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Basic considerations for Monte Carlo calculations in soil

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Abstract

Monte Carlo codes are extensively used for probabilistic simulations of various physical systems. These codes are widely used in calculations of neutron and gamma ray transport in soil for radiation shielding, soil activation by neutrons, well logging industry, and in simulations of complex nuclear gauges for in soil measurements. However, these calculations are complicated by the diversity of soils in which the proportions of solid, liquid and gas vary considerably together with extensive variations in soil elemental composition, morphology, and density. Nevertheless use of these codes requires knowledge of the elemental composition and density of the soil and its physical characteristics as input information for performing these calculations. It is shown that not always all of the soil parameters are critical but depend on the objectives of the calculations. An approach for identifying soil elemental composition and some simplifying assumptions for implementing the transport codes are presented.

Keywords: Monte Carlo; Soil elements; Neutrons; Gammas; Transport

1. Introduction

The extensive increase in the computational power of the desktop computers facilitated a widespread use of Monte Carlo codes for gamma-neutron transport calculations. These are probabilistic codes that simulate step-by-step the processes that guide radiation transport in matter. These codes enable complex system simulations which other-way would be very time consuming, costly, and occasionally impossible to perform. These simulations can be performed with an arbitrary degree of details provided that all the basic data and complete system description are available. One of these codes is the Monte Carlo Neutron Photon (MCNP) transport code, developed in Los Alamos National Laboratory (Breismeister, 1993), that has been widely used for radiation transport in soil. For example, MCNP has been used for evaluating soil activation, radiation shielding in soil, well logging industry, and for design of complex gauges based on nuclear techniques. One such technique, which gained widespread use, is in situ, non-destructive, multi-elemental analysis of bulk geological samples using neutrons (Csikai, 1991; Clayton and Coleman, 1985). MCNP codes require an input file that contains complete information about the radiation source, the geometry of the simulated system, and both the density and the elemental composition of all materials through which the radiation passes. In addition the output tallies to be calculated need to be specified.

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Due to high variability and inhomogeneous nature of soils, special care must be taken when implementing MCNP simulations. The main contributing factors to complexity in using MCNP for in-soil calculations are; (1) soil is a three-phase system in which the solid phase contains organic and inorganic components, (2) the liquid phase carries many different solutes depending on soil mineralogy, (3) the gaseous phase, although generally ignored, may contain gases that strongly absorb neutrons, (4) on a micro-scale soil is a highly inhomogeneous matrix, although on macro scale some homogeneity and uniformity can be assumed, and (5) soil density primarily depends on porosity and water content. These factors are further complicated by the nature of the geological formation being studied, weathering conditions, and depth. For example, it is well established that the composition of a formation at depth differs significantly from that on the surface. These factors make it nearly impossible to provide exact descriptions of the system. Introducing simplifying assumptions that depend on the degree of accuracy required by the final objectives of the calculation to overcome these complexities. However, the validity of these assumptions must be tested and validated either by conducting simple experiments or by performing analyses of the sensitivity of the calculations to perturbations in the assumptions.

Two essential parameters required for MCNP calculations are soil density and elemental composition. These two primary properties, and an assumption about soil uniformity are pivotal when designing gadgets for soil moisture and porosity measurements (Gardner et al., 1971). These properties are also required when gamma spectroscopy of neutron induced gamma radiation, due to delayed, prompt, or inelastic neutron interactions, are used to solve geophysical problems for the well logging industry (Schweitzer et al., 1993; Grau et al., 1993), or when performing non-invasive in situ quantitative analysis of the elements present in soil (Clayton and Coleman, 1985).

We describe the use of Monte Carlo calculations applied to modeling inelastic neutron scattering (INS), a process we are developing as a technique for quantification of carbon in soil. INS analysis of soil carbon can be carried out rapidly (30–60 min) and does not disturb the soil column. This permits re-sampling at the identical spot over time. Each observation provides a value for approximately 75–100 lb of soil. This is large enough to average much of the small-scale heterogeneity in soils (Wielopolski et al., 2000). At present soil carbon is measured by taking soil samples to the laboratory. This conventional process of extracting soil cores disrupts the soil column and the area around the sampling point. Alternative methods for soil sampling, laser induced breakdown spectroscopy (LIBS), (Cramers et al., 2001; Kincade, 2003) and infrared spectroscopy (McCarty et al., 2002). However, these in situ approaches are invasive. In the first case, small volumes of about 50 μl are vaporized and emission spectroscopy is performed in the second case it is basically surface analysis; these methods are therefore not comparable to the INS method. With re-sampling of the identical spot, and averaging over a relatively large volume, small changes in soil carbon content may be detected that, using conventional methods, would be obscured because of soil heterogeneity. For example, for till no till agriculture (Lal et al., 1999) scanning large areas for carbon content will be very useful to assess the changes in carbon content.

2. Soil components

As pointed out the essential soil parameters, in addition to the geometry, required for Monte Carlo simulations are the elemental composition and the bulk density. These are required to calculate the macroscopic transport cross section for neutrons and gamma radiation, i.e., the probability of interaction with the individual elements present in the matrix, and the density is required for finding the number of atoms in a volume of interest and calculating the range of travel for the radiation.

However, the variety of soil types and the multiplicity of their conditions make it but impossible to obtain a simple parameterization descriptive of all soils. Instead, a semi-systematic approach is used to describe the density and composition of the soil surface and/or near surface, down to about 100 cm. In this region the soil is a loose mixture resulting from physical and chemical weathering and biological processes. It is a heterogeneous system consisting of solid minerals, organic matter, and liquid and gaseous components. The proportion of each component varies largely from site-to-site and depends on the climate and stage of soil

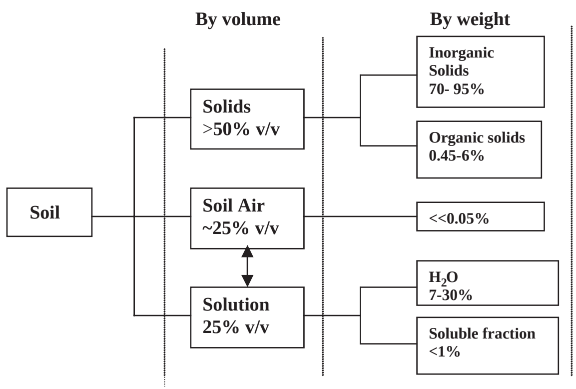

Fig. 1. Soil components with fractional distribution by volume and weight.