Chemical Reactivity Analysis in the PEAC-WMD application

This month we?ll visit the **Chemical Reactivity Analysis** feature and how it is implemented in the PEAC-WMD v5 application.
To give the reader a little background, we have the opportunity to visit with a number of fire service and HAZMAT responders as we attend workshops and conferences around the country. One of the questions that came out from those encounters was ?can you tell me what happens if a certain chemical comes in contact with another chemical?? Obviously this is a problem that arises for many folks dealing with chemical spills and as a corollary to Murphy Law would predict, ?if an ugly accident is going to happen, why not involve more than one chemical??
Some chemicals are pretty nasty all by themselves and others aren?t that bad and we just need to be sure we mitigate the spill and prevent them escaping to the environment. But then we have these situations where more than one chemical is involved and the combination of two or more chemicals can lead to problems beyond what any one of the single chemicals would have presented.
The EPA and NOAA have developed a methodology that has attacked this problem and it provides a reasonable answer to the question of how do the chemicals react and what can be expected. The application or tool is referred to as the Chemical Reactivity Worksheet (http://www.epa.gov/OEM/cameo/react.htm) and can be downloaded for free from the web site.

The EPA/NOAA application is based on initial work that the California Department of Health Services[1] undertook a number of years ago to develop the original data and approach to assessing the reactivity of chemicals. The EPA/NOAA group (Office of Response and Restoration, National Ocean Service, National Oceanic and Atmospheric Administration) headed by Dr. James Farr, have added additional information, refined the data, and approach, the results of which are now displayed in the PEAC-WMD application.

The description of the methodology, its limitations and precautions related to using this feature are adapted from the description provided by EPA/NOAA on their CAMEO web site and an earlier FEMA, DOT and EPA publication[2] that described the California Department of Health Services approach.

The theory behind the **Chemical Reactivity Analysis** is the fact that there are literally tens of thousands of known chemicals used in daily commerce, and since the consequences of only a small fraction of the possible combinations of these materials have been reported in the general literature, none of these information sources can claim (and none do) that combinations of unlisted materials will not produce a hazardous reaction. Thus, although these information sources provide valuable guideposts for evaluating potential chemical compatibility hazards, they are inherently limited in scope, and

cannot always be relied upon to provide the user with desired and/or necessary information.

The initial project undertaken by Hatayama et al. was to provide a user with a ***general*** indication of the ***typical*** effects of mixing a material from one chemical ***family*** with a material from another ***family***. By focusing on the most common families of chemicals, i.e., materials with generally similar molecular structure, and by studying the effects of combining the most reactive chemicals in each family, the researchers were able to produce a relationship that provides an excellent tool to screen lists of chemicals (as might be found at a facility or in a transportation vehicle) for those which may pose an unusual and/or dangerous threat when inadvertently combined (as might occur during some sort of process upset, transportation accident, or mismanaged material transfer operation).

The PEAC-WMD **Chemical Reactivity Analysis** feature will allow the user to choose multiple (two or more) chemicals for analysis, but it will display the potential reactions between only **two** chemicals at a time. There is no ability to assess how a third or additional chemicals when mixed may effect the reactions between the two chemicals being assessed.

Some chemicals, because of their molecular structure, may fall into more than one chemical family. In these cases the **Chemical Reactivity Analysis** will assess the potential reactions for each family against the chemical family(ies) to which the other chemical belongs. We?ll show an example in describing how the feature displays information.

The user should also understand that not all chemicals in the PEAC-WMD database have been assigned a chemical family(ies). If the **Chemical Reactivity** icon [] is not displayed on the screen when an entry in the **List Box** is highlighted, then the material has not yet been assigned a family and cannot currently be added to the **Chemical Reactivity Analysis List**.

The user should also understand that when two chemicals are assessed, there is a potential for multiple results or products from the interaction, meaning there may be more than one result or product. Likewise, there may be no potential reactions predicted from the mixing of two chemicals. If that occurs, the **Chemical Reactivity Analysis** will indicate no potential reactions are expected.

It is **very important** that users of the **Chemical Reactivity Analysis** read and understand the following words of caution before using this feature of the

PEAC-WMD system. These words of caution are adapted from the ?Handbook of Chemical Hazard Analysis Procedures? (referenced above) that provided one of the first public implementations of the Hatayama, et al. developed approach.

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USE CAUTION WHEN USING THE CHEMICAL REACTIVITY ANALYSIS

The **Chemical Reactivity Analysis** is intended to provide an indication of ***some*** of the hazards that can be expected upon mixing of chemical substances. Because of the differing activities of the thousands of compounds that may be encountered, it is ***not possible*** to make any analysis definitive and all-inclusive. It cannot be assumed that members of chemical families not listed in the analysis will be compatible with each other or with listed families. Although the analysis generally will indicated when there is no hazardous incompatibility expected between the families being considered, it cannot be guaranteed that this will always be the case. ***Detailed instructions as to the hazards involved in handling and/or disposing of any given substance should be obtained from the originator of the material or other expert source of information.***

The potential reaction consequences predicted by the analysis are based on pure chemical reactions only at ambient temperature and pressure. Concentration, synergistic, and antagonistic effects have been assumed not to influence the reactions. The reactions have not been validated on actual materials containing individual chemicals.

To the above caution must be added the observation that the analysis is ***solely*** applicable to the combination of ***two*** materials from different families. The addition of one or more other materials to a mixture may (or may not) produce substantially different hazards. The analysis should not be used in any attempt to identify materials that may be self-reactive, i.e., capable of runaway exothermic polymerization, runaway exothermic decomposition, explosion, or other hazardous activity upon simple heating or exposure to air.

How the Chemical Reactivity Analysis works

When the PEAC-WMD application is initially started, the **Chemical Reactivity Analysis List** is empty by default. Once an entry has been selected, either by clicking on the **Chemical Reactivity** icon [] or selecting **Tools|Add to Reactivity List** from the pull down menu (see Figure 1), a dynamic list is created within the PEAC-WMD application that contains the selected entries.
The **Chemical Reactivity Analysis List** can be viewed by clicking on the **Lookup By** pull-down list and selecting **Reactivity Chemicals** from the list, see Figure 2.
Once the user has selected **Reactivity Chemicals**, the **List Box** will display the names of those entries selected for the **Chemical Reactivity Analysis List**, see Figure 2.

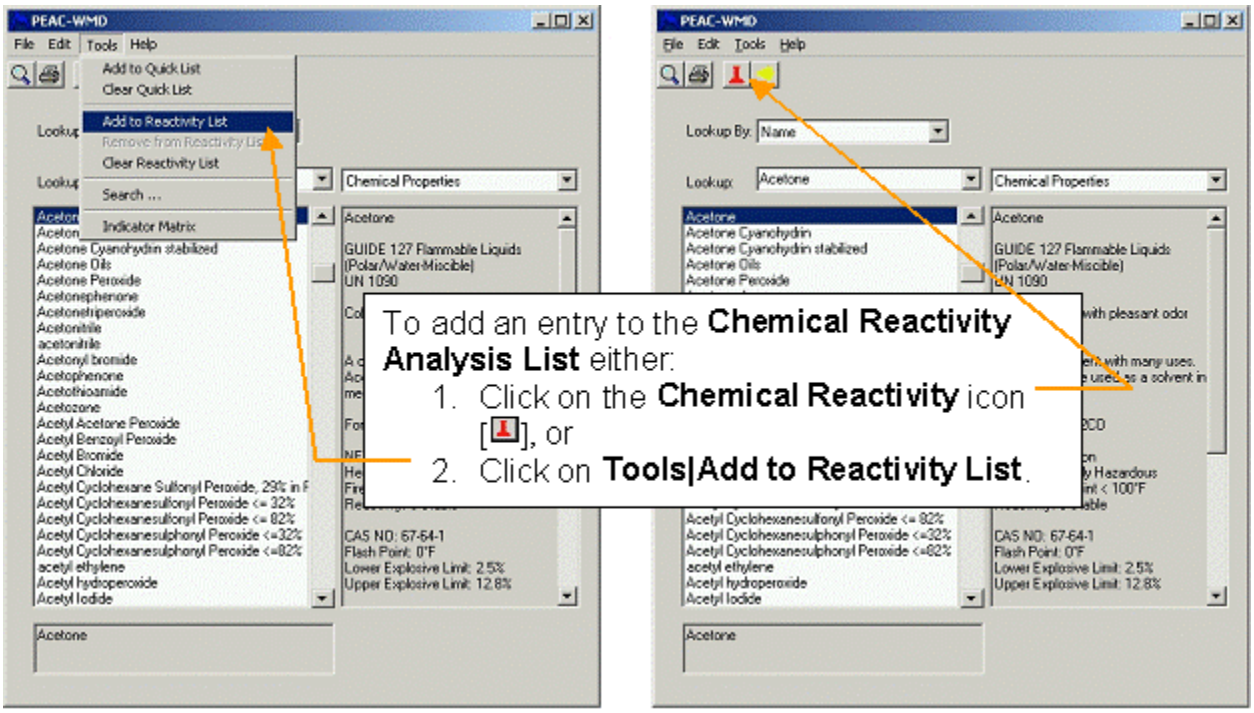

Figure 1 ? Adding to the Chemical Reactivity Analysis List

If the user elects to remove an entry from the **Chemical Reactivity Analysis List**, highlighting the entry in the **List Box** can do this and then clicking on the **Remove Chemical Reactivity** icon [] at the top left of the screen, or click on **Tools|Remove from Reactivity List**, see Figure 2.

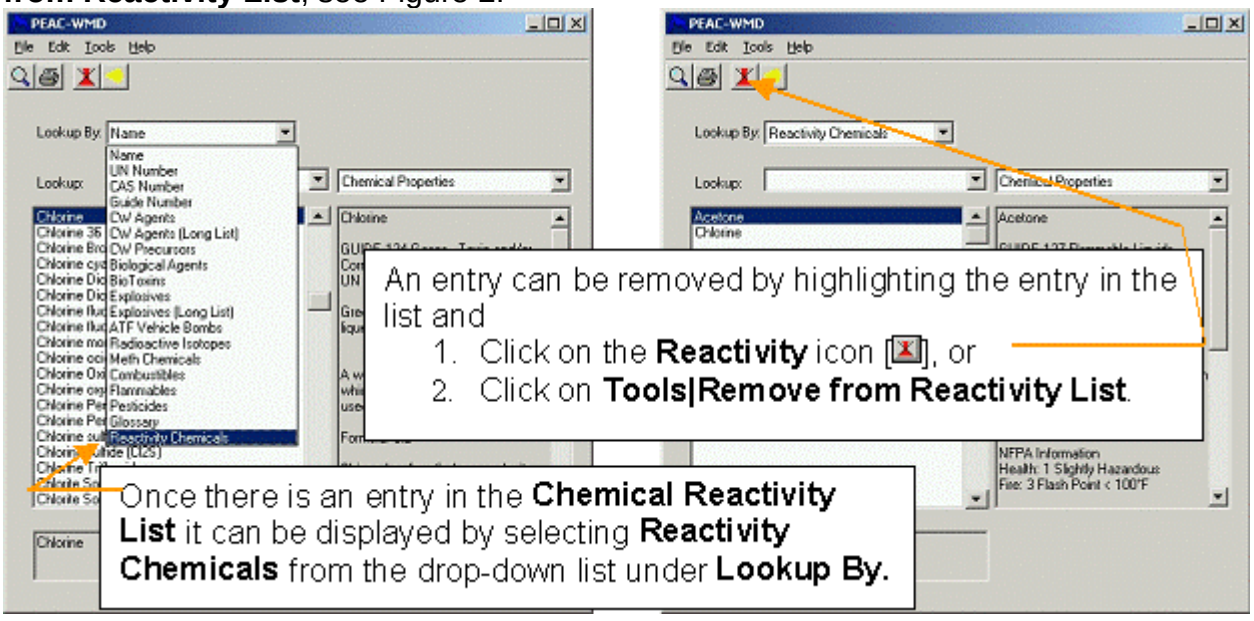

Figure 2 ? Displaying the Reactivity Chemical List and Removing Entries from the List

All the databases of information on each of the chemicals is accessible from the screen as before, CPC, recommended respirators, synonyms and ERG information, even accessing a **PAD Calculator** or accessing the **Explosion Calculator** are available. **Before displaying and assessing the potential reactions that may occur with another chemical, it is <u>important</u> to review two pieces of information related to the individual chemicals selected:** (1) information specific to the hazardous material selected, and (2) the general information related to the **Chemical Family(ies)** the hazardous material fits into. Both of these pieces of information are located in the **Reactivity Information** selection, which can be selected as shown in Figure 3. The first portion of the **Reactivity Information** display is shown in Figure 4, and relates to specific information on the selected hazardous material.

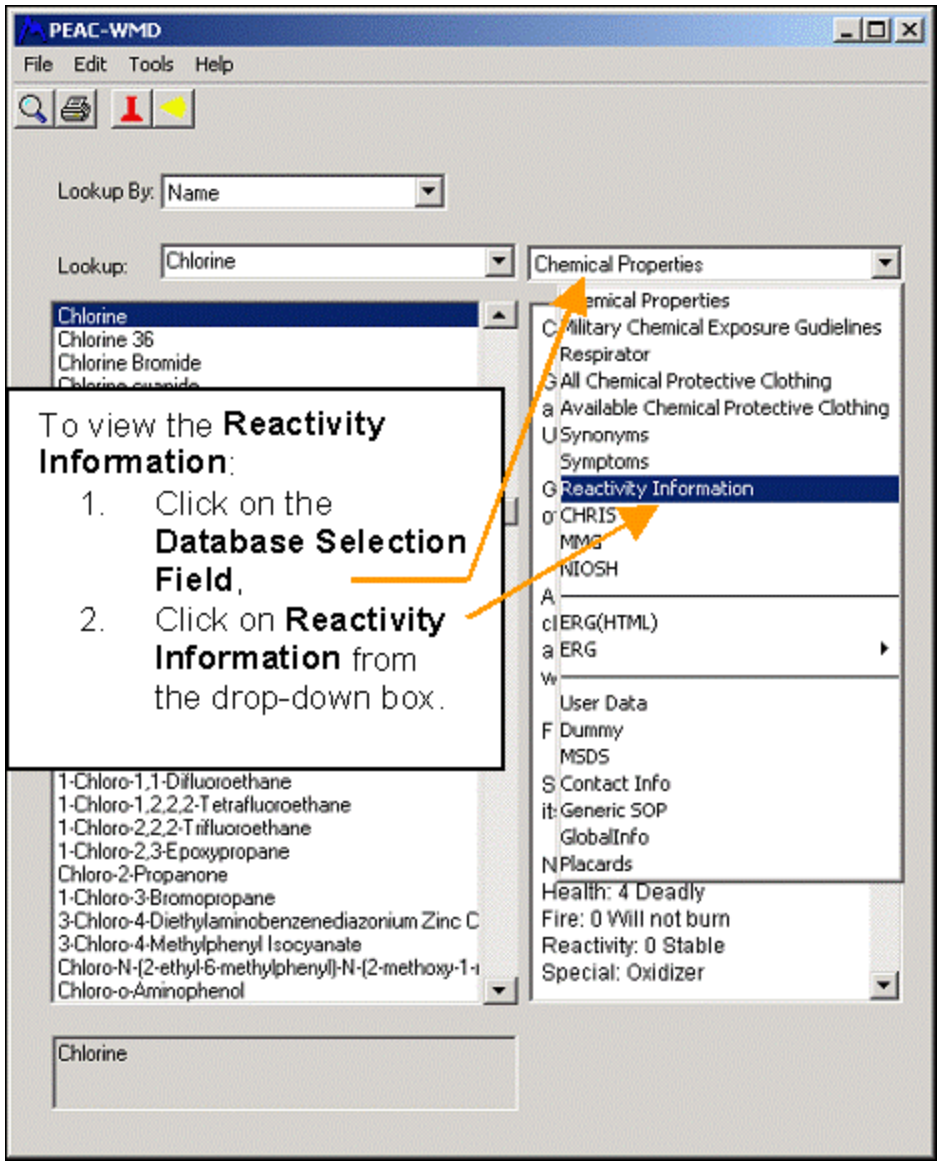

Figure 3 ? Selecting Reactivity Information

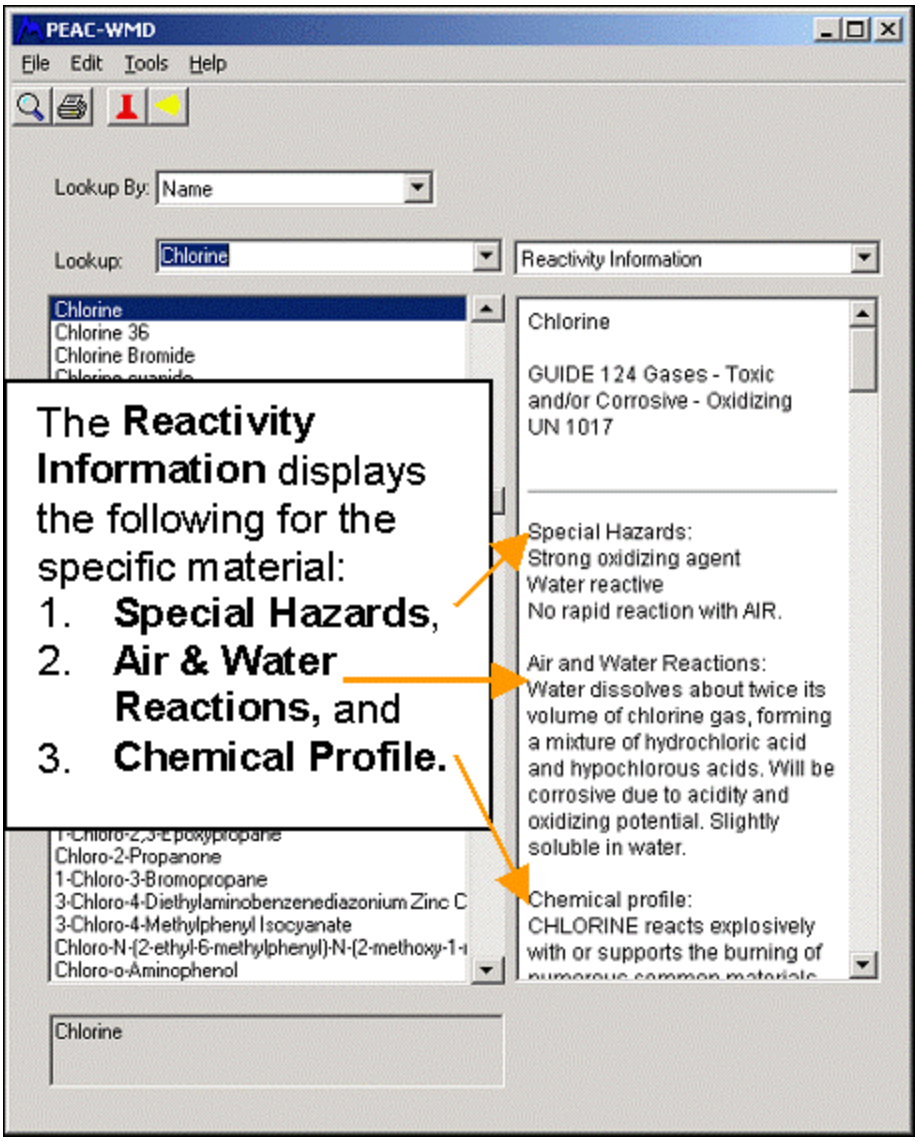

Figure 4 ? First portion of the Reactivity Information is specific to the material

Since air and water are the two most common chemical reactants that a material may come in contact with during an incident, it is important to review what these reactions might be. The first information displayed is the **Special Hazards** associated with this hazardous material. This information is broken into three portions:

1. Special Hazards - which can be none or one or more of the following seven different listings (Highly flammable, Explosive, Polymerizable, Strong oxidizing agent, Strong reducing agent, Peroxidizable compound, or Radioactive material),
2. Either Water reactive or No rapid reaction with water, and
3. Either Air reactive or No rapid reaction with air.

This information provides the user some immediately important information about the **Chemical Family** the selected hazardous material belongs to.

Immediately after the **Special Hazards** are displayed the **Air and Water Reactions**, which are specific for the hazardous material selected.
The next item to be reviewed is the possible reactions for the material selected, which are listed under the **Chemical Profile** header. These first three portions of the **Reactivity Information** database for the hazardous material Chlorine are shown in Figure 4.
Remember ? a specific hazardous material may fall into more than one **Chemical Family** or **Reaction Group**; therefore there may be more than one set of generic information displays regarding the hazardous material to review. To illustrate this fact, using our example of Chlorine as the hazardous material, it falls into two **Chemical Families** or **Reaction Groups**: (1) Inorganic Oxidizing Agents and (2) Strong Halogenating Agents. This is shown in Figure 5, where the **Reactivity Information** database display has been scrolled down below the **Chemical Profile** information for Chlorine to display information for Inorganic Oxidizing Acids. Figure 6, provides an example of the **Reactivity Information** database display for Strong Halogenating Agents which is below the Inorganic Oxidizing Agents information for Chlorine.

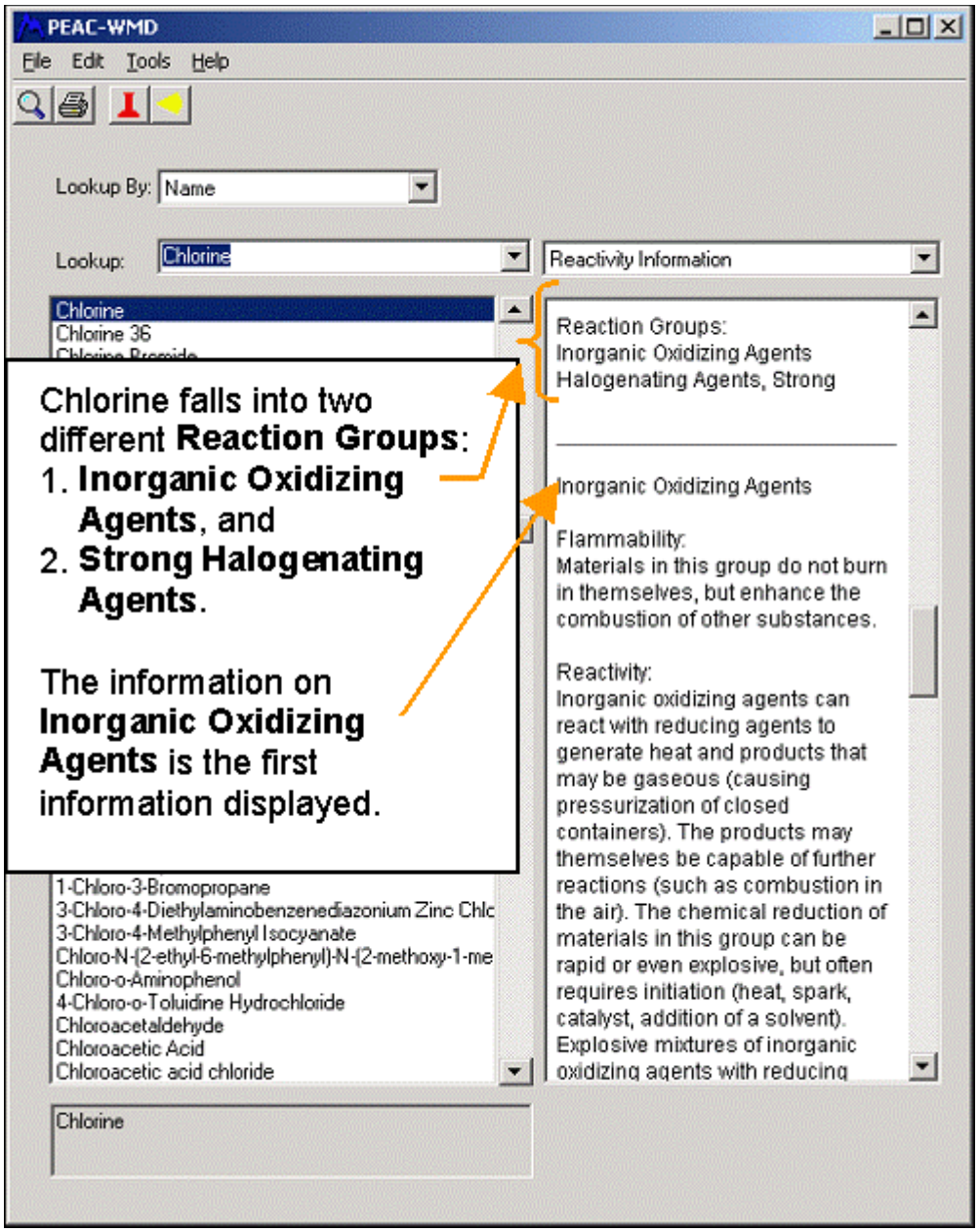

Figure 5 ? Generic information for Inorganic Oxidizing Agents

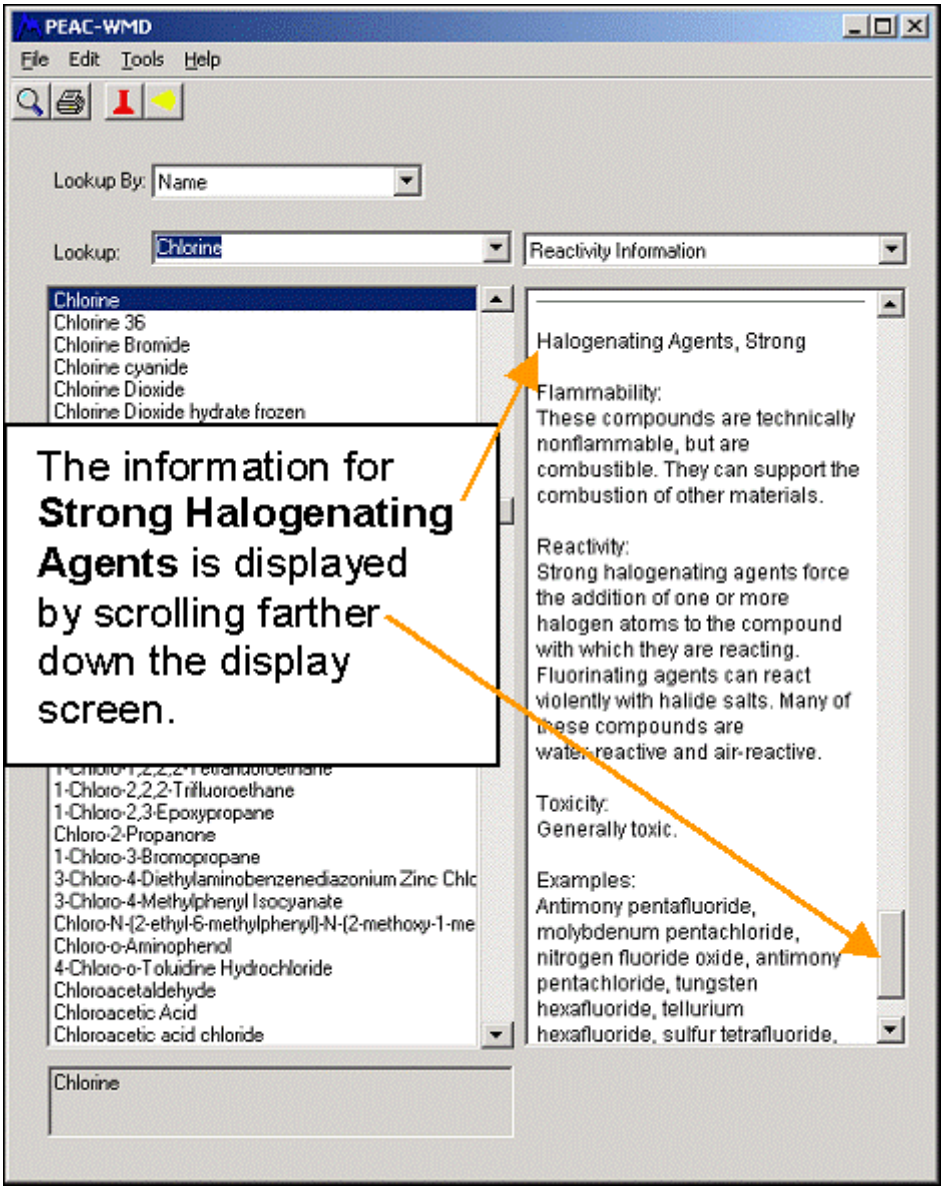

Figure 6 ? Generic information for Strong Halogenating Agents

To demonstrate the feature of assessing chemical reactivity the following materials are selected, Acetone and Bromine. These are selected as shown earlier in Figure 1, by highlighting each material and clicking on the **Reactivity** icon [] to add them to the **Chemical Reactivity Analysis List**. Before accessing the reactivity information related to these two chemicals, the user should review the **Reactivity Information** as described in Figure 3 and 4. To display the potential reactions of Acetone and Bromine, the user should select **Reactivity Chemicals** as shown in Figure 7. The dynamic **Chemical Reactivity Analysis List** is displayed and the user can access the **Reactions** information using the earlier described EPA/NOAA approach by clicking on the **Database Selection Field** and selecting **Reactions** from the drop-down list as shown in Figure 8

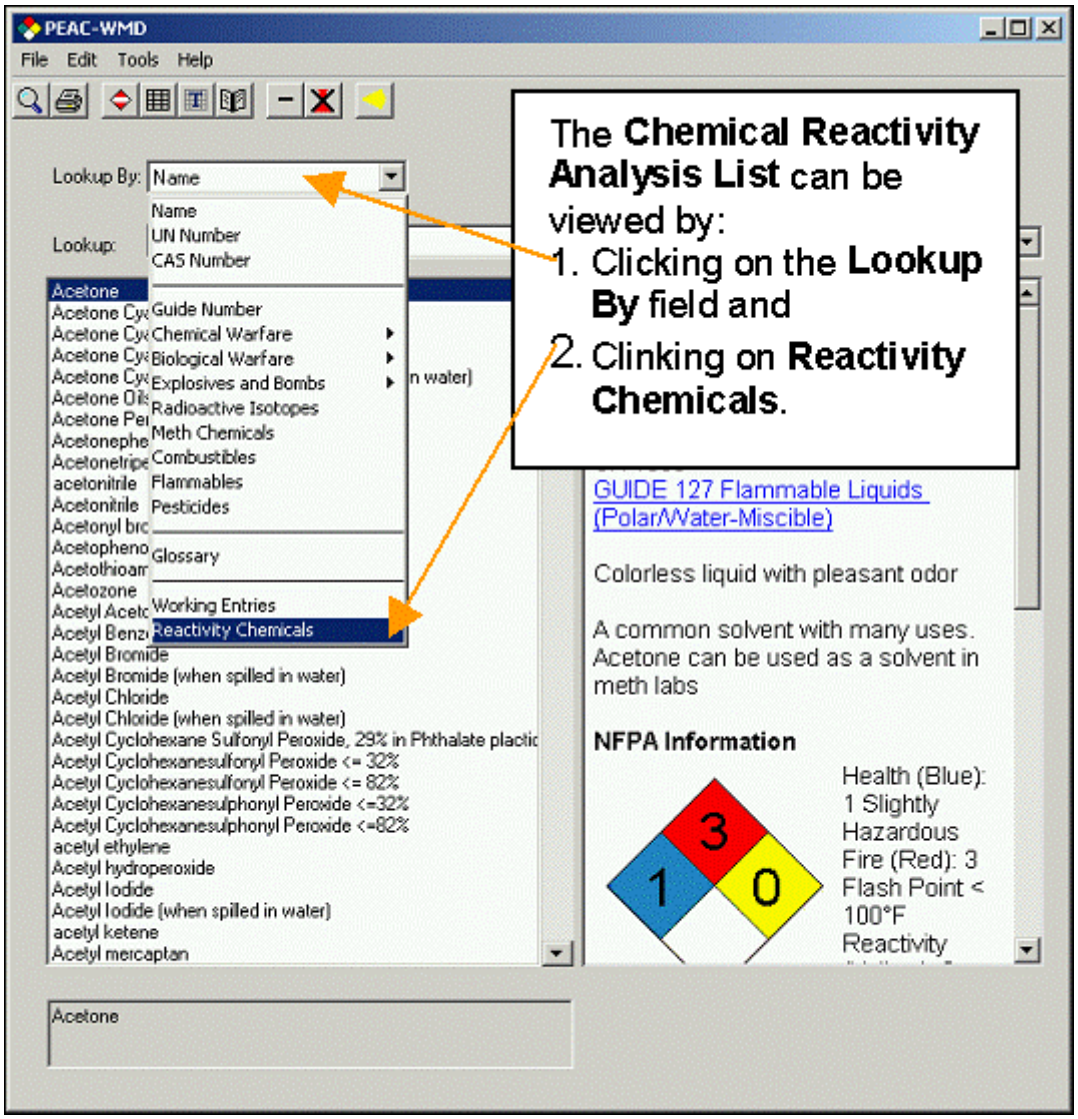

Figure 7 ? Selecting the Chemical Reactivity Analysis List

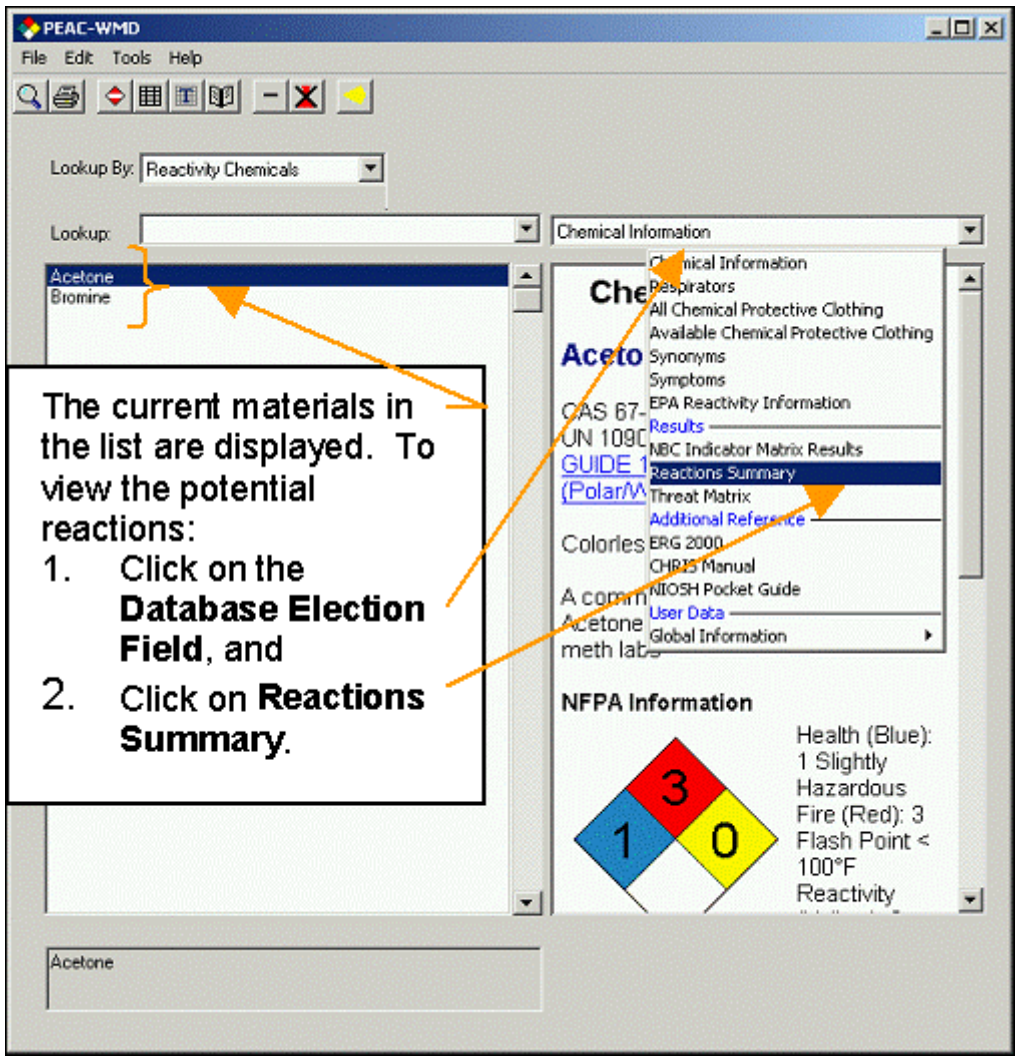

Figure 8 ? Accessing the Reactions information

The **Reactions Summary** display, as shown in Figure 9 displays the following information:

1. A list of what entries are being assessed (maximum of 5 entries are allowed).
2. A summary of all potential reactions is provided. Depending on the number of materials selected and the individual materials selected to be included in the **Chemical Reactivity Analysis** there may be none or multiple potential reactions that can occur. This summary provides a listing of all potential reactions between all the possible combinations of materials that were selected for the **Chemical Reactivity Analysis List.**

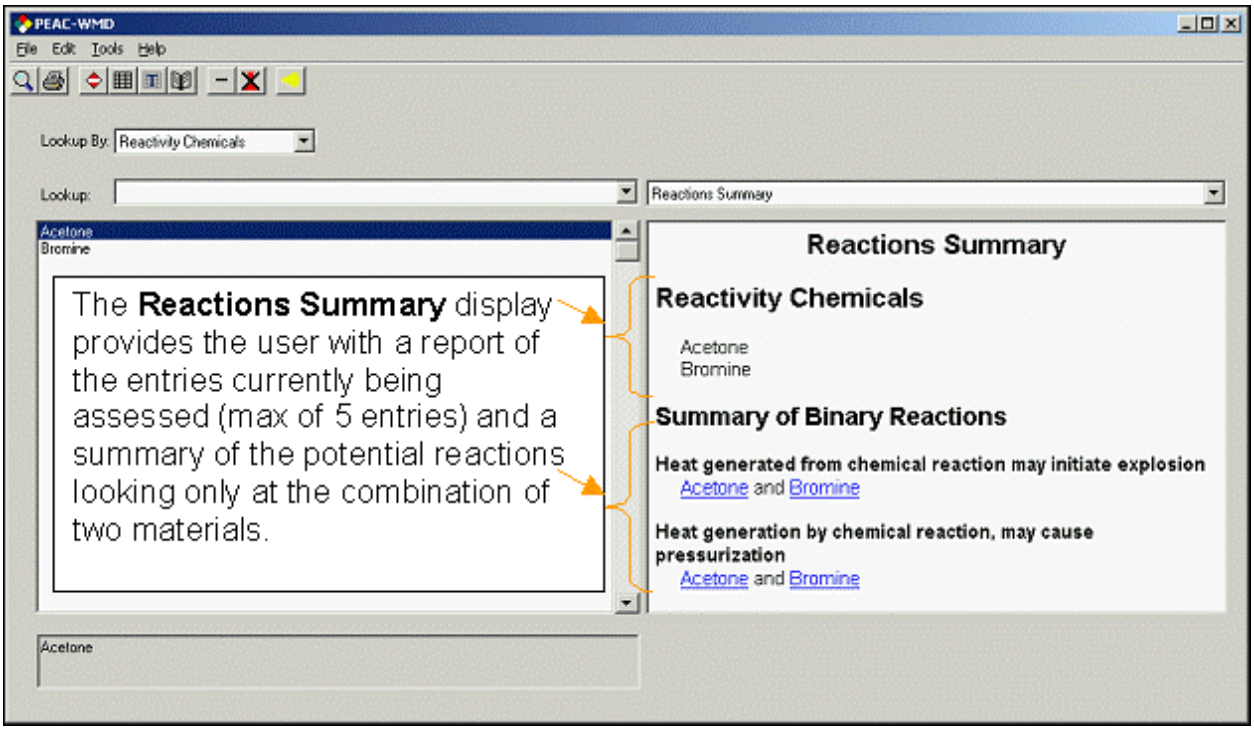

Figure 9 ? Displaying the potential reactions that may occur

To demonstrate an example where no predicted reactions are expected, Figure 10 is the **Reactions** analysis screen for Acetone and Ethanol mixing.

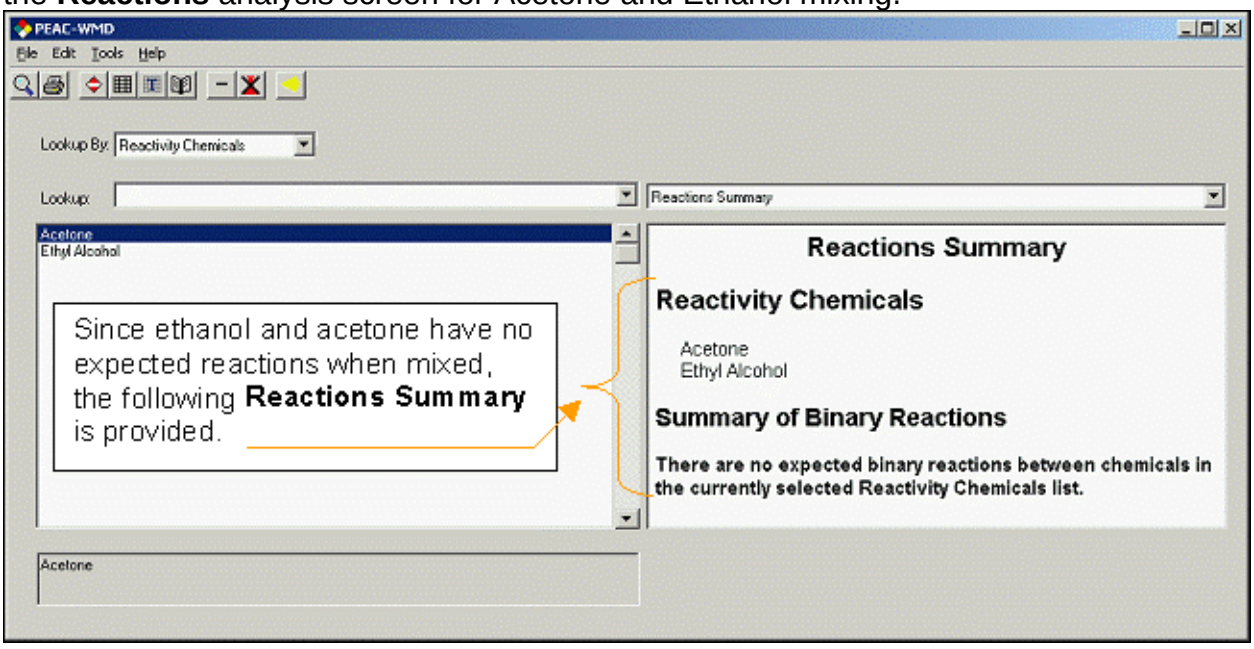

Figure 10 ? Example of materials that are not expected to have reactions

If our newsletter readers, whether a customer or not, have specific questions related to this topic or other topics, please contact AristaTek via our toll free number (877-912-2200) or email us at support@aristatek.com and we?ll work to answer your questions.

[1] Hatayama, H.K., Chen, J.J., de Vera, E.R., Stephens, R., and Storm, D.L., *A Method of Determining the Compatibility of Hazardous Wastes*, EPA Report No. EPA-600/2-8-076, April 1980.

[2] *Handbook of Chemical Hazard Analysis Procedures, Appendix D,* 1989, FEMA (Federal Emergency Management Agency), US DOT (Department of Transportation), and US EPA (Environmental Protection Agency).