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## Standard Guide for the Preparation of a Binary Chemical Compatibility Chart<sup>1</sup>

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### INTRODUCTION

The purpose of this standard is to provide expert guidance to those interested in the task of compiling chemical compatibility (inter-reactivity) charts for the purposes of process safety and reactive chemicals hazard evaluation. This standard does not provide specific answers regarding the inter-reactivity of specific materials. However, it does provide a detailed framework for developing charts based on the current best practices of the chemical industry and it directs the user to sources of reactivity information. It is the E27 Committee's belief that inter-reactivity charts will be increasingly used in industry for day-to-day operations, process hazard reviews, employee education, and emergency response. It is our hope that this standard guide can be useful in that effort.

### 1. Scope

1.1 A binary chemical compatibility chart also called inter-reactivity chart, documents the hazards associated with the mixing of pairs of materials. This guide provides an aid for the preparation 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 in this standard.

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*:<sup>2</sup>

[E537 Test Method for The Thermal Stability of Chemicals by Differential Scanning Calorimetry](#)

[E698 Test Method for Arrhenius Kinetic Constants for Thermally Unstable Materials Using Differential Scanning Calorimetry and the Flynn/Wall/Ozawa Method](#)

[E1231 Practice for Calculation of Hazard Potential Figures-of-Merit for Thermally Unstable Materials](#)

[PS168 Proposed Guide for Estimating the Incompatibility of Selected Hazardous Wastes Based on Binary Chemical Reactions](#)<sup>3</sup>

2.2 *NFPA Standard*:

[NFPA 491 Guide to Hazardous Chemical Reactions](#)<sup>4</sup>

### 3. Terminology

3.1 *Definitions*:

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

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

### 4. Summary of Guide

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

4.2 A summary of the guide follows. Determine the scenario for the determination of compatibility and the degree of reaction that constitutes incompatibility. Both should be identified in the documentation for the chart. Define the materials within the scope of the chart. Define the test, calculation or

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<sup>2</sup> For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

<sup>3</sup> Withdrawn. This chart was subsequently adopted by the U.S. EPA and is widely available by way of the Internet. For example, it may be viewed here: <http://www/sefsc.noaa.gov/HTMLdocs/appendix-H.htm>.

<sup>4</sup> Available from National Fire Protection Association (NFPA), 1 Batterymarch Park, Quincy, MA 02169-7471, <http://www.nfpa.org>.

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 United States governmental regulations forbid incompatible materials to be transported together and require

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 to terminal operators on DOT HM-183 that requires that materials on adjacent compartments of multicompartment tank trucks are compatible. They provide documentation that

| REACTIVITY GROUP |                   |                |                 |                 |                 |                   |
|------------------|-------------------|----------------|-----------------|-----------------|-----------------|-------------------|
| 1                | Hydrochloric Acid | 1              |                 |                 |                 |                   |
| 2                | Sulfuric Acid     | X <sup>1</sup> |                 | 2               |                 |                   |
| 3                | Acetic Acid       | U <sup>8</sup> | X <sup>2</sup>  |                 | 3               |                   |
| 4                | Ethanol           | U <sup>3</sup> | X <sup>4</sup>  | X <sup>4</sup>  |                 | 4                 |
| 5                | Ethylene Diamine  | X <sup>5</sup> | X <sup>6</sup>  | X <sup>7</sup>  | C <sup>12</sup> | 5                 |
| 6                | Water             | X <sup>9</sup> | X <sup>10</sup> | C <sup>11</sup> | C <sup>13</sup> | C <sup>13</sup> 6 |

Legend:

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

NOTE 1—Footnotes/Information Sources:

- (1) Unlikely to be compatible—USCG chart NVC-475 indicates a hazard with non-oxidizing acids plus sulfuric acid.
- (2) Unlikely to be compatible—the Proposed Guide PS168 chart indicates that gas and heat are formed; USCG chart NV 4-75 indicates a hazard when combining sulfuric and organic acids.
- (3) The Proposed Guide PS168 chart indicates that heat is formed; USCG chart NV 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 Proposed Guide PS168 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 Proposed Guide PS168 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.

FIG. 1 Hypothetical Compatibility Chart

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.

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.

5.3 The AIChE organization Center for Chemical Process Safety (CCPS) has recommended the use of this standard in one of their recent monographs (1)<sup>5</sup>. This work is currently available for free download from: <http://www.osha.gov/SLTC/reactivechemicals/index.html>

## 6. Procedure

6.1 *Define the Scenario*—Chemical compatibility depends heavily on the mixing scenario (see Appendix X1). Consider including the following factors in the specification of the mixing scenario, as they, and other factors, may contribute to the assignment of compatibility.

- 6.1.1 Specific quantities of materials,
- 6.1.2 Storage temperatures,
- 6.1.3 Confinement (closed or open system),
- 6.1.4 Atmosphere (air, nitrogen inerted), and
- 6.1.5 The maximum time the materials may be in contact.

6.2 *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 of mixing these materials at a macroscopic scale. These consequences might be, in a worst case, a fast chemical reaction or an explosion, a release of toxic gas, or, in a less severe case, an undesirable temperature rise that might take the mixture above its flash point or cause an unacceptable pressure 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.

6.2.1 Some examples of mixing scenarios and incompatibility definitions include:

6.2.1.1 Ambient temperature in summer, northern climate (approximately 25°C); (5000 gal) scale; insulated, vented storage tank; storage time 7 days maximum, nitrogen padded headspace (chemical transport scenario). Materials considered incompatible if temperature rise greater than 25°C, or grassy reaction.

6.2.1.2 Ambient temperature in a hotter, subtropical climate (approximately 40°C), drum (55 gal) storage of mixed waste for 3 months maximum. Materials considered incompatible if there could be a release from the drum.

6.2.1.3 Room temperature, 4L (1 gal) bottles, loosely capped, 1 month maximum storage time (typical lab waste scenario). Materials considered incompatible if there is an evolution of flammable vapor, toxic gas, or a temperature rise greater than 10°C.

6.3 *Compile Compatibility Chart*—The following steps may be followed for constructing the compatibility chart (see Appendix X2).

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

6.3.2 *Decide on a Hazard Rating Scheme*—Formulate the reference scale for the individual degree of mixing hazard. It may be desirable to have a simple “yes/no” (that is, compatible/incompatible) scale. In some instances, ratings that convey more information may be advantageous. For example, a numerical score of 1, 2, and 3 might be appropriate with 1 indicating a compatible mixture, 2 indicating a moderate hazard (for example, a temperature increase of 10°C or less), and 3 indicating a severe hazard, such as polymerization or spontaneous combustion. Another example of a hazard rating scheme is given in Table 1. Note that in the Table 1 example, the hazard rating scheme also conveys information about procedures for emergency response, but this information need not be included in the chart. The use of color (if available in the charting tool) may also aid in understanding the chart. For example, green could indicate safe, compatible mixtures, red could indicate reactive, incompatible mixtures. It is important to avoid making the chart too complicated.

6.3.3 *Define the Categories*—Defining 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, the chart may group chemicals into natural classifications based on their chemical structure. Examples of these groupings are: mineral acids, aliphatic amines, monomers, water-based formulations, halogenated hydrocarbons,

**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; 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. |

<sup>5</sup> The boldface numbers in parentheses refer to the list of references at the end of this standard.