Designation: C1750 – 21

Standard Guide for
Development, Verification, Validation, and Documentation of Simulants for Hazardous Materials and Process Streams[1]

This standard is issued under the fixed designation C1750; 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.

1. Scope

1.1 *Intent:*

1.1.1 The intent of this guide is to provide general considerations for the development, verification, validation, and documentation of tank simulants for hazardous materials (for example, radioactive wastes) and process streams. Due to the expense and hazards associated with obtaining and working with actual hazardous materials, especially radioactive wastes, simulants are used in a wide variety of applications including process and equipment development and testing, equipment acceptance testing, and plant commissioning. This standard guide facilitates a consistent methodology for development, preparation, verification, validation, and documentation of simulants.

1.2 This guide provides direction on (*1*) defining simulant use, (*2*) defining simulant-design requirements, (*3*) developing a simulant preparation procedure, (*4*) verifying and validating that the simulant meets design requirements, and (*5*) documenting simulant-development activities and simulant preparation procedures.

1.3 *Applicability:*

1.3.1 This guide is intended for persons and organizations tasked with developing simulants to either mimic certain characteristics and properties of hazardous materials or provide representative performance for the phenomenon being evaluated. The process for simulant development, verification, validation, and documentation is shown schematically in Fig. 1. Specific approval requirements for the simulant developed under this guide are not provided. This topic is left to the performing organization. Approval requirements are associated with the design of the simulant, makeup procedures, and final simulant produced.

1.3.2 While this guide is directed at simulants for radioactive materials (for example, nuclear waste), the guidance is also applicable to other aqueous based solutions and slurries.

1.3.3 The values stated in SI units are to be regarded as the standard. The values given in parentheses are for information only.

1.4 This guide is not a substitute for sound chemistry and chemical engineering skills, proven practices and experience. It is not intended to be prescriptive but rather to provide considerations for the development and use of simulants.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

C859 Terminology Relating to Nuclear Materials

2.2 *ASME Standard:*[3]

NQA-1 Quality Assurance Requirements for Nuclear Facility Applications

2.3 *Environmental Protection Agency SW-846 Methods:*[4]

Method 3010A Acid digestion of Aqueous Samples and Extracts for total metals for Analysis by FLAA or ICP Spectroscopy

Method 3050B Acid Digestion of Sediments, Sludges and Soils

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[1] This guide is under the jurisdiction of ASTM Committee C26 on Nuclear Fuel Cycle and is the direct responsibility of Subcommittee C26.13 on Spent Fuel and High Level Waste.

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[2] 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.

[3] Available from American Society of Mechanical Engineers (ASME), ASME International Headquarters, Two Park Ave., New York, NY 10016-5990, http://www.asme.org.

[4] Available from United States Environmental Protection Agency (EPA), William Jefferson Clinton Bldg., 1200 Pennsylvania Ave., NW, Washington, DC 20460, http://www.epa.gov.

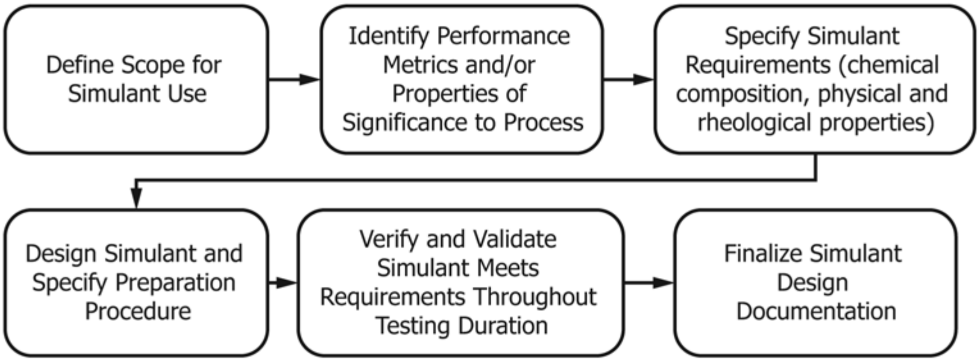

FIG. 1 Simulant Development, Verification, Validation, and Documentation Flowsheet

Method 3051A Microwave Assisted Acid Digestion of Sediments, Sludges and Soils
Method 3052 Microwave Assisted Acid Digestion of Siliceous and Organically Based Matrices
Method 6010C Inductively Coupled Plasma-Atomic Emission Spectrometry
Method 6020A Inductively Coupled Plasma-Mass Spectrometry
Method 9056A Determination of Inorganic Anions by Ion Chromatography

3. Terminology

3.1 Refer to Terminology C859 for additional terminology, which may not be defined below.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *cognizant engineer, n*—lead engineer responsible for overall supervision and direction of simulant development.

3.2.2 *simulant, n*—a solution or slurry that mimics or replicates selected chemical, physical or rheological properties, or both, of an actual process or waste stream and is utilized to reduce hazards and costs associated with working with the actual material.

3.2.3 *simulant development test plan, n*—a document that describes the simulant development process that results in a simulant that meets the usage and design requirements identified in the simulant requirements specification.

3.2.4 *simulant preparation procedure, n*—a document that specifies the step by step process of producing the simulant.

3.2.5 *simulant requirements specification, n*—a document that specifies the simulant use and design requirements.

3.2.6 *simulant validation, n*—establishment of documented evidence that confirms that behavior of the simulant adequately mimics the targeted actual waste behavior or performance; simulant validation can be expressed by the query, "Are you making the correct simulant?" and refers back to the needs for which the simulant is being developed.

3.2.7 *simulant verification, n*—establishment of documented evidence which provides a high degree of assurance that the simulant meets the predetermined design and quality requirements; simulant verification can be expressed by the query, "Are you making the simulant properly?"

3.3 *Acronyms:*

3.3.1 *ASME*—American Society of Mechanical Engineers

3.3.2 *DI*—Deionized Water

3.3.3 *DOE*—U.S. Department of Energy

3.3.4 *GFC*—Glass Forming Chemicals

3.3.5 *HLW*—High-Level Waste

3.3.6 *LAW*—Low-Activity Waste

3.3.7 *N/A*—Not Applicable

3.3.8 *NQA-1*—Nuclear Quality Assurance

3.3.9 *PSD*—Particle Size Distribution

3.3.10 *QA*—Quality Assurance

3.3.11 *QC*—Quality Control

4. Summary of Guide

4.1 This guide provides general considerations on the development, preparation, validation, verification, and documentation of simulants.

4.2 The first step in the process is to define the purpose for which the simulant will be used and to identify the key process performance metrics or properties, or both, relevant to the phenomenon being assessed. The performance metrics/parameters provide a means of comparing simulant performance against that for actual waste (based on available performance or characterization data, or both, for the waste) for the process or phenomenon being evaluated as exemplified by Peterson et al.,[5] Wells,[6] and Lee et al.[7] This first step also includes specifying the target values or range of values for the chemical composition and physical properties (including rheology) of the simulant. The quality assurance requirements are also defined in the first step in accordance with the project requirements for which the simulant is being developed.

4.3 The next step is to define the simulant design requirements. This involves determining the necessary and sufficient

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[5] Peterson, R. A., Wells, B. E., Daniel, R. C., and Russell, R., "Performance-Based Simulants for Hanford Radioactive Waste Treatment Process Testing," *Separation Science and Technology*, February 2021.

[6] Wells, B. E., "Simulant Development for Hanford Tank Farms Double Valve isolation (DVI) Valves Testing," *PNNL-22121*, Pacific Northwest National Laboratory, Richland, WA, 2013.

[7] Lee, K. P., Wells, B. E., and Gauglitz, P. A, and Sexton, R. A., "Waste Feed Delivery Mixing and Sampling Program Simulant Definition for Tank Farm Performance Testing," *RPP-PLN-51625*, Washington River Protection Solutions, LLC, Richland, WA, 2012.

simulant properties to be measured for each affected unit operation. Key simulant properties and acceptance criteria are developed with regard to the project requirements for which the simulant is being developed. Standardized chemical and physical property measurements are referenced.

4.4 The following step is to define an approach for developing the simulant to meet the needs for simulant use while satisfying the design requirements. This approach is often documented in a test plan that includes the methods for validating the use of the final developed simulant and verifying the simulant is acceptable.

4.5 Upon developing an approach and simulant, a procedure for preparing the simulant must be generated and documented. The procedure is focused on providing a means for consistently generating the correct simulant regardless of persons conducting process. The procedure takes into account sequence constituents are added, degree of mixing, and temperature at which processes take place. The development of the preparation procedures must address scale-up associated with fabricating larger batches of simulant, and simulant contamination, degradation, or attrition during testing.

4.6 Once the fabrication of simulant is initiated, the simulant being produced needs to be verified. Verification assures the simulant meets design requirements and addresses the question: was the simulant made properly?

4.7 At the end of the simulant process, documentation for the simulant development process needs to be compiled and finalized. The documentation must meet project requirements for producing records materials and focus on assuring the repeatability of the process.

5. Significance and Use

5.1 The development and use of simulants is generally dictated by the difficulty of working with actual radioactive wastes or hazardous materials, or both, and process streams. These difficulties include large costs associated with obtaining samples of significant size as well as significant environmental, safety and health issues.

5.2 *Simulant-development Scope Statement:*

5.2.1 *Simulant Use Definition:*

5.2.1.1 The first step should be to determine what the simulant is to be used for. Simulants may be used in a wide variety of applications including evaluation of process performance, providing design input to equipment, facilities and operations, acceptance testing of procured equipment or systems, commissioning of equipment or facilities, or troubleshooting operations in existing equipment or facilities. A simulant may be used for single or multiple unit operations. Through the simulant-use definition, the characteristics of the simulant required for development are determined. The characteristics may include chemical, physical, or a combination of these properties. The simulant-use definition should identify the key process performance metrics or properties, or both. It is important to note that a simulant developed to evaluate mobilization and suspension of Material A is not necessarily adequate for assessing component wear or pipeline transport associated with Material A. Both the material and the application (i.e., performance of interest) need to be considered. For example, if pipeline transport of non-buoyant solids in an aqueous liquid is the phenomena being evaluated, solids properties significant to the process performance can be different than those characteristics for the same simulant forming settled sediment that has a yield stress in a vessel, and the associated performance metrics are different. Similarly, significant difference in simulant solid particle performance properties may be required to evaluate waste impact on equipment associated with abrasive wear and fretting. The use of key process performance metrics allows changes in simulant composition to be evaluated and compared with other compositions and the actual waste. The effect of process chemical additions and recycle streams must also be assessed. Wells[6] provides an example of an assessment of an existing simulant designed for an alternative purpose and the resulting development of a performance-based simulant to represent the same process material for evaluating valve wear.

5.2.1.2 The applicable quality assurance requirements should be specified in accordance with the projects quality assurance program. For example, in the U. S. Department of Energy (DOE) complex, these requirements often include a QA program that implements ASME Nuclear Quality Assurance, NQA-1 (latest revision or as specified by project) and its applicable portions of Part II, Subpart 2.7 (latest revision or as specified by project) or Office of Civilian Radioactive Waste Management Quality Assurance Requirements Document: QARD DOE/RW 0333P (latest revision or as specified by project) QA requirements. Simulant-development activities that support regulatory and environmental compliance-related aspects of a waste-vitrification program may need to be performed in accordance with project quality-assurance requirements for generating environmental regulatory data. The use of simulants for project testing that is exploratory or scoping in nature may not need to comply with specific QA requirements.

5.2.2 *Simulant Composition Definition:*

5.2.2.1 Approaches to simulant-composition development will vary depending on the type of simulant required for testing. Simulant compositions may be based on actual sample characterization data, formulated for specific unit operations, or used for bounding or testing the limits of a process or specific piece of equipment. Key properties that are to be simulated should be identified as it may be difficult and unnecessary to develop simulants that exactly mimic all actual process stream properties at once. These key properties may be identified based on the key process performance metrics (see 5.2.1.1) used to evaluate simulant performance relative to the phenomenon being investigated.

5.2.2.2 Compositions for simulants based on actual waste samples should be defined using the available characterization data as the starting point (see Fig. 2). The best available source-term analytical data, including uncertainties, along with a comparison against comparable inventory data, historical process information, or feed vectors must be assessed. This comparison should highlight analytical outlier values that will need to be addressed for an analyte.

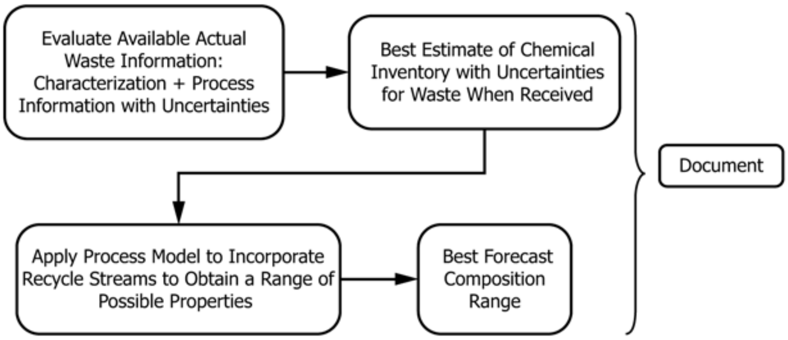

FIG. 2 Flowsheet for Simulant Composition Determinations Based Upon Actual Waste Sample Characterization Data

5.2.2.3 For simulant compositions that mimic flow sheet streams later in the process (after the best available waste source-term analytical information on the incoming waste stream is defined), process flow sheet model runs may be required to provide estimates of the additional stream compositions that incorporate recycle streams from other flow sheet unit operations. Flow sheet runs should consider transient behavior of the process in order to provide a range of compositions such that bounding conditions can be determined. The compositional waste-stream source-term data should be used as inputs to the process model. Any other planned operations that could affect flow sheet compositions being simulated (for example, adjustment of actual-waste-composition data to reflect future waste-feed delivery activities to arrive at the "best forecast composition range") need to be considered. If available, analytical data from actual waste characterization and testing should be compared to waste-stream-modeling results to validate the modeling results. The assumptions and inputs to the process flow sheet used should be described and discussed, and should be incorporated into the simulant requirements specification. By this process, the best-forecast simulant composition range would be traceable to actual waste-characterization data.

5.2.2.4 For simulant compositions formulated for specific unit operations, the composition may be targeted to only the chemical, physical, and rheological properties that are known to affect specific key operating or processing parameters.

5.2.2.5 For a simulant intended to bound the limits of a process or specific piece of equipment, a range of compositions should be developed to define these operational limits. For example, purely physical simulants may be used to determine the rheological bounds between which a specific vessel is able to meet a required process condition. For this approach, multiple simulants may be required to test numerous parameters. A bounding simulant may consist of an existing simulant spiked with specific compounds to test process performance (for example, added organics to test destruction in a melter system) or a purely physical simulant to test the acceptable physical and rheological process limits of a system.

5.3 *Simulant Design Requirements:*

5.3.1 The cognizant engineer should determine the necessary and sufficient simulant properties to measure for each affected unit operation, waste, or recycle stream. These should be the same for both actual waste and simulant waste where the simulant is based upon actual-waste characterization data. Often trace amounts of polyvalent ions or organic constituents can have a significant influence on physical and rheological properties and must be carefully considered. Appendix X1 provides an example of chemical, physical, and rheological properties-measurement matrices for several common unit operations associated with tank waste treatment waste streams that may be considered in developing simulant-design requirements. A similar chemical, physical, and rheological property-measurement matrix should be developed for each specific project or application.

5.3.2 The cognizant engineer should determine how close each measured property must be to the target value for the important analytes, physical and rheological properties. The range of acceptable values may depend on the simulant use as well as the accuracy of the analytical techniques used for measuring the properties. The specified ranges should then become the acceptance criteria for the simulant eventually prepared, to verify the simulant-preparation procedure.

5.3.3 The following key properties may be discussed (as applicable) and documented in the simulant requirements specification:

5.3.3.1 *Key Processing Properties*—The key processing properties to be determined using the simulant should be listed. These may consist of the properties that are measured during testing of a piece of equipment or unit operation. Examples include filtrate flux, decontamination factors, fouling, scaling, pressure drop, and sample homogeneity. The cognizant engineer should consider plant process upset conditions in testing requirements.

5.3.3.2 *Key Chemical Properties*—The chemical properties of the simulant necessary to ensure preparation of a valid simulant should be listed.

5.3.3.3 *Key Physical Properties*—The key physical properties of the simulant should be listed. Examples include density, heat capacity, thermal conductivity, heat of vaporization, PSD, settling rate, wt% settled and centrifuged solids, vol% settled and centrifuged solids, wt% total dried solids, and wt% total oxide.

5.3.3.4 *Key Rheological Properties*—The key rheological properties of the simulant should be listed. These may include yield stress (vane), viscosity measurements obtained from rheogram of shear stress versus strain rate, and evaluation of time dependence associated with response at constant strain rate or constant stress application, or both. Other "strength" related parameters may be pertinent. For instance, erosion (mobilization of the sediment) rate parameters should be investigated for mobilization of the 5.2.1.1 example of a settled sediment that has a yield stress.

5.3.3.5 *Design-basis Range*—Key design assumptions used at the particular point in the plant should also be listed. For example, key design parameters for pumps, agitators, piping, and vessels that would affect the simulant development should be documented.

5.3.4 If simulant melter feeds are to be developed, the cognizant engineer should ensure that the glass-former chemicals (GFCs), used for testing, are consistent with project requirements.

5.3.5 The key simulant properties and acceptance criteria may be documented in the simulant requirements specification, preferably in table format. An example for a LAW Melter Feed is provided in X2.1. Each project is encouraged to develop a similar list.

5.3.6 Standardized chemical, physical, and rheological property measurements for work performed should be used (see Section 2). Use of these property measurements is essential to ensure standardized, comparable results between all actual-waste and simulant-based tests.

5.4 *Simulant Development Test Plan:*

5.4.1 The person or organization assigned to perform the simulant development work may prepare a simulant development test plan that implements the simulant requirements specification. The simulant development test plan describes the proposed simulant development process, the key performance metrics being used, and should indicate what methodologies are planned to verify and validate simulant-property data produced during preparation and testing activities. For complex applications, the test plan may also define a hierarchy for applying or matching performance parameters to guide the simulant development process in cases where compromises between competing factors must be made.

5.5 *Develop Simulant Preparation Procedure:*

5.5.1 Once the simulant requirements specification and the development test plan (if required) have been completed, the performer of the work may proceed with the simulant-development activities in order to produce a standalone simulant preparation procedure. The performer of the work should make sure all simulant design requirements are met when developing the simulant-preparation procedure, for example:

5.5.1.1 Specified ionic forms of waste components to be used.

5.5.1.2 Charge balancing to be completed appropriately.

5.5.1.3 Appropriate substitutes to be used for radioactive species, as required.

5.5.1.4 Matching of pertinent performance parameters and physical properties (for example, phase, morphology, size, and crystalline versus non-crystalline) of solids.

5.5.1.5 Sequence and rate of addition of simulant components to avoid unwanted chemical reactions.

5.5.1.6 Extent of mixing and the need for temperature control (heating/cooling).

5.5.1.7 Actual processing parameters of the simulant important in developing a final simulant (for example, washing, leaching, shearing of solids, or generation and sampling of a submerged-bed-scrubber simulant) are stipulated.

5.5.2 Simulants may be developed following one of several general approaches: attempt to replicate the process that produced the material (for example, waste), replicate key processes that produced the material, obtain individual components that mimic the key properties of the actual material when mixed together, or use materials that are chemically different than the material being represented, but mimic the physical or rheological properties, or both, when mixed together.

5.5.2.1 One approach is to attempt to replicate the process that produced the actual material (for example, waste). This is generally the most difficult approach to implement, but has the greatest chance of replicating a wide variety of material properties. This approach may be able to produce a simulant with specialized properties and produce compounds and particulates that may not be commercially available or may not have been identified during characterization of the actual material of interest. It has the potential to produce a simulant that is highly credible. Use of this approach may be hampered by a lack of knowledge of process conditions that produced the material. For example, nuclear wastes may have been stored for decades with unknown chemical interactions and changed in unknown ways due to aging effects and a chemical evolution that is not fully understood. The processes are often complex, expensive and time consuming to replicate. In practice it is often sufficient to replicate the key processes that produced the material. For example, neutralizing an acidic solution containing soluble components to form a slurry with insoluble precipitates.

5.5.2.2 Another approach is to mix individual commercially available components together to approximate the simulant properties. While this approach is relatively simple to implement it is often hampered by a lack of knowledge of the waste components (speciation) and a lack of commercially available materials. It is also difficult to replicate the particle morphology produced by the originating processes using this approach.

5.5.2.3 Often the optimum approach is to use a combination of the approaches in which some portions of the simulant are produced by replicating the key processes that produced the material and then adding selected components that may be fabricated separately or obtained from commercial sources.

5.5.2.4 For simulants that are developed to mimic only physical or rheological properties, or both, it is often not necessary to replicate the chemical composition of the material. For example, various kaolin/bentonite clays are often used to mimic the rheological properties of nuclear waste slurries.

5.5.2.5 In many cases radioactive components have a negligible impact on the simulant properties and may be ignored. This is due to the relatively low chemical concentration of most radionuclides. Where the radioactive components are important, chemical surrogates may be used. In some cases there may be a stable isotope that may be used. More commonly, an element with similar chemical properties may be used. For example, rhenium is often used as a surrogate for technetium. Rare earth elements are often used as surrogates for the actinides. In general, it is best to use a component from the same group in the periodic table since this will provide the best match of the chemical properties.

5.5.2.6 Where simulants are representing wastes that have been stored for many years and may have undergone significant changes due to aging it may be possible to subject the simulant to an accelerated aging protocol. For radioactive wastes this may involve heating the simulant and perhaps exposing it to radiation.

5.5.2.7 Aging and storage effects on the simulant properties may be an important consideration during the simulant development process. In many applications the simulant may not be used immediately and will be stored for some time. In this case, the effects of storage on the simulant properties should be investigated in order to understand the changes and define appropriate methods of storage. Effects on the simulant may include precipitation of components from solution, dissolution of solid components, changes to the solid phase morphology or PSD, agglomeration of particulates, chemical reaction with air and drying. It may be necessary for climate-controlled storage or the use of inert cover gases, or both, to store the simulant prior to use. The addition of biocides may also be needed to prevent the formation of algae and biological growth that can impact the simulant behavior. The impact of the biocide addition also needs to be assessed during simulant development.

5.5.3 *Considerations for Simulant Scale-up and Fabrication:*

5.5.3.1 Development of the simulant fabrication procedure is often conducted at the bench scale to minimize costs. Depending on the quantity required for testing, scale-up of the fabrication process might be required.

5.5.3.2 Since impurities present in the water and the chemicals may impact the simulant composition and properties, it is recommended that the water and chemicals used at the bench scale be the same as those applied to production batches.

5.5.3.3 Bench-scale work often involves the use of deionized water while large scale production may use process or tap (which could contain chlorine) water obtained from a local source. Since production of large simulant batches may be subcontracted to a chemical supply vendor it is not always known ahead of time what the exact source of water will be. If the water source is expected to be an issue, sufficient water from the same source used for the bench scale work may be shipped to the chemical supply vendor or the use of deionized water may be specified. It's also quite possible that the source of water used by the vendor may be suitable, but this should be demonstrated with a trial batch of the simulant.

5.5.3.4 Bench-scale work often involves the use of reagent grade chemicals while larger scale production may use a lesser grade for cost reasons. Since lower grades of chemicals typically have more impurities or wider range of constituent concentrations, it is desirable to use the same grade of chemical for the laboratory work that is planned for the production batches. Since there may be variability between manufacturers and even batches from the same manufacturer it is best to use chemicals from the same batch from the same manufacturer throughout the development process. This can be especially important for components where a certain PSD or solid surface properties are important. At minimum, using chemicals from the same batch helps eliminate process variables and questions that may arise during the scale-up and production process.

5.5.3.5 The scale-up approach depends on the complexity of the fabrication procedure. For example, simply mixing commercially available solids components can be sufficient if adequate mixing power is available to provide a well-blended mixture. More complicated procedures involving chemical reactions need to be scaled using sound chemical engineering principles for mixing and blending. Variables that need to be considered include: temperature for exothermic or endothermic reactions, order of chemical addition, component solubility at various process steps, rate of addition, and mixing energy. These more complicated fabrication procedures may require one or more intermediate scale-up size batches between the bench- and full-scale fabrication processes.

5.5.3.6 Aqueous-phase-only simulants are relatively simple to produce. The most important considerations are the concentrations of the cations and anions, charge balance and solubility limits during fabrication. Due to analytical uncertainty and incomplete characterization of the actual waste, the charge balance often does not close and adjustments will have to be made to individual component concentrations. The solubility limits during fabrication need to be considered since solids may form which may be difficult to dissolve. This is especially true for fabrication procedures in which the pH varies widely.

5.5.3.7 In some cases a small amount of a radioactive isotope may be added as a tracer. For example, small amounts of ^{137}Cs may be used to monitor the performance of ion exchange processes.

5.5.3.8 Since equipment used for large production batches is often used for a wide variety of other applications it is important to make sure that the vessels are adequately cleaned prior to the start of production. This may involve multiple rinses of the equipment with water or cleaning agents as well as analysis of the solutions to make sure that any significant impurities are not present. Cleaning agents also need to be thoroughly removed from all contacting surfaces prior to addition of simulant components.

5.5.3.9 Another potential area of concern is that the process vessels and equipment may introduce impurities due to corrosion. This risk can be minimized by proper selection of materials for compatibility with the fabrication procedure.

5.5.3.10 Biological growth in susceptible simulants can be controlled through the use of biocides.

5.5.3.11 Testing operations with the simulants may cause degradation or attrition of the material that are not associated with contamination and can be due to aging or interaction with test equipment. Performance metrics can be used to assess the degree of impact any such changes have to the test objectives. Simulant change out or selective dressing can be used should the changes render the simulant performance no longer representative.

5.5.3.12 Simulants can negatively impact test equipment, such as through abrasive wear or chemical compatibility. If these behaviors are not integral to process performance, alternate materials should be selected depending on the test system life cycle.

5.5.4 Care should be taken to make sure that the method of simulant transportation, storage environment, and the containers used to transport the simulants do not impact the simulant properties. The container materials of construction should be compatible with the simulant composition so as to not add corrosion products or leach contaminates into the simulant. Transportation and storage may also subject the simulant to environmental conditions (for example, heat, cold) that may need to be controlled to minimize the impacts of evaporation or freezing.

5.6 *Verify Simulant Meets Design Requirements:*

5.6.1 The performer of the work may document that the simulant has been verified. The documented simulant-verification activities may include:

5.6.1.1 Simulant generated using an approved simulant-preparation procedure;

5.6.1.2 Simulant necessary and sufficient properties were measured and compared to acceptance criteria. This portion of the simulant makeup process can include benchmarking the performance of the simulant against that of the actual material. This can utilize standardize methods, but consideration can also be given to comparing against a known performance of the actual hazardous material unique to the process being evaluated or prior evaluation or handling of the material being represented by the simulant. Examples may include a form of a pour test, mobilization/suspension test, slump test, or settling test that are designed to mimic a known process feed occurrence or observation during characterization of the material. Such tests can be a critical part of the verification process; and

5.6.1.3 All necessary and sufficient properties are within acceptance criteria specifications.

5.6.2 If in the initial testing of the simulant, not all of the necessary and sufficient properties are within the acceptance criteria specified in the simulant requirements specification, the performer of the work may work iteratively with cognizant project personnel to choose a path forward which may include a change to the acceptance criteria. All changes may be documented and controlled by a modified simulant requirements specification or simulant test plan, or both, consistent with project procedures.

5.6.3 All changes to testing may be documented and controlled by a modified simulant requirements specification or simulant development test plan, or both, consistent with project procedures.

5.6.4 For simulants in which the chemical composition is specified, the determination and reporting of the chemical composition of the simulant may rely on both the mass-balance and sample analyses together as a cross check. A batching process/sheet may be written that specifies the following:

5.6.4.1 The technical purity or grade of the beginning chemical constituents. This will require copies of each chemical's purity certifications and may require a confirmation of adsorbed water or waters-of-hydration;

5.6.4.2 The batching sequence and how and when to combine various sub-batches as necessary;

NOTE 1—For typical contaminants such as chloride, these ingredients should be added after the amount already present from the other chemicals added is known.

5.6.4.3 In-process sampling and analyses at key simulant-preparation points, as necessary (for example, analyze a nitrate solution before neutralizing and precipitating solids, or after a precipitation and washing sequence to verify the target values have been reached);

5.6.4.4 Review of completed batching sheet(s) by an independent, qualified individual; and

5.6.4.5 Results of the simulant analyses to verify the final batch composition for acceptance. The vendor or performer of the work should supply the confirmatory analysis results to the project in verification documentation.

5.6.4.6 Following preparation of the simulant, a confirmatory quantitative analysis may be performed on the simulant to verify that all components and their amounts were added correctly. This analysis is a final independent validation of the simulant composition. If the analysis indicates that the amount of an analyte component differs from its target amount by significantly more than the analytical uncertainty for that component, there is reason for concern that an error has occurred with the simulant preparation. Using both the mass balance (that is, batching sheets, chemical addition and weighing confirmation, and calculation verification) and actual chemical composition analysis will increase the probability of producing a simulant with an accurately known chemical composition. This will allow for informed decision making on whether to rely on the calculated or measured analyte value or to re-analyze. For example, an adjustment would not necessarily have to be made to a simulant-batch composition based upon a single out-of-tolerance analytical result if the mass-balance composition and batching sheets corroborated the majority of the analytical results. Disagreement between the measured analytical results and the mass balance or batching sheets due to errors in simulant preparation, however, could lead to a re-analysis and possible re-batching of the simulant. Potential errors in simulant preparation may include (*1*) incorrect chemical quantities or incorrect chemicals being added, (*2*) use of chemicals with poor quality or high levels of impurities, (*3*) use of chemicals with elevated levels of waters-of-hydration from excessive storage, or (*4*) use of starting chemicals that were not reported.

5.6.4.7 The prepared simulant composition should be certified to the previously agreed-upon set of analyte values. Typically, a graded range of analyte composition values is used for simulant preparation work; the graded range should be provided to the performer of the work in the simulant requirements specification before simulant-preparation work begins. An example of a graded range of analyte composition values for preparation of a melter-feed simulant may be ±5 % for major constituents (defined as analytes with concentrations >0.5 wt% on an elemental basis) and ±20 % for minor constituents (defined as analytes with concentrations <0.5 wt% on an elemental basis) known to not have an effect on the melter testing parameters to be studied.