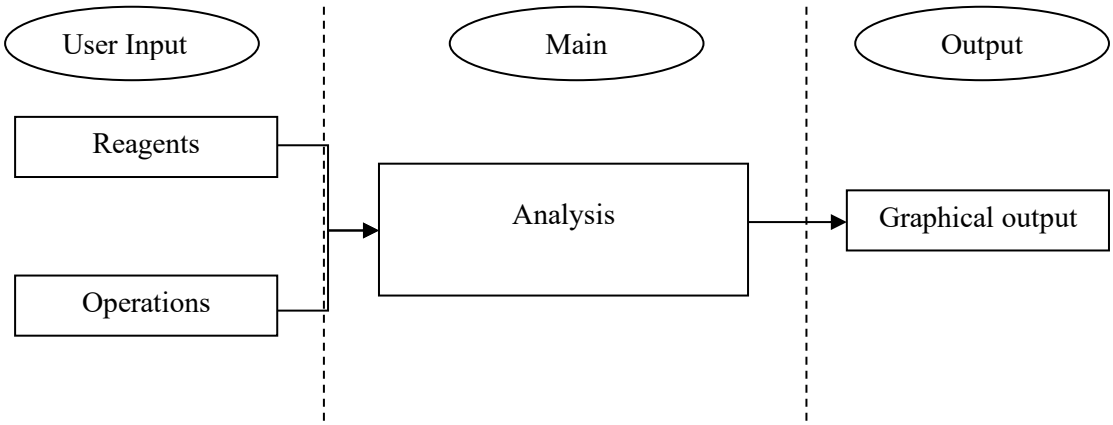

Figure 1: Summary diagram of Analytica Lab

User Input

The user input of Analytica Lab consists of two types; addition of reagents & operations on a sample. The user can add any of the reagents mentioned above. Operations include sub sampling; obtaining a portion from the major sample for the analysis, centrifuging, separation and flame test.

Main Model

The main model of Analytica Lab consists of a Sql Server database and relevant procedures for the analysis. This database consists of physical properties of cations and compounds which are likely to be formed as reagents are added. It contains two data tables known as "Chemical_Compunds" & "Physical_Properties". The structures of the two tables are as follows.

Table 1: Structure of "Chemical_Compounds" data table

compound	reagent_1	reagent_2	-----	-----	reagent_n	operation_1	----	-----	operation_n

Table 2: Structure of "Physical_Properties" data table

compound	state	color	comments

The elements in the compound column in Table 1 are cations and chemical compounds. The table stores data of what compounds are formed upon addition of a reagent or performing an operation. Table 2 stores some physical properties of each compound presenting in the Table 1.

When the user performs an action (eg: addition of a reagent), the code search for possible compounds in the first table (Table 1) and obtains relevant physical properties from the second table. The summary of procedures of the main model can be summarized as follows.

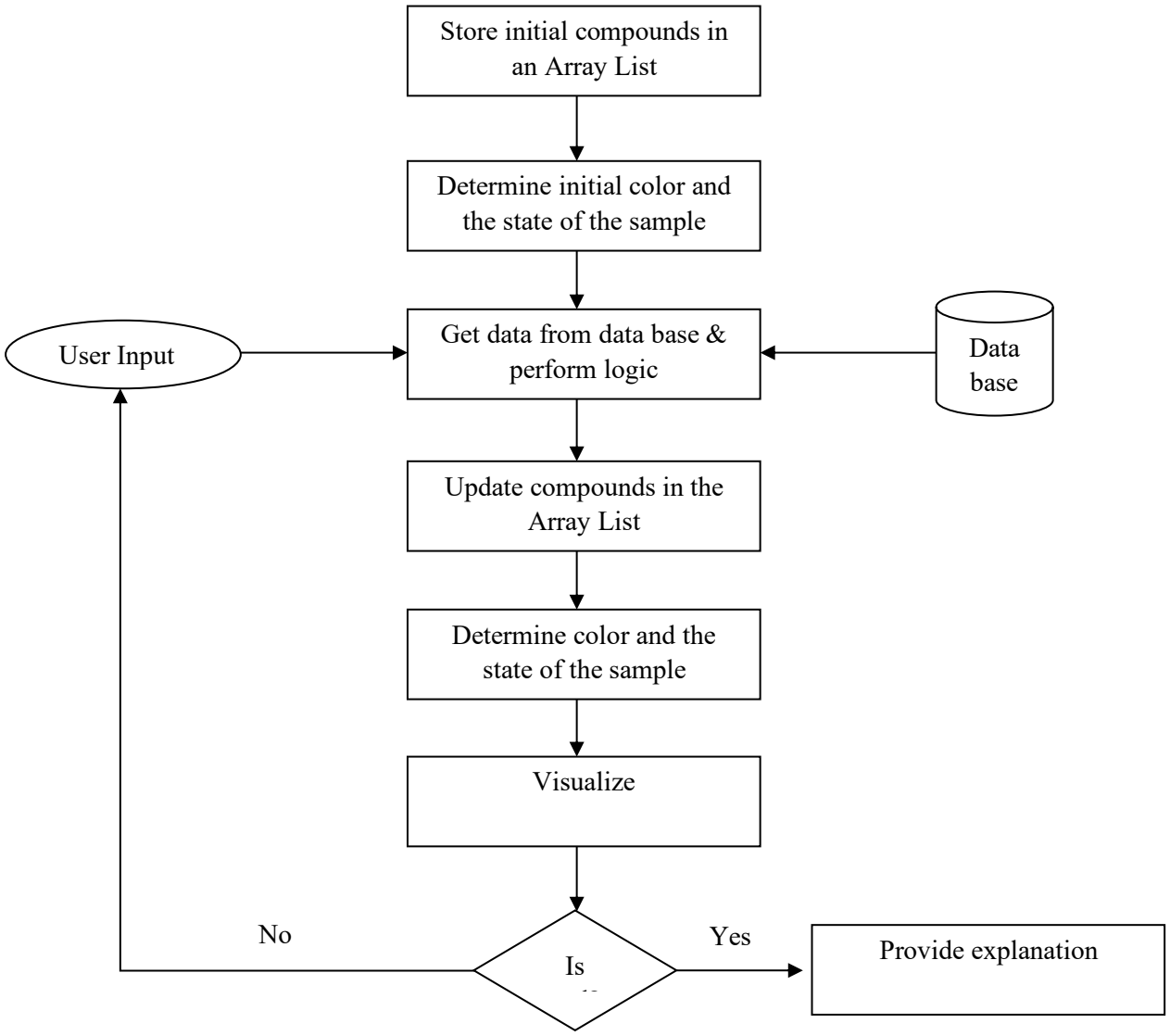

Figure 2: Summary of the Main Model of Analytica Lab

Analytica Lab provides a graphical output of the sample at the end of each user operation and after the program has determined the color and the state of the sample. Also, the changes are displayed in text so that it is convenient for the user to realize the nature of the sample. When the user has finished analyzing the sample or the sample has become wasted, the analysis ends. If requested by the user, the program provides a detailed explanation of the reactions took place at each user operation.