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Standard Test Method for Accelerated Leach Test for Diffusive Releases from Solidified Waste and a Computer Program to Model Diffusive, Fractional Leaching from Cylindrical Waste Forms¹

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1. Scope

1.1 This test method provides procedures for measuring the leach rates of elements from a solidified matrix material, determining if the releases are controlled by mass diffusion, computing values of diffusion constants based on models, and verifying projected long-term diffusive releases. This test method is applicable to any material that does not degrade or deform during the test.

1.1.1 If mass diffusion is the dominant step in the leaching mechanism, then the results of this test can be used to calculate diffusion coefficients using mathematical diffusion models. A computer program developed for that purpose is available as a companion to this test method (Note 1).

1.1.2 It should be verified that leaching is controlled by diffusion by a means other than analysis of the leach test solution data. Analysis of concentration profiles of species of interest near the surface of the solid waste form after the test is recommended for this purpose.

1.1.3 Potential effects of partitioning on the test results can be identified through modeling, although further testing and analyses are required to determine the cause of partitioning (for example, if it occurs during production of the material or as a result of leaching).

1.2 The method is a modification of other semi-dynamic tests such as the IAEA test (1)² and the ANS 16.1 Leach Test wherein elevated temperatures are used to accelerate diffusive release to an extent that would only be reached after very long times at lower temperatures. This approach provides a mechanistic basis for calculating diffusive releases at repository-relevant temperatures over long times, provided that the leaching mechanism does not change with temperature.

1.2.1 Tests can be conducted at elevated temperatures to accelerate diffusive release and provide a mechanistic basis for calculating diffusive releases that would occur at lower temperatures over long times. Tests conducted at high temperatures allow the temperature dependence of the diffusion coefficient to be determined. They also demonstrate that the diffusion mechanism is rate-limiting through the measured extent of diffusive release.

1.2.2 Releases at any temperature can be projected up to the highest cumulative fractional release value that has been measured for that material (at any temperature), provided that the mechanism does not change. The mechanism is considered to remain unchanged over a range of temperatures if the diffusion coefficients show Arrhenius behavior over that range.

NOTE 1—A computer program in which the test results are evaluated using three diffusion models is briefly described in Annex A1 and in the Accelerated Leach Test Method and User's Guide for the "ALT" Computer Program (2). The data are fit with model equations for diffusion from a semi-infinite solid, diffusion from a finite cylinder, and diffusion with partitioning of the species of interest to determine effective diffusion coefficients and quantify the goodness of fit. The User's Guide contains several typographical errors; these are identified in Annex A1.

1.3 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.4 *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 and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 ASTM Standards:³

C1220 Test Method for Static Leaching of Monolithic Waste Forms for Disposal of Radioactive Waste

¹ This test method 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 The boldface numbers in parentheses refer to the list of references at the end of this standard.

³ 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.

D1193 Specification for Reagent Water

2.2 ANSI/ANS Standard:

ANSI 16.1 Measurement of the Leachability of Solidified Low-Level Radioactive Wastes by a Short-Term Test Procedure⁴

3. Terminology

3.1 Definitions:

3.1.1 *cumulative fraction leached*—the sum of the fractions of a species leached during all sampling intervals prior to and including the present interval divided by the amount of that species in the test specimen before the test.

3.1.2 *diffusion coefficient (diffusivity)*—an intrinsic property of a species that relates (1) its concentration gradient to its flux in a given medium (Fick's first law), (2) its spatial rate of change in the direction of the concentration gradient to the time rate of change in its concentration in a given medium (Fick's second law), or (3) its mean square displacement to time in a given medium (the Einstein equation).

3.1.3 *effective diffusion coefficient (D_e)*—the diffusion coefficient as modified by other processes (for example, adsorption) or physical constraints (for example, tortuosity and constrictivity).

3.1.4 *finite cylinder (finite medium)*—a bounded body for which Fick's diffusion equation can be solved.

3.1.5 *incremental fraction leached*—the amount of a species leached during a single sampling interval divided by the amount of that species in the test specimen before the test.

3.1.6 *leachant*—the initial solution with which a solid is contacted and into which the solid dissolves or is leached.

3.1.7 *leachate*—the final solution resulting from a test in which a solid is contacted by a solution and leaches or dissolves.

3.1.8 *leaching*—the preferential loss of components from a solid material into solution leaving a residual phase that is depleted in those components, but structurally unchanged.

3.1.9 *leaching interval*—the length of time during which a given volume of leachant is in contact with a specimen.

3.1.10 *leaching mechanism*—the set of processes that controls the rate of mass transport of a species out of a specimen during leaching.

3.1.11 *matrix material*—the solid material used to immobilize the waste or species of interest.

3.1.12 *reference leach test*—a leach test conducted under defined conditions, the results of which are used as a standard against which the results of other leach tests are compared. In this test method, a reference leach test is one that is conducted at 20°C using demineralized water.

3.1.13 *semi-dynamic leach test*—a leach test method in which the specimen is exposed to fresh leachant on a periodic schedule.

3.1.14 *semi-infinite medium*—a body having a single planar surface and extending infinitely in the directions parallel to the surface and in one direction normal to the surface.

3.1.15 *source term*—in this test method, the concentration of a species of interest in a specimen prior to leaching.

3.1.16 *specimen volume*—for purposes of this test method, the volume of a monolithic specimen calculated from macroscopic measurements of its dimensions by assuming a simple geometric shape, such as a right circular cylinder.

3.1.17 *surface area*—for purposes of this test method, the geometric surface area of a monolithic specimen that is calculated from macroscopic measurements of its dimensions by assuming a simple geometric shape, such as a right circular cylinder.

3.1.18 *waste form*—the waste material and any encapsulating or stabilizing matrix in which it is incorporated.

4. Summary of Test Method

4.1 This test method is a semi-dynamic leach test in which a cylindrical specimen is immersed in a leachant that is completely replaced after specified intervals. The concentration of an element of interest in the recovered test solution is measured after each exchange; this is referred to as the *incremental fraction leached (IFL)*. The accumulated amount of the species of interest in the intervals prior to and including the interval of interest is analyzed to determine if the release from the solid can be described using a mass diffusion model. The amount accumulated through a particular test duration is referred to as the *cumulative fraction leached (CFL)*.

4.2 Tests at a single temperature are adequate to compare the leaching behaviors of different materials.

4.3 The results of tests at repository-relevant temperatures can be extrapolated to long times if data from tests run at elevated temperatures and data from tests run at the reference temperature (20°C) can be modeled using a diffusion model and the diffusion coefficients show Arrhenius behavior.

4.3.1 Elevated temperatures are used to accelerate the release of a species of interest and collect enough data to show that the release is controlled by diffusion and determine the value of the diffusion coefficient.

4.3.2 Tests must be performed at a minimum of three temperatures to verify that the leaching mechanism does not change over that temperature range.

4.3.3 By generating data over a range of temperatures, an Arrhenius plot can be produced to interpolate values of the diffusion coefficient within the temperature range that was tested. Values cannot be extrapolated to temperatures that are higher or lower than the temperature range spanned by the tests.

4.3.4 A computer program that plots the experimental data and a regression curve calculated using a finite cylinder model (2) is available from ASTM (see Note 1). The program provides the value of the effective diffusion coefficient, the modeled *IFL* and *CFL* values, and a measure of the goodness of fit of the model.

⁴ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, <http://www.ansi.org>.

4.4 If the data from the accelerated tests, the reference test, and the fit of the modeled curve agree within defined criteria, the leaching mechanism can be taken to be diffusion-controlled and a diffusion model can be used to calculate releases from full-scale waste forms for long times.

4.4.1 The accelerated leach test provides the maximum cumulative fractional release to which the modeled data can be extrapolated. The maximum cumulative fractional release measured represents the maximum extent of reaction for which the consistency of the mechanism has been verified for that material.

4.4.2 Because the cumulative fraction leached is a function of the specimen surface area-to-volume ratio, the results of tests with the small-scale specimens used in the ALT directly represent leaching from large-scale waste forms having the same aspect ratio.

4.4.3 The effective diffusion coefficient can be used to calculate diffusive releases from waste forms with other shapes.

4.5 If the diffusion model does not fit the data within defined criteria, no extrapolation can be made in time or specimen size. However, other models can be applied to the data to evaluate the leaching process.

4.5.1 A model including diffusion with partitioning of the species of interest between phases having different release behaviors is included in the computer program (2).

4.5.2 The possibility of a solubility-limit to the release of the species of interest is addressed in the computer program (2).

4.6 If the data cannot be fit with a diffusion model within the defined criterion, then graphical comparisons of the data are recommended for added insight: For example, a plot of the cumulative fraction leached (*CFL*) from ALT conducted at an elevated temperature against the *CFL* from ALT conducted at the reference temperature can be used to verify that the accelerated data are consistent with the reference data and that the accelerated test appropriately accelerates the release, even though the release is not diffusion-limited.

5. Significance and Use

5.1 This test method can be used to measure the release of a component from a cylindrical solidified waste form into water at the reference temperature of 20°C and at elevated temperatures that accelerate the rate and extent of leaching relative to the values measured at 20°C.

5.2 This test method can be used to:

5.2.1 Compare releases of waste components from various types of solidification agents and formulations.

5.2.2 Determine the diffusion coefficients for the release of waste components from waste forms at a specific temperature.

5.2.3 Promote greater extents of reaction than can be achieved under expected service conditions within a laboratory time frame to provide greater confidence in modeled diffusive releases.

5.2.4 Determine the temperature dependence of diffusive release.

5.3 Fitting the experimental results with a mechanistic model allows diffusive releases to be extrapolated to long times and to full-scale waste forms under the following constraints:

5.3.1 Results of this test method address an intrinsic property of a material and should not be presumed to represent releases in specific disposal environments. Tests can be conducted under conditions that represent a specific disposal environment (for example, by using a representative groundwater) to determine an effective diffusion coefficient for those conditions.

5.3.2 Projections of releases over long times requires that the waste form matrix remain stable, which may be demonstrated by the behavior of the specimen in ALTs at elevated temperatures.

5.3.3 Extrapolations in time and scale are limited to values that correspond to the maximum *CFL* value obtained in an accelerated test.

5.3.4 The mechanism must be the same at all temperatures used in the extrapolation. The same model that describes the results of tests conducted at elevated temperatures must also describe the results of tests run at the reference temperature of 20°C.

6. Apparatus

6.1 A forced-air environmental chamber or a circulating water bath capable of controlling leachant temperatures to within 1°C of the target test temperature shall be used.

6.2 *Balance*—The balance shall be accurate to 0.1 % of the test load.

7. Reagents and Materials

7.1 *Leachant*—The leachant can be selected with regard to the material being tested and the information that is desired. Demineralized water, synthetic or actual groundwaters, or chemical solutions can be used. The effects of the leachant solution on the species of interest (that is, the species for which the diffusion coefficient is to be measured) and the solid must be considered. For example, the leachant should not degrade the host solid. In general, the leachant should be devoid of the species of interest to minimize solution feedback and solubility limit effects. If the leachant does contain a non-negligible amount of the species of interest, blank tests should be conducted to provide background concentrations to calculate the amounts released from the solid by using the concentrations measured in the tests. If demineralized water is used, it must meet or exceed the standards for types II or III reagent water specified in Specification **D1193**.

7.2 *Leaching Containers*—Leaching containers shall be made of a material that does not react with the leachant, leachate, or specimen. It is particularly important to select materials that are not susceptible to plate-out of species of interest from solution. High density polyethylene has been found to be a suitable container material. The top of the container shall fit tightly to minimize evaporation. The mass of the vessel must be checked before sampling to verify that evaporative losses are less than 1 % of the leachant mass (or volume) over every test interval.

7.3 *Specimen Supports*—Supports for the specimens shall be made of a material that does not react with the leachant, leachate, or specimen and is not susceptible to plate-out. The method of support should not impede leaching by contacting more than 1 % of the surface area of the specimen. Moreover, the support should not interfere with the removal and replacement of the leachate.

7.3.1 It is often convenient to suspend the waste form from the cover of the leaching container using monofilament string.

7.3.2 Alternatively, samples can be placed on perforated or mesh stands.

7.4 *Sample Containers*—Containers to hold aliquots of leachate for storage prior to analysis should not be susceptible to plate-out of radionuclides. The container must allow for adequate preservation of the leachate and specimen.

7.5 *Stirrers*—Stirrers are used to homogenize the leachate solution prior to removing aliquots for analysis.

7.6 *Filtration Equipment*—If filtration of visible particulates in the leachate is required, the filter medium should be capable of removing particulates that are 0.45 μm in diameter or larger. Disposable syringe filters are recommended. Tests must be conducted to determine if the filter and the filtration apparatus adsorb a significant amount of the species of interest. It may be necessary to pre-condition each filter with a sacrificial volume of the leachate solution to saturate sorption sites in the filter.

8. Specimens

8.1 Right circular cylindrical specimens shall be used with a diameter-to-height ratio between 1:1 and 1:2. This shape is used to facilitate modeling the test results. A convenient size is 2.5 cm diameter by 2.5 cm height. Smaller specimen sizes should not be used to avoid producing nonhomogeneous samples.

8.2 To the extent possible, the specimens should be prepared using the same techniques as those used to produce full-scale waste forms. For example, the curing conditions used to prepare laboratory-scale specimens should match those used for actual waste forms as closely as possible, especially the temperatures experienced by the large waste forms.

8.3 Specimens shall be representative of the full-scale solidified waste form. Particular attention should be paid to ensuring that the species of interest is homogeneously distributed in the material being tested. Test specimens can be cut from a larger sample or cast individually.

8.4 Many solids prepared by casting form a skin on the outer surface during preparation that has different characteristics than the bulk material. The effect of the skin must be determined and differentiated from the bulk property. This can be done by conducting separate tests using samples with surfaces that are representative of the structure of surfaces of large waste forms, such as surfaces that are cast against container walls, and tests with samples having cut or polished surfaces that expose the bulk material to the leachant. The effect of the skin can be determined from differences in the derived diffusion coefficients for materials with and without the skin.

8.5 A minimum of three replicate tests should be conducted at each temperature if results are to be used to predict long-term behavior.

8.6 The dimensions, weight, composition, curing history, and other pertinent information that could affect performance shall be recorded for each specimen.

8.7 Accurate determination of the amount of the species of interest in the specimen at the start of the leach test shall be made and recorded.

8.8 If a specimen is prepared in a mold, any excess material should be removed from the specimen prior to weighing it.

8.8.1 If the quantity of the species of interest in the specimen (that is, the source term) was determined before the specimen was removed from the mold, the amount of that species that remained in the mold (plus material removed as excess) shall be determined and the amount accounted to be in the specimen adjusted.

9. Procedure

9.1 The dimensions of each specimen shall be measured with a calibrated device (for example, digital calipers) to the nearest 0.01 cm. At least two measurements of the diameter shall be made at the top and bottom of the specimen and two measurements of the height at diametrically opposite locations. The geometric surface area and volume are calculated by modeling the specimen as a right circular cylinder and using the arithmetic averages of the measured diameters and heights.

9.1.1 The surface area and volume of the specimen are used to calculate the diffusion coefficient (see A1.3.2.1).

9.1.2 The uncertainty in the surface area and volume of the specimens contribute to the uncertainty in the diffusion constant and should be quantified, for example, by using the propagation of errors method or, preferably, that developed by the International Committee for Weights and Measures (CIPM) and promulgated by NIST (3) ; see Annex A2.

9.1.3 The surface area and volume used to model the results can be adjusted to take into account deviations in the specimen shape from an ideal right circular cylinder based on additional measurements and geometric calculations.

9.2 *Leachant Volume*—The leachant volume is selected based on the specimen surface area and an estimate of the leach rate. The volume must be low enough that the solution concentrations that are generated during the test can be analyzed, but high enough that solution feedback effects on leaching are negligible (that is, so that the chemical gradient between the solid and solution remains nearly constant). The solution mass can be measured and used to calculate the volume if the solution density is known.

9.2.1 The solution volume is not used directly in the calculation of the diffusion constant, but is used to calculate the mass of the species of interest from the measured solution concentration.

9.2.2 The specimen surface area-to-solution volume must remain the same for all test intervals in an ALT to ensure that any impacts of solution feedback and solubility limitation are similar during each test interval.

9.2.3 The specimen size and solution volume must be selected by compromising the benefits of using a large specimen (ease of fabrication, uniformity of specimens, ease of sampling reacted materials, etc.) with the complications of large solution volumes (handling, analytical limitations, waste disposal, etc.).

9.2.4 The effects of solution feedback and solubility limits can be identified (or mitigated) by conducting tests at different specimen surface area-to-leachant volume ratios. Solution feedback effects are expected to be more significant at higher temperatures and surface area-to-leachant volume ratios.

9.2.5 For example, to replicate the standard conditions in the Test Method **C1220** static leach test, the leachant volume (in cm³) used for each interval must be 10× the surface area of the specimen (in cm²) as calculated below:

$$\frac{\text{Specimen surface area (cm}^2\text{)}}{\text{Leachant volume (cm}^3\text{)}} = \frac{1 \text{ cm}^2}{10 \text{ cm}^3} = 0.1 \text{ cm}^{-1} \quad (1)$$

9.2.5.1 This ratio requires a very large volume of water for specimens of even moderate size. For example, a 2.5 × 2.5 cm cylindrical specimen having a surface area of 29.45 cm² would require 294.5 mL of solution for each of the 11 test durations. Specimens that are much larger than this and tests at lower surface area-to-leachant volume ratios will require volumes of water that need sophisticated means of wastewater handling (such as peristaltic pumps for draining the containers), since large volumes may be too unwieldy for pouring.

9.2.6 Large volumes of leachant can make analysis challenging, even for major constituents of the specimen, and present unnecessary waste disposal costs. Under these circumstances, higher specimen surface area-to-leachant volume ratio may be used. The leach rates of some waste form materials may be low enough that a specimen surface area-to-leachant volume ratio higher than 0.1 cm⁻¹ must be used to generate measurable solution concentrations.

9.2.7 The user must verify that solution feedback effects or solubility limits do not affect the results. Solution feedback effects (or solubility limits) are considered negligible if the same value of D_e , within experimental uncertainty, is obtained for tests conducted at different specimen surface area-to-leachant volume ratios.

9.3 *Temperature*—For materials and formulations that have not been tested previously, leach tests shall be conducted at a minimum of three temperatures to establish that the leach rate increases systematically with higher temperatures. One temperature must be 20°C. The other temperatures should be selected based on knowledge of the material being tested. For example, the recommended maximum temperature is 50°C for cementitious materials, which is below the threshold of anomalous releases observed previously (3). Temperatures above 50°C can be used if it is demonstrated that the leaching mechanism does not change.

9.3.1 The controlled-temperature device must maintain a temperature within 1°C of the desired temperature throughout the test (except for short-term perturbations with the vessels are removed for sampling). The temperature shall be recorded

either before the vessel is placed in the device at the beginning of a test interval or before it is removed at the end of a test interval.

9.3.2 The time required for the device to return to the set temperature after it is opened (for example, to emplace or remove a test vessel) should be noted, even though the vessel may not have attained that temperature. The time required to heat the specimen to relatively high test temperatures may be a significant fraction of the first two test intervals (2 and 5 hours).

9.4 *Leachant Replacement*—Leachant replacements shall take place at the following time intervals: 2 hours, 5 hours, 17 hours, and 24 hours, and then daily for the next 10 days, for a total test duration of 11 days. The times at which the specimen is removed from the leachate and placed in the fresh leachant should be noted to the nearest minute. The times at which the vessel is removed from and emplaced in the controlled-temperature device should be noted to the nearest minute. The use of an electric clock or a watch is adequate.

9.4.1 If the specimen is suspended from the top of the container, the most convenient method for changing the leachant is to lift off the cover (with the specimen still attached) and place it on a new container with the appropriate volume (or mass) of fresh leachant. The new leachant may be pre-heated to the test temperature (if practical). The new container can be sealed and placed into the temperature-controlled environment immediately. During leachant changes, the specimen should be exposed to air for as short a time as possible. Rinsing the sample prior to transfer is not necessary.

9.4.2 If the specimen is at the bottom of the test container, the leachate can be decanted into a collection container and the sample recovered with forceps and placed immediately into another test container with pre-heated leachant (is not necessary to rinse the specimen). The new test container can be sealed and placed into the controlled-temperature device.

9.4.3 The mass of the assembled vessel shall be measured before the vessel is placed in the controlled-temperature device at the start of a test interval and when the vessel is removed at the end of the test interval. The difference in mass provides a measure of the loss of leachate solution due to evaporation (see 7.2).

9.5 *Acid Strip*—At least one vessel bottom shall be subjected to an acid strip at the end of a test interval to verify that the species of interest is not sorbing to the vessel. If the amount sorbed is not negligible, the vessel shall be acid-stripped after every sampling, and the amount of the species of interest recovered in the acid strip shall be added to the amount in the leachate.

9.5.1 Discard any remaining leachate solution from the vessel and rinse with demineralized water.

9.5.2 Fill vessel with an amount of demineralized water equal to or greater than the amount of leachate that was removed.

9.5.3 Add the appropriate amount of concentrated ultrapure nitric acid to produce a 2 volume% acid solution.

9.5.4 Cap the container and agitate, then let settle for several minutes.

9.5.5 Collect a sample of the acid strip solution for analysis.

9.6 *Leachate Sampling*—Immediately after opening the vessel, the old leachate should be stirred thoroughly and sampled quickly to minimize any artifacts that could occur during cooling (for example, precipitation). Several aliquots may be required at each sampling for desired analyses.

9.6.1 If the specimen is suspended from the vessel lid, place the lid on the vessel with fresh water and initiate the next test interval before removing aliquots of the leachate for analysis.

9.6.2 If the specimen is placed on a stand at the bottom of the vessel, stir solution and remove aliquots of the leachate for analysis before initiating the next test interval.

9.6.3 The solution aliquots should be collected and preserved in ways appropriate for the analytical technique(s) to be employed.

9.6.4 If particulates are visible in the leachate, it is necessary to account for the quantity of the species of interest associated with them.

9.6.4.1 If the particulates form by spalling from the specimen, they should be removed prior to analyzing the solution and the species of interest associated with the spalled material should be excluded from the amount released.

9.6.4.2 If the particulates formed after the species of interest were leached, two approaches can be used. One requires filtration of the leachate and subsequent analysis of both the filtrate and the particulate material on the filter. The other is to acidify the leachate to dissolve the particulates and thereby include the associated species of interest in the analyzed solution. One or both methods can be used (for example, analyze filtered and unfiltered solutions), depending on the information desired.

9.7 *Analysis and Standards*—Analysis of the leachate for the species of interest shall be conducted by standard methods and using appropriate calibration standards. If necessary, standards should be prepared to match the matrix elements in the samples. For radioactive specimens, a series of waste reference solutions can be prepared by diluting an aliquot of the original solution (or waste) that was used to make the specimens for comparative analysis. The analytical results for the test samples can then be compared directly to analytical results for these reference solutions to calculate fractional releases without the need for absolute standards, detector efficiencies, or decay corrections.

9.8 *Standard Test*—One or more ALTs with an equivalent specimen shall be conducted at 20°C for use as a standard for comparison with ALTs conducted at other temperatures and ALTs conducted with other materials. Triplicate standard tests at 20°C are required if the results will be used to project releases to long durations or larger waste forms.

9.9 *Blank Test*—Depending on the species of interest, a blank test with either no specimen or with a specimen that does not contain the species of interest is recommended to provide background solutions to help detect contamination that may occur during the procedure or provide background levels for leachants that contain the species of interest.

10. Calculations

10.1 *Incremental Fraction Leached*—The incremental fraction of species i leached (IFL) during test interval n is calculated by using Eq 2:

$$IFL = \frac{i^a_n}{i^a_0} \quad (2)$$

where:

i^a_n = the quantity of species i measured in the leachate from the n th test interval, and

i^a_0 = the quantity of species i in the specimen at the beginning of the test.

In the case of radionuclide i , both terms must be corrected for radioactive decay to the beginning of the test.

10.1.1 It may be necessary to calculate the value of i^a_n from the measured solution concentration using the leachant volume. In that case, the uncertainty in the measured concentration and the uncertainty in the leachant and leachate volumes must be taken into account. (See Annex A2.)

10.1.2 The average rate of release for any interval can be calculated by dividing IFL by the duration of that interval. The rate can then be divided by the surface area of the specimen to obtain the average fraction released per area per time. This allows comparisons of tests conducted with samples having different surface areas.

10.2 *Cumulative Fraction Leached*—The cumulative fraction of species i leached through the j th interval (CFL_j) is calculated by using Eq 3:

$$CFL_j = \frac{\sum_{n=1}^j i^a_n}{i^a_0} = \sum_{n=1}^j IFL_n \quad (3)$$

NOTE 2—The indices for the species and interval are excluded for convenience hereafter.

10.2.1 Plotting the CFL value for each interval against the cumulative time provides a graphical comparison of data from various tests with each other and with modeling results. An example of this type of plot is shown in Fig. 1.

10.3 *Effective Diffusion Coefficient*—The results of this test method can be used to determine the effective diffusion coefficient (D_e) for the release of the species of interest based on a model. A computer program has been developed at Brookhaven National Laboratory to calculate a best fit effective diffusion coefficient (D_e) based on the equations for diffusion from a semi-infinite medium or from a finite cylinder (4). The ALT computer program also evaluates the possible influence of partitioning and solubility limits on the diffusive release. That program is available from ASTM for use with this test method (2); see also (5, 6). The computer program determines the value of the effective diffusion coefficient by regressing analytical expressions for diffusion from a semi-infinite solid and from a finite cylinder to the CFL determined from the test results. The analytical expressions are provided in Annex A1. The uncertainty in the diffusion coefficient can be calculated using the formula for diffusion from a semi-infinite solid.

10.4 *Agreement with Models*—The CFL values calculated using values of D_e determined from the data using the diffusion