CRW 2.0: A Representative-Compound Approach to Functionality-Based Prediction of Reactive Chemical Hazards

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The NOAA Chemical Reactivity Worksheet (CRW) has provided a user-friendly yet powerful method of qualitatively predicting reactive chemical hazards since its introduction in 1998, and has seen use in spill response, storage management, and process safety for intentional chemistry. The CRW predicts reaction hazards based on a database of 6000+ common industrial chemicals, classified by major reactive groups, using 43x43 matrix of organic and inorganic reactive groups, modified from the earlier "EPA Method for Determining the Compatibility of Hazardous Mixtures." CRW output describes the hazards qualitatively; e.g., "Spontaneous ignition of reactants or products due to reaction heat," or "Combination liberates non-flammable, non-toxic gas. May cause pressurization." The CRW also provides summaries of properties and special hazards for many of the compounds in the database.

CAMEO Chemicals, a new web-based database, includes an extensive overhaul (Version 2.0) of the CRW. Earlier versions of the CRW had a limited set of references and limited information about specific reactions, and this information could only be found in each compound's profile, increasing search time for assessing reaction specifics, and providing little information that could be used to mitigate the chance of false-positives—the CRW is designed to be conservative in its predictions, and will indicate an incompatibility even if only a few reactions are found between two functional groups. Version 2.0 improves the database based on an extensive literature survey of potentially hazardous reactions for representative members of all 43 listed functional groups, with primary literature references available for many of the hazards predicted, and many errors and omissions corrected. This paper describes the methodology for the literature search, rationale for changes to the operation of the database, extent of the new documentation, and remaining design limitations of the product.

Introduction

Since 1998, the NOAA Chemical Reactivity Worksheet[1] (CRW) has provided an easy-to-use method of predicting incompatibilities due to inadvertent mixing of common chemicals, and hazardous reactions of industrial chemicals, providing information on the interactions of over 6,000 common industrial compounds and mixtures. It has found applications in prediction of storage compatibility, intentional chemistry/process safety, and response to hazardous chemical release incidents. It has been implemented both as a stand-alone product, and as a part of the CAMEO suite of emergency response and planning software.

The CRW bases its reactivity predictions on a two-dimensional matrix containing 43 different organic and inorganic reactive groups, a classification for inorganic compounds which are not described by any of the other groups, nine special hazards (e.g. polymerization, explosive, water-reactive, etc.), a non-reactive classification, and an unknown classification. The special hazards are based on a set of special hazards developed for the EPA Method for Determining the Compatibility of Hazardous Mixtures[2] (EPA Table), although additional hazards such as air-reactive and peroxidization have been added; these groups are intended to inform the user when a compound has particularly high intrinsic reactivity. The “unknown” group is intended to list when a compound cannot be classified using the stated reactive groups, since insufficient classification information is provided in a particular mixture’s Department of Transportation (DOT) records, or where composition of a mixture may vary. Compounds are assigned to one or more reactive groups based on chemical structure and functionality, and binary pairs of individual functional groups are used to determine reaction hazards[1]. Such an approach provides first-order predictions without having to determine hazards for every pair of materials in the database. Determination of hazards for every pair would require up to 18 million

individual entries, many of which have little or no available reactivity information. Additionally, extensive reworking of the product would be needed each time a new compound were added.

While the reactive-group based approach can provide useful predictions with negligible computational cost, earlier versions of the CRW provided insufficient documentation about how a pair of functional groups was determined to be incompatible. Some literature citations could be found under each compound's "Chemical Profile," a section of a compound's entry about properties and special hazards[1], but there was no direct access to citations from the reactive hazard report generated by the CRW, and no cross-referencing between compounds, increasing difficulty of accessing the documentation.

The new CRW (Version 2.0), available through NOAA's new CAMEO Chemicals web portal[3], addresses the documentation issue by providing literature citations for hazardous reactions of representative compounds for each reactive group, arranged as hazard statements for each binary pair of groups. These extended hazard statements are now available for the majority of binary pairs and provide guidance to users in interpreting the CRW's predictions.

Representative Compounds Approach

The 43 functional groups selected for the CRW are intended to cover a wide range of both organic and inorganic reactions to maximize the scope and accuracy of the CRW's predictions. Many representative industrial compounds can be found for each group. However, those compounds can produce different degrees of hazards due to factors beyond the target functional group. The process below describes how representative compounds were chosen for the literature search used to overhaul the CRW's predictive matrix.

Compounds within each group can have varying lengths of hydrocarbon chains, amounts of branching or cyclization, degrees of substitution, levels of conjugation for unsaturated

compounds, or counter-ions for salts. These structural differences can affect kinetic behavior at reaction centers, making generalization of hazards or lack of hazards to an entire reactive group non-trivial. Some of these structural differences, such as primary, secondary, and tertiary alcohols and amines, may warrant further study of kinetic effects, and possible revision of the reactive groups.

Classification is further complicated by many common industrial compounds possessing multiple functionalities. For example, the CRW classifies acrolein as both an aldehyde and an unsaturated hydrocarbon, and hydroxylamine as both an amine and a strong base[4]. If a compound is multiply classified, the group suspected to contribute most to the compound's reactivity is listed first in that compound's CRW entry.

In order to resolve the multiple-classification dilemma, only mono-functional compounds were chosen as representative for a functional group, since most of the multifunctional compounds in the database are assigned to multiple reactive groups, covering reactions that would occur at those groups. The mono-functional compounds that were chosen possessed varying hydrocarbon chain lengths and degrees of branching for organic molecules, or different counter-ions or substituents. If conjugation or aromaticity would be expected to influence the reactivity of a group, such as with some highly polymerizable aldehydes (acrolein, crotonaldehyde) and nitriles (acrylonitrile), a few representative unsaturated compounds were also chosen for that functional group.

Furthermore, since 1-carbon (C1) organic molecules of certain functionalities (e.g. formic acid, formaldehyde, methanol, and haloforms) have a different oxidization state on the carbon than other molecules with the same functional group, and less steric hindrance, their reactivity may be enhanced. Examples of enhanced reactivity for one-carbon compounds include formic acid's K_a being an order of magnitude larger than acetic acid[5] and the enhanced activity of

methyl substrates in S_N2 reactions[6]. Therefore, since the CRW is intended to predict a worst-case scenario, C1 compounds were always selected as one of the representative compounds for each functional group. The increased reactivity and common industrial use of C1 and C2 compounds made them an ideal starting point for choosing representative compounds, although compounds up to between C4 and C8, or up to four aromatic nuclei for aromatics, were evaluated for each organic functional group, such as the three different butanols for alcohols, hexanes and octanes for alkanes, and cyclohexanone for ketones.

Between 4 and 10 representative compounds were chosen for each functional group, and all reactions of those compounds with any one other compound, under mild conditions, (<373K, <3atm) and without the presence of other compounds to act as catalysts (binary reactions only), were used to revise the CRW's binary compatibility table and to build a new set of documentation for the CRW. Table 1 includes lists of representative compounds for several functional groups.

Table 1: Example representative compounds for four reactive groups

Inorganic Non-Oxidizing Acids	**Aldehydes**	**Alcohols & Polyols**	**Active Metals**
Hydrochloric acid	Formaldehyde	Methanol	Calcium
Hydrobromic acid	Acetaldehyde	Ethanol	Magnesium
Hydrofluoric acid	Acrolein	2-Propanol	Zinc
Phosphoric acid	Crotonaldehyde	n, sec, and t-Butanols	Iron
	Benzaldehyde	Ethylene Glycol	Nickel
		Glycerol	Cobalt
			Titanium
			Aluminum

All reaction predictions assume concentrated solutions, pure solids, or a significant partial pressure of a gas, unless specified otherwise. Highly forcing conditions were excluded from the binary compatibility predictions due to the CRW's focus on response and storage compatibility, although higher temperature and pressure reactions are often listed in compounds'

chemical profiles. However, reactions at nonstandard but relatively mild conditions were included, reflecting the wide range of ambient temperatures present in various locations in the United States, to better reflect hazard conditions in the event of a spill or fire, and to provide an additional safety margin. An example hazard statement can be seen in Figure 1, at the end of the Results section.

Literature Search Methodology

The documentation for CRW 2.0 was based entirely on a survey of available literature; no new laboratory work was conducted to assess reactivity. Most of the sources used are also commonly available, or a more extensive excerpt from the source is commonly available in secondary literature.

Once representative compounds were chosen, a preliminary research phase was conducted using two well-known chemical engineering encyclopedias, the *Kirk-Othmer Encyclopedia of Chemical Technology*[5], and *Ullmann's Encyclopedia of Industrial Chemistry*[7]. Examination of these articles helped determine whether or not sufficient information would be available for a 'representative' compound, and if not, what might be a better compound to choose. The preliminary phase also provided citations for papers that may be useful in analyzing reactivity hazards, which were later used in the specific phase. When specific reactivity information was found in the encyclopedias, it was also recorded for use in the CRW documentation.

The second phase in the documentation research consisted of examination of general sources, including textbooks on organic (*Solomon & Fryhle's Organic* Chemistry[6]*)* and inorganic chemistry *(Mellor's Modern Inorganic Chemistry*[8]), and specific monographs on individual functional groups or chemistry of an element, including Saul Patai's *Chemistry of the*

Functional Groups series[9]. While specific documentation of hazardous reactions was rarely found in these sources, the general survey phase enabled better interpretation of reactive hazards reported in other sources.

Once sufficient background information was available to interpret reports of reactivity incidents, the main source used to compile the hazard documentation was *Bretherick's Handbook of Reactive Chemical Hazards*[10], which contains an extensive, cross-referenced annotated bibliography of literature about hazardous reactions, major accidents in the chemical industry, and laboratory accidents. The less-comprehensive, but still extensive *National Fire Prevention Association Publication 491M*[11], covering hazardous reactions relevant to fire prevention, was also used as a supplemental secondary source for building the hazard statements.

Initially, two other secondary sources common in hazardous materials literature, *Sax's Dangerous Properties of Industrial Materials*[12], and *The Sigma-Aldrich Library of Chemical Safety Data*[13], were examined as sources for hazard documentation, but while valuable as quick-references for safety data, neither of those sources contained sufficient information about conditions under which hazardous reactions occurred nor citations of a primary source. Furthermore, hazard classifications were often broad and difficult to elaborate upon, so use of those two sources rapidly desisted, although some better-supported citations are present in the hazard statements.

The preliminary, secondary-source search was followed by a search of primary sources if the secondary-source information was ambiguous or insufficiently complete. Abstracts of papers obtained through Chemical Abstract Services were the most common verification source, with full-texts of papers examined only if a hazard was still ambiguous or a particular paper seemed probable to have extensive information about additional hazards. Other verification sources

included the *Manufacturing Chemists' Association (MCA) Safety Data Sheets*[14], and the MCA *Case Histories of Accidents in the Chemical Industry*[15].

If verification information was unavailable or a particular reaction was still ambiguous, CRW staff used information of physical and chemical properties of the compounds, from sources such as *The Merck Index*[16], *Hawley's Condensed Chemical Dictionary*[17], *NIST WebBook*[18] and the *CRC Handbook of Chemistry and Physics*[19], and best available chemical judgment to decide how to classify hazards.

Literature Search Results

The representative-compound search significantly increased the amount of available documentation for the CRW. Of 540 binary pairs with at least one hazardous reaction listed, 297 (55 %) now have links to citations for at least one of the hazards, and all of the known hazards for many of the binary pairs have been documented.

Several reactive groups, including oxidizing acids, alcohols, bases, active metals, ethers, and inorganic oxidizing agents, now have a particularly extensive amount of documentation (>80% of known interactions with other CRW reactive groups documented and cited). However, documentation is very limited (<40% documented) for other important reactive groups, including carbamates, cyanides, thiocarbamates, isocyanates, and nitrides/phosphides/silicides/carbides, and somewhat sparse (<60%) for others such as organic sulfides, peroxides, and carboxylic anhydrides, due to a lack of information about specific reactive hazards.

For some of the groups with less documentation, such as nitriles and peroxides, large amounts of general reactivity information was available, but not the specific information needed to assign hazard classes. For other groups, such as carbamates, isocyanates, and organic phosphates, extensive toxicology, synthesis, and environmental fate information is readily

available in the hazardous materials literature, but little documentation of reactive accidents or hazards of the use of those compounds in intentional chemistry could be found. A third set of groups, including organometallics and salts, contain such a wide variety of compounds that drawing general conclusions was difficult.

Another new property of the documentation is a brief description of conditions for many of the reactions. Representative reactions were chosen to be under mild conditions that could be expected in a storage or spill situation, but solvent information was listed, if relevant, for some of the reactions. The temperatures under which a reaction is known to occur are typically listed as ranges (see Table 2), although specific temperatures were used in some hazard statements. Reactions taking place over 373K were not used to determine binary pair hazards, nor were reactions at pressures greater than 3 atm.

Table 2: Temperature Ranges for Classification in CRW Documentation

Classification	Temperature Range
Cryogenic	<173K
Low	173-273K
Ambient	274-308K
Slightly Above Ambient	309-323K
Slightly Elevated	324-343K
Elevated	344-373+ K

While the documentation was intended to remove gaps from previous versions as well as add new information, non-documented hazards from older versions of the CRW were NOT expunged, unless compelling reasons for reclassification or removal were found in the literature. This is because the CRW takes a very conservative approach to reactive hazards, and a documentation check for one of the listed, but currently undocumented hazards would reveal the lack of citations, and allow users to make a decision whether or not to disregard the hazard. An example hazard statement appears below.

Figure 1: Example Binary Combination Hazard Statement

Documented reactions of Inorganic Non-Oxidizing Acids and Inorganic Oxidizing Agents:

> **HCl reacts with oxidizing agents (e.g. H2O2, V2O5), including air, to produce Cl2 gas** (Hisham, M.W.M., T.V. Bommaraju, 2004, Hydrogen Chloride. In *Kirk-Othmer Encyclopedia of Chemical Technology*, John Wiley & Sons, Inc.)**. Reaction of HCl and KMnO4 evolves toxic Cl2 gas** (Curry, J.C. 1965. *School Sci. Rev.* 46(160):770)**, and can be explosive, possibly due to the formation of Cl2O gas** (Ephraim, 1939, 162)**. Reaction of concentrated hydrofluoric acid and anhydrous KMnO4 is exothermic and violent** (Black, A.M. et al. 1974. *Journal of the Chemical Society*, Dalton Trans. 977.)**. Hydrofluoric acid forms powerful oxidizer HgF2 with HgO; reactions involving a HF/HgO mixture and organic materials must be run at low temperature to avoid a runaway reaction** (Ormston, J. 1944. *School Sci. Rev.* 26(98):32.)**. Reaction of HBr and ozone accelerates to explosion, even at -104ºC** (Lewis, B. et al. 1931. *Journal of the American Chemical Society* 53:3565)**. HF, HCl, HBr, and HI, whether aqueous or anhydrous, ignite on contact with fluorine.** (Mellor, 1940, Vol. 2, 12). **HCl reacts violently with AgClO4 in carbon tetrachloride solution** (Lewis, R.J., Sr. 1992. *Sax's Dangerous Properties of Industrial Materials, 8th Edition.* New York: Van Nostrand Reinhold. pp. 1893)**.**

CRW Design Improvements

Re-researching the reactive groups in the CRW provided not only an opportunity to expand the product, but also to error-check and optimize the compatibility table, Reactive Group Profiles, and the Chemical Profiles of several compounds.

First, a number of compounds were misclassified, or questionably classified, in earlier versions, and 22 compounds have now been reclassified to different reactive groups or had additional reactive groups added to their profile.

Second, a number of minor errors have been corrected within reactive group profiles, and 143 new or updated citations for reactions have been added to individual compounds' Chemical Profiles if the reaction were relevant to the compound but could not be generalized to a reactive group. However, reactions added to a binary pair's hazard statement were not added to chemical profiles in this release since the information is available in the hazard report. CRW 2.0 will also

have the ability to display all of the hazardous reactions for a reactive group in a single list, for examining general incompatibilities instead of only binary pairs.

Third, the reaction hazard codes used to generate hazard reports have been streamlined. Several unused or redundant reaction hazards have been removed, and identified reactions merged with other hazards or assigned new hazards. One new hazard was also added, and several hazards have been rewritten for clarity. The coding system was also simplified such that only one code related to gas generation, violent reactions, or fire hazards would be used for any particular binary pair, with lesser hazards implied by the more stringent hazard statements; e.g. if two chemicals are likely to ignite on contact (code B4), they also pose a fire hazard (code B1). Additionally, exothermic reactions that may be vigorous or violent have now been flagged as such (the code for violent reactions was unused until Version 1.7), or if an explosive reaction hazard is present, the appropriate explosion code. Conversely, reactions that were already defined as explosive have also been defined as exothermic if they were not already.

Finally, the CRW has been previously criticized[20] for its high rate of returning false-positives, including hazards that seem nonsensical. These erroneous results are due to both the limitations imposed by a binary compatibility matrix, and "worst case" assumption for CRW predictions; the CRW is designed to be very conservative in returning a "no reaction" result. Few documented reactions (usually two) are needed to declare a reactive hazard between two reactive groups, and therefore CRW 2.0 will still have a high false-positive rate. However, since most of the hazards returned by CRW 2.0 are now extensively documented, the false-positives are now mitigated by the user's ability to view documentation and determine if the reactions found for the representative compounds that we used to determine the hazard are relevant to the compounds the user intends to work with. The extent of the new documentation is summarized in Tables 3 and 4. Since the old CRW did not include extensive documentation, the false-positive deficiency

in CAMEO Chemicals/CRW 2.0 should be significantly lower than in any previous version, however the CRW should still not be the sole source for process safety data, and in a process safety use, ambiguous positive results should be confirmed through MSDS info, additional literature searches, thermodynamic modeling, or experiment. Known issues regarding the CRW are discussed further in the next section.

Table 3: Documentation Quality Summary

Grade	# of Reactive Groups
A (> 80% documented)	5
B (60-79%)	14
C (40-59%)	12
D (< 40%)	12

Table 4: Five Best and Worst Documented Reactive Groups

Best Documented Groups	% Documented	Worst Documented	% Documented
Ethers	90	Organometallics	19
Inorganic Oxidizing Acids	88	Chlorosilanes	22
Inorganic Oxidants	86	CFCs	25
Alcohols	82	Phenols	25
Active Metals	81	Thiocarbamates	26

Remaining Design Limitations/Deficiencies of the CRW

While the CRW 2.0 update greatly expands upon the capabilities of the already-effective CRW, several deficiencies that could be addressed by future versions or are better covered by other products, remain. Some could be addressed by incremental updates using current methodology, and others are due to the simplifying assumptions used to develop a working product that can handle such a wide variety of reactions.

First, 40% of the pairs with a reactive hazard listed in the CRW are currently undocumented, and finding other secondary-source documentation for those reactive pairs may be difficult for users wishing to verify an undocumented CRW prediction. However, many of these reaction hazards seem intuitive and/or match the predictions of other compatibility tables; for example, the CRW has no documentation for a reaction of strong reducing agents and

amines, but the EPA Table[3] and the upcoming Reactivity Management Roundtable (RMR) Simplified Storage Compatibility Table[21] predict an incompatibility. Deficiencies for less-common reactions have generally been mitigated by the new documentation.

Second, predicting products is currently beyond the scope of the CRW, although future versions may include a feature for identifying gasses generated in a reaction. Some products, especially gasses, and some explosive products, are listed in the CRW 2.0 reaction documentation, but the CRW does not predict the identity of many dangerous products generated by reactions. Furthermore, such a lack of product prediction contraindicates the addition of a recursive search for interaction of reaction products with other products or reactants in a mixture, whether or not the first reaction is hazardous. Since reactions with gaseous products can lead to particularly severe incidents, such as the 1995 Powell Duffryn fire and spill in Savannah, Georgia, where H_2S evolution was a major concern[22], a feature for predicting gasses generated by reactions will likely be added to a future version of the CRW.

Third, the CRW does not currently provide quantitative or semi-quantitative information about reaction thermodynamics or kinetics; however, users can obtain thermodynamic information about reactions with other common safety products such as CHETAH[23]. This feature deficiency in the CRW could be addressed by other products, or by incorporating basic thermodynamic prediction and/or quantitative structure-activity relationship (QSAR) functionality into a future version of the CRW.

Fourth, since the CRW functions by comparing binary reactions of reactive groups, based on (usually) monofunctional representative compounds, reactions specific to multifunctional compounds may be neglected, as are reactions involving three or more compounds, or presence of a catalyst, potentially leading to false-negatives[20]. Effects of de-activating groups and

inhibitors may also be ignored, leading to false positives. Non-binary reactions are considered to be outside of the current scope of the CRW.

In order to utilize the CRW most effectively, users should read all documentation for the CRW before use, in order to understand its limitations, and when interpreting reaction predictions, consult the chemical profiles for individual compounds and/or use a source that does include catalyzed reactions and reactions involving more than two reactants, such as *Bretherick's*, *NFPA 491M*, the major chemical engineering encyclopedias, or primary literature.

Conclusion

Use of representative compounds to draw general conclusions about the reactivity of functional groups enabled significant improvements to the CRW, including verification of many of the hazards previously identified by the CRW, and addition of hazard statements for many new dangerous combinations, without having to re-research more than a few hundred of the 6000+ compounds in the database. Researching hazards for the selected compounds, and re-examining the database also allowed correction of a significant number of errors and omissions from earlier versions, and allowed optimization of the hazard codes and user interface. While CRW 2.0 still has several deficiencies, the addition of hazard statements generated from representative compound information greatly expands upon the utility of the product.

Some CRW 2.0 features, including the revised compatibility matrix, are already implemented through the current release of Cameo Chemicals, accessible at (http://cameochemicals.noaa.gov.) Other features, such as access to the documentation for binary reactions and revised chemical profiles, are pending implementation, and should be available in late 2007.

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