CRW v 4.0.2 – Update (*Release Date*)

The fourth generation of the Chemical Reactivity Worksheet (CRW) was released for public distribution in March of 2016. Download statistics indicate wide global interest and usage with very few problems being reported.

Recently, it was discovered that, for a few reactive group combinations, the CRW did not accurately predict potential hazardous reactions. Upon notification of this, a thorough review of all reactive group combination hazard predictions was conducted.

This update contains the following modifications:

1. Revised hazard predictions for the reactive groups in question
2. Updated default chemical database (CAMEO chemicals)
3. Updated Excel macro for converting CRW compatibility chart data into an Excel file format.
4. Refinements to the Custom Chemical entry module.
5. Fixed MacOS CRW4 application launch problem.
6. Corrected a programming error that predicted one or more potential hazards for a chemical mixed with itself. The CRW continues to indicate which chemicals and reactive groups can be self-reactive.

Details for each of these modifications are listed below:

1) There were 17 chemicals in the chemical database whose reactive group assignments were thought to be inconsistent with the possible predicted hazards in combination with other chemicals. In each of the 17 cases, the assigned reactive group "Reducing Agents, Mild" (Group #50) was changed to "Reducing Agents, Strong" (Group #45). By placing these records into Group 50 allowed certain known hazards to not be predicted by the CRW. A full listing of the edits can be found below. (pdf doc).

1a) The CRW Team also reviewed and made edits to the some potential gas predictions. Making the gases listed for any combination of reactive groups more consistent and complete. Users need to bear in mind that the list of gases are potential depending on the individual compounds users may mix together i.e. for Acids Oxidizing - for Sulfuric Acid you get SOx , while Nitric Acid yields NOx gases. There is a pdf file listing the 456 reactive group pairs whose gas hazard predictions were reviewed (and in some cases edited).

2) The CRW uses NOAA's CAMEO chemical database for its default chemical library. As such, an attempt is made to keep the CRW chemical information as current as possible. Included in this update is NOAA's current version of the CAMEO chemical database.

3) Some CRW users have a need to move chemical mixture compatibility charts into a Microsoft Excel environment. To accommodate this need, an Excel macro file that facilitates this process is included in the CRW4 installer package. It was recently reported that the included file does not work when using Excel 2013. A corrected macro (compatible with previous and current versions of Excel) is included in this update.

4) In order for the CRW to understand and properly manage custom chemical information added by CRW users, the program uses characters such as carriage returns to detect and incorporate custom chemical names and synonyms. Errant entry of such characters can adversely affect the successful synthesis of compatibility charts for mixtures where custom chemicals are included. Additional "traps" and safeguards have been implemented in this update to prevent and/or detect the presence of such errant characters.

5) Some MacOS users have reported the failure of the CRW4 application to launch when the CRW4 application icon is double-clicked on. While this problem can be overcome by dragging-and-dropping the CRW4.cr4 data file icon onto the CRW4 application icon, a fix for this problem is included in this update.

6) Most chemicals and reactive groups are stable and do not present a reactive hazard when the chemical is pure or a given reactive group is homogeneous. As such, the "diagonal" gray line of cells indicates chemical/reactive group stability. The CRW does consider three reactive groups to be potentially self-reactive. They are:

- Acrylates and Acrylic Acids
- Conjugated Dienes
- Polymerizable Compounds

For any chemical associated with one or more of these reactive groups, or for any of these three reactive groups, the CRW will present a "SR" (self-reactive) designation on the Compatibility Chart "diagonal" that lists these chemicals and/or reactive groups. This distinction is illustrated in the default "Reactive Group Matrix" mixture included in the CRW tool.