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

This standard is issued under the fixed designation E 2012; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

INTRODUCTION

In 1982, ASTM Committee D-34 on Hazardous Waste proposed the compatibility chart PS 168 that is discussed in this standard. ASTM Committee E-27 (sponsors of this standard guide) raised several issues as to the accuracy of parts of the chart that ultimately led to the withdrawal of the proposed standard and the tacit agreement of E-27 to take over further development. As time passed, it became increasingly clear that a consensus chart, agreeable to all, and comprehensive enough to be useful to the chemical industry was and still is a difficult task. Consequently, Committee E-27 embarked on an easier but nonetheless very useful task that provides expert guidance to those who might be interested in the task of compiling compatibility information without actually dictating the answers to specific binary reactivity questions. This standard is the result of that effort. It is the 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 call inter-reactivity chart, compares the hazards associated with the mixing of two different 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:*

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]

PS 168 Proposed 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]

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, that is, 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

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

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

[3] Discontinued. See 1986 *Annual Book of ASTM Standards*, Vol 11.04.

[4] Available from the National Fire Protection Association, One Batterymarch Park, PO Box 9101, Quincy, MA 02269-9101.

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 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.

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

SUBSTANCE

1	Hydrochloric Acid (35%)	1					
2	Sulfuric Acid (90%)	R[1]	2				
3	Acetic Acid	?[8]	R[2]	3			
4	Ethanol	NR[3]	R[4]	NR[15]	4		
5	Ethylenediamine	R[5]	R[6]	R[7]	NR[12]	5	
6	Water	R[9]	R[10]	NR[11]	NR[13]	R[14]	6

Legend:

R	Reactive under the stated scenario - **incompatible**
NR	Non-Reactive under the stated scenario - **compatible**
?	**unknown** - assume incompatible until further information is obtained

Footnotes/Information Sources:

1 Unlikely to be compatible - USCG chart NVC 4-75 indicates a hazard with non-oxidizing acids plus sulfuric acid. Heat of mixing may be significant.
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 Primary alcohols do not react with aq. HCl at ambient temperature.
4 Heat of solution followed by reaction to form ethyl hydrogen sulfate.
5 Lab experiment 980001(50/50 mix) resulted in a significant heat of neutralization.
6 Lab experiment 980002 (50/50 mix by volume) resulted in a XXX C adiabatic temperature rise.
7 Organic acids and amines are generally incompatible due to acid/base neutralization heat.
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). Violent reaction with splattering if water is added to the acid.
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 materials to be compatibile.
14 Mildly exothermic hydrate formation.
15 Very slow, nearly thermoneutral, equilibrium-limited esterification at ambient temperature.

FIG. 1 Hypothetical Compatibility Chart

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). 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. Incompatible if there could be a release from the drum.

6.2.1.3 Room temperature, _L (1 gal) bottles, loosely capped, 1 month maximum storage time (typical lab waste scenario). 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, and so forth. One limitation with this manner of chart construction is that for a number of classes, certain binary combinations might be known to be compatible whereas other combinations within the 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 what materials are present at a site and which ones should be included in the chart.

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.
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 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 emergency response groups once evacuation is underway or complete.

6.3.4 *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.

6.3.5 *Document How the Decisions Are Made*—Backup and supporting data should be easily accessible for chart users and to 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.

6.3.6 *Label the Chart*—Date the chart and ensure that title 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 with the