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Standard Guide for
Comparison of Techniques to Quantify the Soil-Water (Moisture) Flux[1]

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1. Scope

1.1 This guide describes techniques that may be used to quantify the soil-water (or soil-moisture) flux, the soil-water movement rate, and/or the recharge rate within the vadose zone. This guide is not intended to be all-inclusive with regard to available methods. However, the techniques described do represent the most widely used methods currently available.

1.2 This guide was written to detail the techniques available for quantifying soil-moisture flux in the vadose zone. These data are commonly required in studies of contaminant movement and in estimating the amount of water replenishing a renewable ground-water resource, that is, an aquifer. State and federal regulatory guidelines typically require this information in defining contaminant travel times, in performance assessment, and in risk assessment. Both unsaturated and saturated flow modelers benefit from these data in establishing boundary conditions and for use in calibrations of their computer simulations.

1.3 This standard is one of a series of standards on vadose zone characterization methods. Other standards have been prepared on vadose zone characterization techniques.

1.4 *This guide offers an organized collection of information or a series of options and does not recommend a specific course of action. This document cannot replace education or experience and should be used in conjunction with professional judgment. Not all aspects of this guide may be applicable in all circumstances. This ASTM standard is not intended to represent or replace the standard of care by which the adequacy of a given professional service must be judged, nor should this document be applied without consideration of a project's many unique aspects. The word "Standard" in the title of this document means only that the document has been approved through the ASTM consensus process.*

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

2. Referenced Documents

2.1 *ASTM Standards:*

D 653 Standard Terminology Relating to Soil, Rock, and Contained Fluids[2]

D 1452 Practice for Soil Investigations and Sampling by Auger Boring[2]

D 2216 Test Method for Laboratory Determination of Water (Moisture) Content of Soil and Rock by Mass[2]

D 3404 Guide to Measuring Matric Potential in the Vadose Zone Using Tensiometers[2]

D 4643 Test Method for Determination of Water (Moisture) Content of Soil by the Microwave Oven Heating [2]

D 4696 Guide for Pore-Liquid Sampling from the Vadose Zone[2]

D 4700 Guide for Soil Sampling from the Vadose Zone[2]

D 4944 Test Method for Field Determination of Water (Moisture) Content of Soil by the Calcium Carbide Gas Pressure Tester Method[2]

D 5126 Guide for Comparison of Field Methods for Determining Hydraulic Conductivity in the Vadose Zone[2]

D 5220 Test Method for Water Content of Soil and Rock In-Place by the Neutron Depth Probe Method[2]

3. Terminology

3.1 *Definitions:*

3.1.1 *chlorine-36, ^{36}Cl*—a radioactive isotope of chlorine, containing one extra neutron in the nucleus, and a decay half-life of 300,000 years.

3.1.2 *deuterium, ^{2}H*—a stable isotope of hydrogen, containing one extra neutron in the nucleus.

3.1.3 *oxygen-18, ^{18}O*—a stable isotope of oxygen, containing two extra neutrons in the nucleus.

3.1.4 *recharge flux, (LT^{-1})*—the soil-moisture flux of water moving through the vadose zone, beneath the zone of evapotranspirative uptake, which eventually replenishes water to an underlying aquifer.

3.1.5 *soil-moisture flux, (LT^{-1})*—synonymous with specific discharge.

3.1.6 *specific discharge, (LT^{-1})*—the rate of flow of water through a porous medium per unit area measured at a right angle to the direction of flow. **(D 653)**

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[2] *Annual Book of ASTM Standards,* Vol 04.08.

3.1.7 *specific flux, (LT^{-1})*—synonymous with specific discharge.

3.1.8 *tritium, ^{3}H*—a radioactive isotope of hydrogen, containing two extra neutrons in the nucleus, and a decay half-life of 12.3 years.

3.2 Definitions of other terminology used in this guide may be found in Standard D 653.

4. Summary of the Guide

4.1 The quantitative techniques described for assessing soil-moisture flux are:

4.2 *Water Balance Methods*—The water balance method is based on the mass balance of input/output parameters in the hydrologic budget. The hydrologic budget for any given locale may be summarized in terms of the influence of the following factors/phenomena: precipitation, runoff, infiltration, evapotranspiration, interflow, sources/sinks, and recharge rate. Soil-moisture flux may be estimated by determining all parameters in the hydrologic budget (for example, precipitation rate) except the desired flux term, which is solved by differencing the water balance equation. One or more of the parameters needed in the water balance method are typically difficult to estimate, and therefore cause significant uncertainties when estimating soil-moisture flux with this method.

4.3 *Chloride Mass-balance Method*—The chloride mass-balance method is similar to the water balance method in that mass balance concepts are employed. However, the chloride mass-balance approach relies upon the transport of chloride in soils to predict soil-moisture flux based on a knowledge of chloride deposition at the land surface. The uncertainties associated with chloride deposition and transport are much less than the uncertainties associated with estimating components of the hydrologic budget.

4.4 *Soil-Physics Based Approaches*—A multitude of soil-physics based approaches exist to quantify the soil-moisture flux. These techniques rely upon indirect measures of soil-water movement, for example, physical data such as moisture content and pressure head, as input to mathematical equations to solve for the flux. The Darcy's Law approach is most commonly used, with variants on this method employed in infiltration quantification, for example, Green and Ampt equation. A more rigorous approach to estimating the soil-moisture flux is to employ Richard's equation, a transient, non-linear formulation describing flow through unsaturated porous media. Unsaturated hydraulic characteristic data required as input to these soil-physics based methods can be very uncertain with regard to spatial variability and/or measurement error.

4.5 *Bomb-pulse Tritium and Chlorine-36 Methods*—Environmental tracers may also be used to estimate the soil-moisture flux. Tritium (a radioactive isotope of hydrogen) and chlorine-36 (a radioactive isotope of chlorine) exist today in the environment because of natural processes in the earth's atmosphere. However, the atmospheric nuclear testing which occurred in the late 1950s and early 1960s created much higher concentrations of these radioisotopes in atmospheric fallout than normal. By sampling the concentrations of these radioisotopes in subsurface soils one can determine the extent of infiltration over the past 30 to 40 years, and therefore quantify the soil-moisture flux.

4.6 *Stable Isotope Methods*—Another environmental tracer technique employs knowledge of naturally occurring deuterium (a stable isotope of hydrogen) and oxygen-18 (a stable isotope of oxygen) in the water molecule and how transport processes occur in subsurface soils. Because deuterium and oxygen-18 are natural components of the water molecule, and their behavior during evaporation and transient temperature phenomena are understood, the soil-moisture flux may be quantified based on this knowledge.

4.7 *Other Tracer Techniques*—Other tracer techniques exist to quantify the soil-moisture flux. In this category, techniques are discussed which physically introduce a tracer, or chemical constituent, into infiltration water or directly into the subsurface to monitor soil-water movement over a specified time frame. Tracers such as bromide, chloride, certain organic compounds, certain short-lived radionuclides, and tritium may be used in these types of tests. Obviously, the application of tracers in a man-made experiment has limitations on the length of analysis time. These techniques are best used to investigate shorter time-frame infiltration and soil-water movement rates, as well as adsorption phenomena.

5. Significance and Use

5.1 The determination of the soil-moisture flux is one of the fundamental needs in the soil physics and hydrology disciplines. The need arises from requirements for defining recharge rates to ground water for water supply predictions, for contaminant transport estimates, for performance/risk assessment studies, and for infiltration testing purposes. The techniques outlined in this guide provide a number of alternatives for quantifying soil-moisture flux and/or the recharge rate for various purposes and conditions. This guide is not intended to be a comprehensive guide to techniques available for quantifying soil-moisture flux, but rather a "state-of-the-practice" summary. Likewise, this guide is not intended to be used as a comprehensive guide to performance of these methods, those detailed methods may come at a later time. Techniques that might be useful for the implementation of these methods, for example, sampling network design, are not part of this guide, but may come at a later time.

5.2 All of the techniques discussed in this guide have merit when it comes to quantification of the soil-moisture flux. Factors influencing the choice of methods include: need/objectives; cost; time scale of test; and defensibility/reproducibility/reduction in uncertainty. If the need for soil-moisture flux information is crucial in the decision making process for a give site or study, the application of multiple techniques is recommended. Most of the techniques identified above have independent assumptions associated with their use/application. Therefore, the application of two or more techniques at a given site may help to bound the results, or corroborate data distributions. The uncertainties involved in these analyses are sometimes quite large, and therefore the prospect of acquiring independent data sets is quite attractive.

5.3 As stated above, each of these techniques for quantification of soil-moisture flux has assumptions and limitations associated with it. The user is cautioned to be cognizant of those limitations/assumptions in applying these techniques at a given site so as not to violate any conditions and thereby invalidate the data.

5.4 In general, the tracer techniques for quantifying soil-moisture flux will have less uncertainty associated with them than do the soil-physics based modeling approaches because they are based on direct measures of transport phenomena, rather than indirect measures of soil characteristic data/parameters. However, the forward problem of predicting future soil-water movement rates or transient behavior is best served by the modeling applications. The tracer methods may be used to calibrate, or supply boundary condition data to, the modeling techniques.

5.5 Published reviews of these methods are also available in the literature **(1, 2, 3)**.

6. Quantitative Techniques

6.1 This standard is not intended for use as a specific guide to field operations, but as a guide to choosing one or more appropriate methods for quantifying the soil-moisture flux, soil-water movement rate, and/or the recharge rate. Therefore, issues regarding the selection of sampling locations and the adequacy of sampling, for example, sampling network design, are outside the scope of this guide.

6.2 *Water Balance Methods*

6.2.1 *Theory*

6.2.1.1 The technique that was typically employed in water resources planning to estimate the rate and amount of recharge to an aquifer was the water balance approach. In this method, all inputs and outputs to the aquifer are estimated, for example, precipitation, evapotranspiration, surface runoff, pumping, discharge, and interflow, and the interrelationship between the parameters derived from simple mass-balance concepts. The water balance equation for a given watershed may be represented as follows:

$$R = P + I - ET + Sr_{on} - SR_{off} + L_{on} - L_{off} - \Delta S \quad (1)$$

where:

R = recharge rate or soil-moisture flux below the root zone [L/T],
P = precipitation rate [L/T],
I = irrigation water application [L/T],
ET = evapotranspiration rate [L/T],
SR_{on} = surface water runon [L/T],
SR_{off} = surface water runoff [L/T],
L_{on} = interflow (water laterally entering the zone of interest) [L/T],
L_{off} = interflow (water laterally leaving the zone of interest) [L/T], and
ΔS = change in soil moisture storage [L/T]. The water balance equation is then solved for the recharge rate.

6.2.1.2 The main drawback to this approach is that parameters such as evapotranspiration are very difficult to measure or estimate. There is a large amount of uncertainty in evapotranspiration estimates. This uncertainty in the input parameters then translates into a large uncertainty in the recharge estimate. Therefore, independent methods for estimating the recharge rate have been developed. The water balance method may be used to solve for any of the parameters shown in Eq 1, given estimates for the other parameters. There may be some applications (discussed below) which may employ other methods to estimate the recharge rate and then to solve for evapotranspiration, for instance. The water balance approach is basically a mass balance method. Eq 1 has also been used in more simplified form for smaller scale, test-specific applications to define soil-moisture flux. Infiltration techniques, such as the instantaneous profile (IP) method **(4)**, rely on water balance methods to estimate soil-moisture flux. The IP method, and its variants, are generally used to quantify hydraulic characteristic data, such as the unsaturated hydraulic conductivity as a function of moisture content. In so doing, the soil-moisture flux is quantified by a mass balance method and used as input to a mathematical/graphical procedure to determine the hydraulic characteristic data. Data requirements generally include the determination of moisture content and pressure head in situ. Neutron logging, Time Domain Reflectometry, Resonant Frequency Capacitance, and cross-hole gamma methods may be used to quantify changes in soil moisture with time (ASTM D18.21.89.16 and D18.21.89.17). Tensiometers are used for the determination of the pressure head changes during the IP test (Guide D 3404). In the IP method, the drainage portion of the infiltration test is the most important data gathering sequence, when inflow, surface runoff, interflow, discharge, and evapotranspiration are essentially zero. Therefore, changes in soil-moisture storage with time can be equated to soil-moisture flux.

6.2.1.3 Another application of the water balance method is in the use of weighing lysimeters **(5)**. The concept of a weighing lysimeter is relatively simple. Typically, a cylinder is emplaced in the ground filled with soil approximating the stratigraphy of the surrounding soil. The cylinder may be set on a weighing pan to quantify changes in weight/mass due to precipitation, evapotranspiration, and recharge/outflow. The lower boundary flux condition must be maintained equivalent to the surrounding media if natural conditions are to be approximated. Care must be taken in the construction of lysimeters to ensure that the potential for preferential flow along sidewalls is minimized. Weighing lysimeters are typically used to define evapotranspiration components.

6.2.2 *Applications*—Water balance methods are the simplest means of estimating the soil-moisture flux or recharge rate, but also probably the least accurate. The need for obtaining the soil-moisture flux, as well as the acceptable uncertainty, would help dictate the usefulness of this approach. The typical applications would be: *a*) to estimate the amount of renewable resource in a ground-water supply, that is, aquifer, for consumptive and/or industrial use, or agricultural activities, and *b*) to estimate boundary conditions for numerical flow simulations, where the flow simulations are performed for a specific need such as estimating travel times in an aquifer, or a pathways analysis in a performance and/or risk assessment, and *c*) to estimate the evapotranspiration rate by independently estimating the recharge rate (with techniques described below) for risk assessment purposes, that is, air pathway releases of volatile contaminants, and *d*) to estimate the soil-moisture flux during real-time infiltration testing, for example, IP method.

6.2.3 *Monitoring and Operating Procedures*

6.2.3.1 The water balance approach relies on independent measures/estimates of various parameters to calculate a residual parameter in a mass-balance equation. Typically, the recharge rate is the parameter of interest, but other techniques (described below) may also be used to estimate the recharge rate, thereby allowing other parameters to be estimated, for example, evapotranspiration rate.

6.2.3.2 The parameters typically estimated in the water balance method include precipitation, evapotranspiration, surface runoff, pumping/discharge rates, interflow, and changes in soil-moisture storage. Precipitation rates are quantified using conventional meteorological monitoring equipment.

6.2.3.3 Evapotranspiration rates can be estimated by several methods. First, there are empirical techniques based upon meteorological and soil moisture data **(6)**. These empirical techniques are fraught with uncertainty, and therefore precision and bias become a major issue in evaluating the adequacy of such methods. The second approach used in estimating evapotranspiration rates is the use of weighing lysimeters **(5)**. The basic concept behind a weighing lysimeter is that a volume of soil is placed in a caisson, emplaced in the ground with a weighing scale beneath it, and measurements of water gain/loss made through time. The caisson may contain specific plant types or bare soil. Differences in the weight of the caisson through time can be attributed to changes in the mass balance of water movement in the caisson. Outflow and inflow measurements are made, as well as soil moisture measurements to estimate the changes in soil-moisture storage. The analysis is essentially the water balance approach, only on a much smaller scale compared to that mentioned above. The problem with the weighing lysimeter methods is the applicability of measurements to actual field conditions. The boundary conditions of the caisson may not be entirely representative of the actual field conditions because of the lower boundary flux/head potential, constraints on multi-dimensional flow potential, and preferential flow potentials along the sidewalls. In addition, the evaporation rate may be estimated using stable isotope methods (discussed below), but are not conducive to quantifying transpiration.

6.2.3.4 Surface water runoff can be measured through stream gauging or by empirical modeling methods based on surface roughness and hydrologic characteristics. Some concerns exist regarding precision and bias for these methods, but generally the relative uncertainties are less than those associated with estimating evapotranspiration.

6.2.3.5 Interflow occurs when water is either entering or leaving the confines of the defined watershed as leakage from an adjacent watershed or an adjacent aquifer. Typically, interflow is estimated through the use of potentiometric surface maps (to quantify the hydraulic gradient) and hydraulic characteristic data, for example, transmissivity, to calculate inflow/outflow rates. Interflow may also be important as it pertains to lateral movement of moisture into and out of a defined vadose zone profile.

6.2.3.6 The change in soil-moisture storage may be quantified by a number of soil-moisture monitoring devices. Neutron logging, Time Domain Reflectometry (TDR), Resonant Frequency Capacitance, and cross-hole gamma methods may be used to quantify changes in soil moisture with time (ASTM D18.21.89.16 and D18.21.89.17).

6.2.4 *Analysis, Interpretation, Accuracy, and Reporting*—The application of the water balance method through the use of Eq 1 is done to estimate soil-moisture flux. In reporting the results, statements should be made regarding the conditions during monitoring/sampling events, the location of the sampling site and its attributes, for example, topography, terrain, vegetative cover, etc., a summary of the monitoring data, for example, meteorological and soil-moisture data, the accuracy and precision of the data used in evaluating Eq 1, as well as a general qualitative analysis of the representativeness of the results.

6.3 *Chloride Mass-balance Method*

6.3.1 *Theory*

6.3.1.1 The chloride mass balance method is a geochemical technique which has been widely used throughout the world to quantify the soil-moisture flux, due to its low cost and ease of use **(7, 8, 9)**. Two major assumptions are made in applying this technique. The first assumption is that the average rate of chloride deposition from precipitation to the soil is constant. The second assumption is that the chloride moves vertically by piston displacement, that is, no preferential flow paths, below the root zone. Under steady state conditions, the flux of chloride deposited at the land surface is equivalent to the flux of chloride beneath the root zone. Care must be taken to estimate the depth of the root zone, although no exact method is available. In semi-arid or arid environments the task is especially problematic due to the sometimes extreme depths that certain plants can develop root systems. Visual inspection of soil cores and/or analysis of pressure head profiles are sometimes used to estimate root zone depth. A methodology for determining root zone depth is beyond the scope of this guide, but might be included in a future test method to describe the actual application of this technique. Therefore:

$$R = P\,C_p / C_s \qquad (2)$$

where:

R = the average recharge rate, or soil-moisture flux, below the root zone [L T^{-1}]

P = average precipitation rate [L T^{-1}]

C_p = average chloride concentration in precipitation and dry fallout [M L^{-3}]

C_s = the average chloride concentration in the soil [M L^{-3}]

6.3.1.2 In addition to estimating the soil-moisture flux below the root zone, the chloride mass-balance approach may be used to estimate soil-water age with depth in the profile. The following equation may be used to estimate soil-water age:

$$t_n = \int_{z=n}^{z=0} C_s\,\theta / C_p\,P \qquad (3)$$

where:

θ = the moisture content, and

n = the total depth increment of the sampled soil profile at which a soil-water age is desired.

6.3.2 *Applications*—The chloride mass-balance method is generally applicable for quantifying soil-moisture flux below the root zone in non-humid locales. The application of the technique requires destructive soil sampling and subsequent analysis of the soil core for moisture content and chloride concentrations with depth through the profile.

6.3.3 *Monitoring and Operating Procedures*

6.3.3.1 The chloride mass-balance method relies on the determination of chloride concentrations and moisture content with depth in the soil profile. Care should be taken to ensure that the sampling event is performed when the soil profile is in quasi-steady state conditions, or in other words, the sampling should not take place following any major infiltration/wetting/redistribution events. Sampling following wetting events will tend to bias the results toward overestimation of the average soil-water flux, and underestimation of the average soil-water age. The topographical relief at the site should be evaluated for its potential impact to the method results. One of the assumptions behind the chloride mass-balance approach is that one-dimensional piston displacement is the dominant transport mechanism. If the topographical relief is great enough then multi-dimensional flow may be occurring in the subsurface, thereby potentially invalidating the results.

6.3.3.2 The moisture content and chloride concentration data are acquired from analysis of soil core samples, which are collected by destructive core sampling (Guide D 4700 or Practice D 1452, as appropriate). Moisture content determinations should be done in accordance with Test Method D 2216. Chloride concentrations are quantified by leaching the chloride from the soil sample, and the leachate analyzed by a titration technique or an Inductively Coupled Plasma/Mass Spectrometry (ICP/MS) analytical method to achieve the proper analytical sensitivity. Estimates of chloride deposition rates and concentrations at the land surface must be made from long-term meteorological information. These estimates may be somewhat uncertain, and the user should qualify the results based on this knowledge.

6.3.4 *Analysis, Interpretation, Accuracy, and Reporting*—The application of the chloride mass-balance method through the use of Eq 2 and 3 is done to estimate soil-moisture flux and the soil-water age with depth in the profile. Graphical display of the data is useful, and should include plots of chloride concentrations versus depth in the profile, cumulative chloride versus depth in the profile, cumulative chloride versus cumulative water content, and soil-water age versus depth in the profile. In reporting the results, statements should be made regarding the conditions of the soil sampling event, the location of the sampling site and its attributes, for example, topography, terrain, vegetative cover, etc., the subsurface sampling intervals, the accuracy and precision of the laboratory methods used to determine the moisture content and chloride concentrations, as well as general qualitative analysis of the representativeness of the results.

6.4 *Soil-physics Based Approaches*

6.4.1 *Theory*

6.4.1.1 A soil-physics based approach may be used to quantify the soil-moisture flux from measured or estimated hydraulic characteristic data. Soil-physics based approaches rely on the measurement of soil characteristics, for example, soil moisture, unsaturated hydraulic conductivity function, as input to a mathematical formulation for soil-moisture flux. The parameters measured are generally not direct measures of soil-water movement. Therefore, these techniques are indirect methods of estimating soil-moisture flux. Oftentimes, the data needs for these mathematical formulations are subject to significant uncertainty, due to spatial and/or temporal variability, and/or measurement error.

6.4.1.2 The most common, and basic, formulation for soil-moisture flux in porous media is Darcy's Law. Darcy's Law is the fundamental basis for many of the other techniques that exist for quantifying the soil-moisture flux. Therefore, it is appropriate to begin this discussion with a summary of the Darcy's Law approach. The mathematical basis for this analysis is the unsaturated form of Darcy's Law:

$$q = -(K(\theta,\psi))\, i = -(K(\theta,\psi))\,(dh/dz) = -(K(\theta,\psi))\,\frac{d(\psi+z)}{dz} \qquad (4)$$

where:

q = darcian flux [L/T],
$K(\theta,\psi)$ = unsaturated hydraulic conductivity [L/T], as a function of volumetric water content, θ [L^3/L^3], or pressure head, ψ [L],
i = hydraulic gradient [L/L], and $i = dh/dz$
h = total head [L], and $h = (\psi+z)$
z = depth below land surface [L]

6.4.1.3 Several assumptions must be met in order to apply Darcy's Law to estimating the soil-moisture flux. First, the profile must be under steady state conditions, that is, the water content and pressure head distributions at depth are slowly varying in time. Second, the soil water must be moving essentially in one dimension, vertically downward or upward, depending on the analysis. Third, when estimating the recharge rate, that is, the soil-moisture flux contributing to recharge of the underlying aquifer, the data must be from below the root zone in order to preclude any evapotranspiration uptake from affecting the results. A special case of the Darcy's Law approach is sometimes applicable if one can demonstrate that a unit-gradient exists. In this case the hydraulic gradient is equal to one, implying gravity drainage is dominant, and the solution to Eq 4 is simplified to be merely a calculation of the unsaturated hydraulic conductivity as a function of moisture content or pressure head.

6.4.1.4 Data are required as input to the Darcy's Law mathematical formulation in order to solve for the soil-moisture flux. These data include moisture content, pressure head, saturated hydraulic conductivity, and the unsaturated hydraulic conductivity function, that is, as a function of pressure head and/or water content. These data are determined from in situ measurements, in situ testing, and/or laboratory testing of core samples (D18.21.89.16, D18.21.89.17, Practice D 1452, Test Method D 2216, Guide D 3404, Test Method D 4643, GuideD 4696, Guide D 4700, Test Method D 4944, Guide D 5126 and Test Method D 5220). Care must be taken in performing laboratory analyses that preferential flow along the sidewalls of the sample does not occur, thereby causing errors in the hydrologic estimates.

6.4.1.5 An important point that is quite often overlooked in modeling soil-water movement is that the uncertainty in the unsaturated hydraulic conductivity function is generally quite large. Uncertainty in hydraulic conductivity estimates is generally due to both measurement error and spatial variability.

Depending on the scope of the investigation, the user may want to address the nature of uncertainty in the hydraulic conductivity estimates by conducting a sampling program that allows the user to evaluate spatial variations as well as measurement accuracy/precision (Guide D 5126). (Note: issues related to sampling network design are beyond the scope of this guide) Once the data have been assimilated regarding a statistical sampling, or distribution, for example, mean and standard deviation estimates, of hydraulic conductivity values, the user can use one of several techniques to evaluate the range of soil-water movement rate estimates using Darcy's Law. One possible technique is to bound the soil-water movement rate calculations using the highest and lowest values of the hydraulic conductivity values, paired with the appropriate moisture content and soil-water tension data. This will yield some point estimates of soil-water movement rate which span a range of outcomes, thereby giving the user a measure of uncertainty in the soil-water movement rate. Another approach to addressing uncertainty is that of using a probabilistic method, such as stochastic or Monte Carlo techniques. The approach taken with probabilistic methods is that of propagating input parameter uncertainty, for example, hydraulic conductivity, into a full estimate of uncertainty in the needed output estimate, for example, soil-water flux. In the case of Monte Carlo techniques, many Darcy's Law simulations would be run, each time varying the value of the hydraulic conductivity function within the range and distribution measured. In this manner a set of soil-water flux estimates is obtained, which can also be described statistically by a range and distribution. The number of Monte Carlo runs necessary to quantify the distribution, or uncertainty, in the soil-water flux estimates will be dependent upon the range of uncertainty in hydraulic conductivity, and therefore does not allow one to formulate a general rule about the number of simulations required. Commercial spreadsheet and flow modeling software exist to apply Monte Carlo techniques and to analyze data for statistical purposes, for example, parameters to describe a distribution, like mean and standard deviation. The probabilistic methods provide a more quantitative estimate of uncertainty than simple bounding calculations, but can sometimes be a significant calculation burden in comparison. The need for quantifying uncertainty will be dependent upon the nature and scope of the investigation. It would be difficult to formulate a decision rule as to when it is appropriate to perform uncertainty analyses, because each investigation will have a different importance tied to the soil-water flux estimates and the possible outcomes or actions taken on the basis of those estimates.

6.4.1.6 Extensions of the basic Darcy's Law formulation exist to predict infiltration rates and wetting front advancement. There are a multitude of formulations to describe various ponding and natural gradient infiltration scenarios. Typically, analytical or quasi-analytical solutions exist to implement these mathematical formulations.

6.4.1.7 Green and Ampt **(10)** developed some of the early solutions to the infiltration equations describing a sharp wetting front advance through soils. A variation by Horton **(11)** is as follows:

$$v = \frac{di}{dt} = v_f + (v_i - v_f)\, e^{-\beta t} \tag{5}$$

where:
v = infiltration rate [L T^{-1}]
i = cumulative infiltration [L]
v_i = initial infiltration rate [L T^{-1}]
v_f = final infiltration rate [L T^{-1}]
β = physical constant
t = time [L]

The final infiltration rate, *vf*, may be approximated by K_o, the saturated hydraulic conductivity of the soil, as $t \to \infty$. The main sources of uncertainty in this equation are the initial infiltration rate estimate (which can be quite large at early time), and the estimation of the constant β. In addition, this equation describes infiltration across a wetted soil surface. Wherever subsurface flow is not vertical below the wetted surface, the soil-water flux will not equal the infiltration rate at the surface. Care must be taken in using this approach when ponding at the soil surface is intermittent and variably saturated flow conditions are likely.

6.4.1.8 Alternatively, Philip **(12)** proposed an infiltration equation of the following form:

$$v = \frac{di}{dt} = \frac{1}{2} S\, t^{\frac{-1}{2}} + A \tag{6}$$

where:
S = sorptivity [L $T^{-½}$]
A = physical constant

The sorptivity term may be estimated with such methods as the air-entry permeameter technique (Guide D 5126). The physical constant, *A*, may be approximated by K_o, the saturated hydraulic conductivity of the soil, as $t \to \infty$. This equation is subject to some of the same cautionary considerations as listed for Horton's equation.

6.4.1.9 The most rigorous soil-physics based approach that may be applied pertains to the use of Richard's equation. By application of the continuity equation to Darcy's Law, Richard **(13)** derived the following expression to describe transient flow through unsaturated porous media:

$$\frac{\partial\theta}{\partial t} = \nabla \cdot [K(\theta,\psi)\, \nabla H] \tag{7}$$

Applications of this equation generally take the form of non-linear numerical models requiring the use of computers to iteratively solve the equation with the appropriate boundary and initial conditions. These models provide estimates of vadose zone flow, and some include estimates of soil-moisture flux or pore velocity. Application of a Richard's equation-based model allows the user the ability to evaluate transient, near-surface processes, and spatial variability issues in a more rigorous fashion than with a Darcy's Law approach. Additional data requirements become necessary with the application of Richard's equation, such as the soil-moisture characteristic curve, that is, moisture content versus pressure head relation. There can be a significant amount of uncertainty associated with the application of such a numerical model, given that it is a non-linear mathematical model, that the input parameters are subject to uncertainty in spatial and temporal variability, as well as measurement error.

6.4.1.10 Yet another soil-physics approach to estimating the soil-moisture flux is the application of solute transport equations to solve for the flux. This application involves the sampling of contaminant and/or tracer data in the subsurface, followed by the inverse solution of a solute transport equation to estimate the soil-moisture flux **(14)**.

6.4.2 *Applications*

6.4.2.1 The soil-physics based approaches, in general, may be applied under most any environment, be it humid or arid. The key to these applications is that the area of study be a porous media and that estimates of hydraulic characteristic data are available, for example, soil-moisture retention curve. This guide does not specifically address fracture flow or preferential flow considerations, which are considered exceptions to the general practice. Methods do exist to address soil-moisture flux where fracture/preferential flow may be important, but are not covered here.

6.4.2.2 Given the uncertainties associated with input data/parameters to these soil-physics based models, the user is encouraged to characterize the hydraulic characteristics as well as possible. Spatial variability and measurement error are key contributors to this uncertainty. Long-term measurements of moisture content and pressure head in the subsurface are oftentimes needed to evaluate the soil-moisture flux as a result of seasonal changes in the hydrologic budget.

6.4.3 *Monitoring and Operating Procedures*

6.4.3.1 In order to apply any of the soil-physics methods described above, information regarding the soil hydraulic characteristics must be measured/obtained. Some of these data are obtained through either field or laboratory testing. The hydraulic characterization of "undisturbed" core samples includes the determination of the initial moisture content, the soil-moisture characteristic curve, that is, pressure head versus water content relationship, bulk density, porosity, sorptivity, saturated hydraulic conductivity, and grain-size distribution. The unsaturated hydraulic conductivity function is determined from an in-situ instantaneous profile test, one-step outflow tests in the laboratory, or from the soil-moisture characteristic curve (with methods such as van Genuchten's **(15)** curve-fitting model, using the mathematical formulation of Mualem **(16)**). In applying the Darcy's law formulation in a deterministic fashion it is recommended that the effective unsaturated hydraulic conductivity across any depth interval be the harmonic mean of the individual K estimates **(17)**.

6.4.3.2 In addition to the hydraulic characteristic data/parameters, information on the spatial/temporal variability of moisture content and pressure head are also needed. Measurements of moisture content may be done with neutron logging, Time Domain Reflectometry, Resonant Frequency Capacitance, and cross-hole gamma methods (ASTM D18.21.89.16 and D18.21.89.17). Tensiometers and thermocouple psychrometers may be used for the determination of the pressure head (Guide D 3404). It should be noted that the absence of change in moisture content or pressure head measurements with time does not imply that no soil-moisture flux is apparent, but that steady-state conditions may preside.

6.4.4 *Analysis, Interpretation, Accuracy, and Reporting*

6.4.4.1 The application of soil-physics based methods to estimate soil-moisture flux is quite varied and useful. In reporting the results, statements should be made regarding the conditions of any soil sampling/monitoring events, the location of the sampling site and its attributes, for example, topography, terrain, vegetative cover, etc., the subsurface sampling intervals, the accuracy and precision of the laboratory/field methods used to determine the hydraulic characteristics, as well as general qualitative analysis of the representativeness of the results.

6.5 *Bomb-pulse Tritium and Chlorine-36 Methods*

6.5.1 *Theory*

6.5.1.1 The distribution of bomb-pulse tritium and chlorine-36 with depth in the profile can be analyzed to determine the soil-water movement processes that have occurred over the past 30 years. The atmospheric nuclear testing performed in the late 1950's and early 1960's has left us with a unique signature of the soil water in the vadose zone that is approximately 30 to 40 years old. Therefore, determining the maximum depth of infiltration of the bomb-pulse tritium and chlorine-36 allows us to calculate the modern day soil-moisture flux and/or recharge rate **(7)**. Chlorine-36 has a half life of 300,000 years, and tritium has a half life of 12.3 years.

6.5.1.2 The soil water extracted from the core samples (Guide D 4700) is analyzed for its tritium concentration with a liquid scintillation counting technique. The chloride from the soil samples is processed into AgCl for subsequent analysis of the 36Cl on a Tandem Accelerator Mass Spectrometer.

6.5.2 *Applications*

6.5.2.1 The bomb-pulse tritium and chlorine-36 techniques are applicable in arid as well as humid climates. The depth of the vadose zone in humid regions may be a factor, however, in locating the bomb-pulse peaks. If a relatively high recharge rate exists in a shallow water-table environment the peak may have passed into the saturated zone within the last 30 years.

6.5.2.2 The time of sampling for the bomb-pulse tracer techniques is of importance. Seasonal changes in precipitation and infiltration may affect the analysis of the results. If one is trying to quantify long-term behavior of soil-moisture flux the sampling should be done during quasi-steady state conditions, that is, at a time when significant rainfall events are not occurring. These tracers may be used to evaluate transient soil-water movement phenomena, if that were the need, because the relative depth of the peak may change somewhat depending on the season and the impact of evapotranspiration and infiltration.

6.5.2.3 The difference between the bomb-pulse tritium and chlorine-36 peaks in a given soil profile may be used to identify the relative importance of vapor-phase versus liquid-phase movement of soil water. If the tritium peak is at a greater depth than the chlorine-36 peak, then there is likely to be a net enhancement of downward water movement in the upper portion of the soil profile.

6.5.2.4 In addition to the applications listed above, these tracers may be used as indicators of preferential flow potential. The presence of bomb-pulse levels of tritium and chlorine-36 deeper in the profile may be indicative of preferential flow components, possibly due to macropore or fracture flow phenomena.

6.5.3 *Monitoring and Operating Procedures*

6.5.3.1 Data acquisition for the bomb-pulse tritium and chlorine-36 techniques is mainly a destructive sampling activity. Discrete samples should be collected through hand sampling, push tube sampling, coring, or via drilling/sampling (Practice D 1452). Care must be taken not to allow cross-contamination of soil samples from one depth horizon to another, because the concentrations of these isotope species are relatively low compared to other geochemical indicators. Therefore, mixing of samples from different depths could cause significant errors in results, and difficulties in interpretation.

6.5.3.2 Once core samples have been collected, a series of analytical procedures are required to obtain the necessary data for application of these techniques. First the samples should be well sealed in air-tight containers to prevent the possible evaporation of soil water, thereby altering both the moisture content and the tritium concentration. The sample is brought to the laboratory for extraction of the water. Viable extraction, or distillation, techniques include vacuum distillation and azeotropic distillation. Care should be taken during the extraction process to limit any possible fractionation of the water that would cause alteration of the isotopic composition of the tritium. If vacuum distillation is used to extract the water, essentially all of the water must be liberated from the sample to avoid adverse fractionation potential. In the azeotropic distillation method, a purification step is needed to sorbed the toluene or kerosene out of the water so as not to adversely impact the ratio mass spectrometer analyses. Also, data analysis of water content can be performed with the distillation data, if the volume of soil and water are recorded. The extracted water is then analyzed for tritium concentration using a liquid scintillation counting method. The soil from which the water was extracted is then leached of chloride. The chloride concentration may be determined at this juncture to combine this technique with the chloride mass balance method. The leached chloride is then put through a process to make silver chloride, AgCl **(7)**. The AgCl is then analyzed on a Tandem Accelerator Mass Spectrometer (TAMS).

6.5.4 *Analysis, Interpretation, Accuracy, and Reporting*

6.5.4.1 The application of radioisotope methods to estimate soil-moisture flux is a fairly new technique which is quite useful. In reporting the results, statements should be made regarding the conditions of any soil sampling/monitoring events, the location of the sampling site and its attributes, for example, topography, terrain, vegetative cover, etc., the subsurface sampling intervals, the accuracy and precision of the laboratory/field methods used, as well as general qualitative analysis of the representativeness of the results. Graphics showing the distribution of the isotopic species with depth in the profile are quite valuable in the interpretation of the results.

6.6 *Stable Isotope Methods*

6.6.1 *Theory*

6.6.1.1 Several stable isotope methods may be used to quantify soil-moisture flux. Techniques exist to estimate the liquid and vapor flux of water in the unsaturated zone, as well as to quantify the soil-moisture flux associated with the evaporation process. First, Knowlton's **(18)** stable isotope method is based on theoretical work presented by Allison **(19)**. Knowlton's method is a tracer technique used to estimate the transport of the isotopic species deuterium (D or ^{2}H) and ^{18}O in the water molecule ($H_2{}^{18}O$ and $HD^{16}O$), which in turn allows for the quantification of the liquid flux, the vapor flux, and the recharge rate. The main assumption in the development of this mathematical model is that quasi-steady state conditions exist with regard to soil-water movement. Practically speaking, this means that the field sampling should be done during a lengthy period of little or no major precipitation events that could cause significant infiltration. Therefore, the isotope profile should be slowly changing in time. In the arid southwest, this requirement is generally met between late spring and mid summer, prior to the 'rainy season' in July and August. An additional assumption must also be met, that the soil water is moving essentially in one dimension, vertically. Significant lateral soil-water movement would invalidate this model. The model may be applied for either isothermal or non-isothermal conditions. With non-isothermal conditions the vapor flux is more readily quantified. The mathematical model used to describe the shape of the deuterium profile is:

$$R\,(\delta_D - \delta_D{}^{Rec}) = ((h\,N_{sat}D^v)\,/\,\rho)\,(\epsilon_D + \eta_D)\left[\frac{d\,[ln\,(h\,N_{sat}\,(\epsilon_D + \eta_D)]}{dz}\right] \tag{8}$$

$$-(D + ((h\,N_{sat}\,D^v)\,/\,\rho))\,\frac{d\,(\delta_D)}{dz}$$

where:

R = recharge rate [L/T]

δ_D = standardized isotope ratio at any depth [permil]

δ^{Rec} = standardized isotope ratio of the recharge water at depth [permil]

h = relative humidity

N_{sat} = saturated water vapor density in air [M/L^3]

D^v = effective diffusivity of water vapor in air [L^2/T]

D = effective self-diffusion coefficient of water [L^2/T]

ρ = density of liquid water [M/L^3]

ϵ_D = equilibrium enrichment factor

η_D = diffusion ratio excess

z = depth below land surface [L]

6.6.1.2 A discussion on how to estimate or determine these parameters is provided by Knowlton **(18)**, along with a sensitivity analysis. A non-linear least squares analysis is applied to solve Eq 2 for the recharge rate. Data required as input to the model include the stable isotope ratios and water content distributions with depth. In addition to estimating the recharge rate, the stable isotope data may be used to quantify or identify other soil-water movement processes. First, the data may be used to quantify the distribution of the liquid and vapor flux with depth in the profile **(18)**. The potential for vapor-phase movement of volatiles might therefore be assessed in this manner.

6.6.1.3 Second, the stable isotope data may also be used to quantify the evaporation rate according to techniques developed by Allison and others **(19)**. There are essentially four methods outlined by Allison and others, all of which require knowledge of the distribution of deuterium and/or oxygen-18 and water content with depth in the profile. One of the methods is suitable for non-isothermal conditions, and therefore the transient temperature distribution within the soil profile would also be required.

6.6.1.4 A third alternative application of the stable isotope data is to help define whether the soil water at depth has been isotopically altered due to infiltration of water from a treatment, storage, or disposal facility. For a case where water of unknown composition, that is, possibly contaminated, is disposed of in a facility and infiltrates, the extent of vertical migration of the water might be assessed with stable isotopes. In a deep vadose zone where the fluid has migrated a finite distance below the facility, this type of characterization might offer a means of convincing a regulator that the imminent threat of contaminants reaching the underlying aquifer is small. Therefore, the likelihood that the regulator would allow vadose zone monitoring in lieu of drilling expensive monitoring wells might be enhanced.

6.6.1.5 A fourth application of stable isotopes to quantify the soil-moisture flux exists for use in more humid climates. This technique relies on the use of the stable isotopes as tracers of soil-water movement. The distribution of deuterium and oxygen-18 ratios in precipitation generally changes with the season, due to the temperature dependence of these isotopic species in the water molecule. In regions where precipitation, and hence infiltration, occurs essentially year round, for example, humid climates, the distribution of the isotope species with depth in the profile should reflect a series of maxima and minima corresponding to summertime and wintertime infiltration events, respectively. These data can then be used to quantify the soil-moisture flux because the time and depth of infiltration for any given wetting period are known **(20)**.

6.6.1.6 A fifth application for stable isotopes exists for quantifying the recharge rate, or the deep soil-moisture flux. This technique, by Allison and others **(21)** involves the comparison of paired values of deuterium and oxygen-18 for samples in the subsurface with the isotope ratios of precipitation, that is, the meteoric water line relationship. The stable isotope ratios within the subsurface are generally higher than that of precipitation, due to enrichment during evaporation processes. The offset of these data from the precipitation ratios is proportional to the recharge rate. This method is most applicable in areas where recharge is not great, for example, arid or semi-arid locales.

6.6.2 *Applications*—The techniques described above should provide stable isotope methods for a variety of applications where quantification of the soil-moisture flux is required. In semi-arid or arid zones, Knowlton's method **(18)** is useful to quantify the liquid flux, vapor flux, and the recharge rate. Allison and others have techniques for quantifying the evaporation rate, which may be applied in most any climate. Stable isotopes may also be used to identify whether soil water in the vadose zone has been isotopically altered due to artificial infiltration, for example, contaminant migration, which in turn could be used to interpret the depth of penetration of such an infiltration scenario. The fourth application described above applies for quantifying soil-moisture flux in humid climates. The distribution of the stable isotope ratios with depth in the profile may be interpreted to yield information about seasonal infiltration/recharge events. The fifth application identified above for stable isotope methods is Allison's method for quantifying the recharge rate in arid or semi-arid locales. This method relies on the interpretation of an offset between precipitation and subsurface soil-water stable isotope ratios.

6.6.3 *Monitoring and Operating Procedures*—In these stable isotope methods, the distribution of deuterium, and/or oxygen-18, and water content with depth are required to estimate the soil-moisture flux, and/or the recharge rate. These data are acquired from destructive core sampling (Guide D 4700). Soil samples collected during the coring operation and stored in Mason jars are subjected to a vacuum distillation procedure **(18)** or azeotropic distillation to extract the soil water. The soil water is then processed with a CO_2/H_2O equilibration technique or hydrogen reduction method prior to analyzing the stable isotope ratios of $^{18}O/^{16}O$ (referred to as oxygen-18) and $^{2}H/H$ (referred to as deuterium), respectively. The stable isotope ratios are determined on a ratio mass spectrometer. For the non-isothermal applications described above, the temperature distribution with depth in the profile is also required. These data might be obtained from monitoring in-situ temperature thermistors or from analytical/numerical modeling of heat flow **(18)**. Transient effects may be evaluated with these various stable isotope techniques. Therefore, routine destructive sampling at a site may be desired if the quantification of soil-water movement, recharge, and/or evaporation are desired if the transient behavior is needed.

6.6.4 *Analysis, Interpretation, Accuracy, and Reporting*

6.6.4.1 The application of stable isotope methods to estimate soil-moisture flux is a fairly new technique which is quite useful. In reporting the results, statements should be made regarding the conditions of any soil sampling/monitoring events, the location of the sampling site and its attributes,for example, topography, terrain, vegetative cover, etc., the subsurface sampling intervals, the accuracy and precision of the laboratory/field methods used, as well as general qualitative analysis of the representativeness of the results. Graphics showing the distribution of the isotopic species with depth in the profile are quite valuable in the interpretation of the results.

6.7 *Other Tracer Techniques*

6.7.1 *Theory*

6.7.1.1 Other tracer techniques exist to quantify the soil-moisture flux. These techniques generally involve emplacing a tracer, for example, bromide, in the feed water of an infiltration experiment or to physically emplace the tracer in the subsurface and to monitor the rate of movement of the tracer through either soil-water extraction techniques (Guide D 4696) or destructive sampling (Guide D 4700).

6.7.1.2 Tracers that have been used extensively for transient testing purposes include bromide and chloride. Chloride and bromide are conservative tracers, and do not volatilize or adsorb readily onto the soil.

6.7.1.3 Other tracers which have been used effectively include o-TFMBA (orthotrifluoromethyl benzoic acid), PFBA (pentafluorobenzoic acid), and 2,6-DFBA (2,6difluorobenzoic acid) **(22)**. These three tracers are anionic organic acids, and generally travel with the velocity of the water, and are not significantly inhibited by soil texture, for example, clays, and/or adsorbed. Still other techniques which have been used for tracers include fluorescent dyes.

6.7.1.4 Short-lived radioactive tracers have also been used to quantify soil-water movement rates. Some of the candidate tracers include chromium-51 (with a half-life of 28 days), cobalt-58 (with a half-life of 72 days), bromine-82 (with a half-life of 1.5 days), and iodine-131 (with a half-life of 8 days) **(23)**. Regulatory approval on the use of these radioactive tracers would generally be required.

6.7.1.5 The use of artificially applied tritium as a tracer has also been done **(24)**. Tritium has a half-life of 12.3 years, and is therefore more persistent than the radioisotopes mentioned above. Again, regulatory approval on the use of this radioactive tracer would generally be required.

6.7.1.6 Care should be taken when using radioactive tracers that the amount of tracer used does not constitute a health hazard in terms of total activity and dose to exposed workers.

6.7.2 *Applications*

6.7.2.1 The use of the applied tracer techniques outlined in this section is generally in support of relatively short-term testing. The application of these tracers is generally done in infiltration water or directly into the subsurface to monitor the behavior of soil-water movement. Either destructive sampling or pore-water extraction methods are used to obtain samples for concentration data through time in the experiments. The analysis of the concentration data is dependent on the type of tracer used. Acid tracers may be analyzed by liquid chromatographic techniques, whereas radioactive tracers may be analyzed by liquid scintillation counting or gamma spectroscopy.

6.7.3 *Monitoring and Operating Procedures*

6.7.3.1 The acquisition of data for transient tracer methods generally requires destructive sampling/coring [Practice D 1452 and Guide D 4700] or pore-liquid sampling [Guide D 4696]. Analytical determinations of the concentrations of the tracers from any given sample is dependent upon the type of tracer used, whether it is an acid, a salt, or a radioactive constituent.

6.7.4 *Analysis, Interpretation, Accuracy, and Reporting*

6.7.4.1 The application of transient tracer methods to estimate soil-moisture flux is quite useful. In reporting the results, statements should be made regarding the conditions of any soil sampling/monitoring events, the location of the sampling site and its attributes, for example, topography, terrain, vegetative cover, etc., the subsurface sampling intervals, the accuracy and precision of the laboratory/field methods used, as well as general qualitative analysis of the representativeness of the results. Graphics showing the distribution of the tracer with depth in the profile through time are quite valuable in the interpretation of the results.

7. Keywords

7.1 boundary condition; recharge flux; soil-moisture flux

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