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Standard Guide for Preparation of Binary Chemical Compatibility Chart[1]

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1. Scope

1.1 A binary chemical compatibility chart (also called inter-reactivity chart) compares the hazards associated with the mixing of two different materials. This guide provides an aid for the preparation of these charts. It reviews a number of issues that are critical in the preparation of such charts: accurate assessment of chemical compatibility, suitable experimental techniques for gathering compatibility information, incorporation of user-friendliness, and provision for revisions.

1.2 The uses of chemical compatibility charts are summarized.

1.3 This guide also reviews existing public domain compatibility charts, the differences therein, and their advantages and disadvantages.

2. Referenced Documents

2.1 *ASTM Standards:*

E 537 Test Method for Assessing the Thermal Stability of Chemicals by Methods of Differential Thermal Analysis[2]

E 698 Test Method for Arrhenius Kinetic Constants for Thermally Unstable Materials[2]

E 1231 Practice for Calculation of Hazard Potential Figures-of-Merit for Thermally Unstable Materials[2]

P 168 Guide for Estimating the Incompatibility of Selected Hazardous Wastes Based on Binary Chemical Reactions[3]

2.2 *NFPA Standard:*

NFPA 491 Guide to Hazardous Chemical Reactions[4]

2.3 *Federal Standard:*

46 CFR Compatibility of Cargoes[5]

3. Terminology

3.1 *Definitions:*

3.1.1 *compatibility*—the ability of materials to exist in contact without specified (usually hazardous) consequences under a defined scenario.

3.1.2 *scenario*—a detailed physical description of the process whereby a potential inadvertent combination of materials may occur.

4. Summary of Practice

4.1 A binary chemical compatibility chart indicates whether, under a given set of conditions (the scenario), combination of two materials does or does not yield a specified undesired consequence.

4.2 Determine the scenario for the determination of compatibility and the degree of reaction that constitutes incompatibility. Both should be identified in the title of the chart. Define the materials within the scope of the chart. Define the test, calculation, or judgment that is used to make a decision. List the materials as both columns and rows of a grid. At the intersections of the grid, note whether the materials are compatible. To avoid duplicate entries, a triangular chart is required. If a decision on compatibility was not by the standard means (as defined by the user) or the scenario differs, indicate by footnote the basis for the decision or the change in scenario. The chart should be dated and the author identified. See Fig. 1 for an example of a binary compatibility chart.

5. Significance and Use

5.1 Various governmental regulations require that incompatible materials not be transported together and that chemical reactivity be considered in process hazard and risk analysis. A chemical compatibility chart is one tool to be used to satisfy these regulations. Binary compatibility charts are useful teaching tools in general education in the chemical plant or laboratory and for areas and operations where commonly performed tasks might lead to chemical mixtures, such as might occur during co-shipment in compartmentalized containers, storage in a common area, or compositing waste. Compatibility information is essential during process hazard reviews (for example, HAZOP). These charts may provide guidance on DOT HM-183 to terminal operators, which requires that materials on adjacent compartments of multicompartment tank trucks are compatible. They provide documentation that the potential for inadvertent mixing as a potential source of heat and gas evolution from chemical reactions has been considered in sizing relief devices. Compatibility charts serve as check lists for use during process hazard reviews, and the preparation of the chart itself often brings attention to potential hazards that were previously unknown.

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[1] This test method is under the jurisdiction of ASTM Committee E-27 on Hazard Potential of Chemicals and is the direct responsibility of Subcommittee E27.02 on Thermal Stability and Condensed Phases.

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[2] *Annual Book of ASTM Standards*, Vol 14.02.

[3] Discontinued; see 1988 *Annual Book of ASTM Standards*.

[4] Available from National Fire Protection Association, One Batterymarch Park, Quincy, MA 02269.

[5] Available from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

	REACTIVITY GROUP	1	2	3	4	5	6
1	Hydrochloric Acid	1					
2	Sulfuric Acid	X[1]	2				
3	Acetic Acid	U[8]	X[2]	3			
4	Ethanol	U[3]	X[4]	X[4]	4		
5	Ethylene Diamine	X[6]	X[6]	X[7]	C[12]	5	
6	Water	X[9]	X[10]	C[11]	C[13]	C[13]	6

Legend:

X	incompatible
C	lab compatibility testing revealed no hazard
U	unknown - further evaluation needed

Footnotes/Information Sources:

1 Unlikely to be compatible - USCG chart NVC 4-75 indicates a hazard with non-oxidizing acids plus sulfuric acid.

2 Unlikely to be compatible - the P-168 chart indicates that gas and heat are formed; USCG chart NVC 4-75 indicates a hazard when combining sulfuric and organic acids.

3 The P-168 chart indicates that heat is released; USCG chart NVC 4-75 only indicates a hazard with furfuryl alcohol plus non-oxidizing mineral acids; testing should be conducted on this combination.

4 Unlikely to be compatible - see P-168 chart.

5 Lab experiment 980001 resulted in a XXX C adiabatic temperature rise.

6 Lab experiment 980002 resulted in a XXX C adiabatic temperature rise.

7 Organic acids and amines are generally incompatible.

8 The P-168 and USCG charts indicate no hazard; most likely compatible, but lab testing should be performed.

9 Heat of mixing may be a concern in some circumstances. The maximum adiabatic temperature rise is XX C (see XYZ Encyclopedia of Chemical Technology).

10 Heat of mixing may be a concern in some circumstances. The maximum adiabatic temperature rise is XX C (see XYZ Encyclopedia of Chemical Technology).

11 Lab experiment 98005 showed that mixing acetic acid and water is endothermic at room temperature.

12 Lab experiments 98003 and 98008 indicate that the materials do not generate heat or gases when mixed nor when heated to 100 C. Although the USCG chart NVC 4-75 indicates that some alcohols and amines are incompatible, ethylene diamine has been found to be compatible with many alcohols; see Appendix of USCG Guide.

13 Plant experience has shown that these materials do not generate heat or gases when mixed. In addition, no condition is known that would cause the materials to be combined at elevated temperature.

NOTE 1—Scenario: Ambient temperature mixing under adiabatic, non-vented conditions. Time of mixing is 4 h.

NOTE 2—Definition of incompatibility: Adiabatic temperature rise greater than 25°C, or a gassy reaction.

FIG. 1 Hypothetical Compatibility Chart for Process Y at Site X

5.2 A binary chart only considers pairs of materials and, therefore, does not cover all possible combinations of materials in an operation. A common third component, for example acidic or basic catalysts, may be covered by footnoting the potential for catalysis of a reaction between otherwise compatible materials, but the form of the chart does not ensure this. There may be reactive ternary systems that will escape detection in a binary chart.

6. Procedure

6.1 The following is a step-by-step procedure, which may be followed, to prepare a compatibility chart.

6.1.1 *Define the Scenario*—Chemical compatibility depends heavily on the mixing scenario. The scenario is a detailed physical description of the process and conditions whereby a potential inadvertent combination of materials may occur. Consider including the following in the specification of the mixing scenario:

6.1.1.1 Specific quantities of materials,

6.1.1.2 Storage temperatures,

6.1.1.3 Confinement (closed or open system), and

6.1.1.4 The maximum times the materials may be in contact.

6.1.1.5 These factors (and others) may contribute to the assignment of compatibility. Further discussion of the scenario dependence of compatibility may be found in Appendix X1.

6.1.2 *Define Incompatibility Within the Scenario Framework*—An effective chart should clearly convey the criteria for defining two materials as incompatible. In a general sense, chemical incompatibility implies that there may be undesirable consequences when mixing these materials at a macroscopic scale. These consequences might be in a worst case a fast chemical reaction or an explosion, or in a less severe case, an undesirable temperature rise, which might take the mixture above its flash point or cause an unacceptable pressure

TABLE 1 An Example of Hazard Levels and Typical Associated Emergency Response Actions

Hazard Rating	Hazard Level	Suggested Emergency Response
0	Minimal	Report inadvertent mixing event to supervision; no further action necessary.
1	Caution	Report event to supervision; devise and implement plan(s) to manage the situation; no emergency procedures to be initiated.
2	Danger	Report event to supervision; prepare to initiate unit emergency plan if needed; notify personnel in immediate area; consider halting normal activities until extent of situation is fully assessed.
3	Severe danger	Report event to supervision; initiate unit emergency plan; notify all plant personnel; cease normal activities until extent of situation is fully assessed; consider need to evacuate the plant; report event to plant industrial security and other ex-plant Emergency Response groups.
4	Extreme danger	Initiate unit emergency plan; notify all plant personnel to evacuate the area; cease normal activities, if possible, before evacuating; report event to plant industrial security and other ex-plant Emergency Response groups once evacuation is underway or complete.

increase in the system. If, however, the tank where the mixing will occur is inerted with nitrogen, and the material has an acceptably low vapor pressure increase, then even this temperature rise might not pose a practical problem. Consequently, a working definition of incompatibility needs to be formulated before compatibility judgments can be effectively and accurately made. Examples of mixing scenarios and incompatibility definitions are given in 6.1.2.1-6.1.2.3.

6.1.2.1 Ambient temperature in summer, northern climate (~25°C); 5000 gallon scale; insulated, vented storage tank; storage time seven days maximum, nitrogen padded headspace (chemical transport scenario). Incompatible if temperature rise greater than 25°C, or gassy reaction.

6.1.2.2 Ambient temperature in a hotter, subtropical climate (~40°C), drum (55 gal) storage of mixed waste for three months maximum. No release from the drum is allowed.

6.1.2.3 Room temperature, gallon bottles, loosely capped, one month maximum storage time (typical lab waste scenario). No evolution of flammable vapor, toxic gas, and no temperature rise greater than 10°C.

6.1.3 *Compile Compatibility Chart*—The following steps may be followed for constructing the compatibility chart. Appendix X2 contains additional information related to the preparation of a chart.

6.1.3.1 *State the Scenario*—In the preparation of a compatibility chart, consider stating explicitly on the chart both the scenario and the scenario based definition of incompatibility.

6.1.3.2 *Decide on a Hazard Rating Scheme*—The reference scale for the individual degree of mixing hazard needs to be formulated. In certain instances, it may be desirable to have a simple *yes (compatibile)/no (incompatible)* scale (*yes* meaning the mixture is compatible). In other instances, ratings that convey more information may be advantageous. For example, a numerical score of *1*, *2*, and *3* might be appropriate with *1* indicative of a compatible mixture, a *2* might indicate a moderate hazard (such as, a temperature increase of 10°C or less), and a *3* might indicate a severe hazard (such as polymerization or spontaneous combustion). Another example of a hazard rating scheme is given in Table 1. Note that in this example, the hazard rating scheme also conveys information about procedures for emergency response, but it may be decided not to include this information in the chart. The use of color (if available in the charting tool) may also aid in the ease of understanding the chart. For example, green for safe, compatible mixtures; red for reactive, incompatible mixtures. Care must always be exercised to avoid making the chart too complicated, because its practical usefulness might be lost.

6.1.3.3 *Define the Categories*—The definition of categories for the chart is an important part of chart construction. For small plants and operations, each chemical may be included in the chart and the resulting chart may still be of manageable size. For more general compatibility charts, for example, for a large manufacturing site, construct a chart by grouping chemicals into natural classifications based on their chemical structure. Examples of these groupings are mineral acids, aliphatic amines, monomers, water-based formulations, halogenated hydrocarbons, and so forth. One limitation with this manner of construction is that for a number of classes, certain binary combinations might be legitimately known to be compatible whereas other combinations within these same two groups may not be. It may be best to provide the worst case compatibility rating in the actual chart with a separate list of compatible exceptions. It may be prudent to include additional useful compatibility information, such as compatibility of chemicals with materials of construction, water (from process streams or from rain in diked areas), cleaning agents, sealants, and adsorbents. *Heat* might be considered as an entry to flag particularly heat sensitive materials, such as polymerizable monomers. Consultation with a wide variety of personnel (management, engineers, operators, and so forth) may aid in the determination of which materials are present at a site and which ones should be included in the chart.

6.1.3.4 *Consider the Hazards for All Binary Combinations*—The potential hazard for each and every binary mixture needs to be carefully considered. Avoid using blanks (empty cells) in compatibility charts since blanks may indicate that there is no hazard or, simply, that the hazard is unknown. Clearly distinguishing between a non-hazard and an unknown hazard is an important consideration. See Appendix X2 for sources of compatibility information.

6.1.3.5 *Document How the Decisions Are Made*—Backup and supporting data should be easily accessible for chart users and should allow for easier chart updates. If testing was performed to make a decision about a particular binary combination in a chart, then a reference to this test should be included in the chart.

6.1.3.6 *Label the Chart*—Make sure that the chart is dated and that the title of the chart clearly states the purpose of the chart, such as *Chemical Compatibility Chart for the Styrene Polymerization Plant A–104, last updated 9/98*. Scenarios may differ from process to process, and if the chart is not specifically labeled as to the intended use, there is a danger that the