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Conversion and Modification of the MLSOTL and DFSOIL Codes

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Research after the Chernobyl nuclear accident has revealed that the greatest contribution to the long-term external dose rates after the accident in both the urban and rural environment comes from radionuclides deposited onto the ground surface. The migration of these radionuclides into soil with time is important for the estimation of the external dose rates from the ground.

Two computer codes, MLSOIL and DFSOIL, have been originally developed at ORNL in USA for modelling the migration of radionuclides in an undisturbed agricultural land and calculating the resultant external dose rates. It is possible to apply these codes to an open area in the urban environment as well. Therefore, MLSOIL and DFSOIL were converted and modified to make the implementation of the codes easy. Input data files were also prepared for radionuclides important for the assessment of a nuclear accident. Finally the modified versions of both codes were verified to have the intended calculational functions.

Keywords: Chernobyl Nuclear Accident, Long-term External Dose Rates, Urban and Rural Environment, Migration into Soil, Computer Codes

#### MLSOIL及びDFSOILコードの変換と機能拡張

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(1995年6月23日受理)

チェルノブイル事故後の研究によると、事故後の都市及び農村環境における長期的な外部被曝 線量率は、地表面に沈着した放射性核種に起因することが明らかになった。この際、時間に伴う 沈着核種の下層土壌への浸透は、汚染表面からの外部被曝線量率の推定の際に重要である。

2つの計算コードMLSOILとDFSOILは、本来、未攪乱の農耕地における核種の浸透及びそれによる外部被曝線量率を推定するために、米国のオークリッジ国立研究所で開発された。これらのコードを都市環境における屋外にも適用することが可能である。従って、MLSOILとDFSOILの実行を容易にするために、両コードの変換と機能拡張を行った。また、原子炉事故時の評価の際に重要な核種に関して入力データファイルを整備した。さらに、コードの拡張版が意図した計算機能を有していることを確認した。

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#### 1. Introduction

In case of a severe accident at a nuclear power plant, radioactive materials released to the atmosphere would be deposited on the ground surface by dry and wet deposition. The deposited radionuclides play an important role in the radiation exposure to the public. Research after the Chernobyl nuclear accident has revealed that the greatest contribution to the long-term external dose rates after the accident in the urban environment comes from radionuclides deposited onto open areas such gardens and parks<sup>1)</sup>. In rural areas, on the other hand, deposited radionuclides contribute to not only the external dose rates but also contamination of foodstuffs. The food contamination results from direct deposition of airborne radionuclides and root uptake for a long period.

Radionuclides deposited on the ground surface migrate into soil with time. The speed of the migration depends upon physical and chemical forms of deposited materials, the characteristics of soil and the meteorological conditions. The soil shields against the radiation from radionuclides in soil. The activity concentration in a root zone is influenced by the property of soil. Therefore, the change of the vertical distribution of radionuclides in soil with time is important for the estimate of both the external dose rates from the ground and food contamination via root uptake. Considering these situations, two computer codes, MLSOIL and DFSOIL<sup>2)</sup>, were developed at Oak Ridge National Laboratory (ORNL) in USA to estimate the migration of deposited radionuclides into soil and the resultant external dose rates.

The MLSOIL code uses a five-compartment linear transfer model to describe the migration of radionuclides into soil resulting from the deposition on the ground surface. The model takes account of the migration through the soil as well as radioactive decay of radionuclides to be assessed and buildup of their daughters. The element-specific transfer coefficients used in this model are a function of the  $k_d$  values and environmental parameters. The  $k_d$  value is defined as the ratio of the radionuclide concentrations in the solid and liquid phases. MLSOIL also calculates the long-term external dose rates from the radionuclides in the soil.

The DFSOIL code computes dose-rate conversion factors for each of the five soil layers, which are used in MLSOIL. The factors determine the external dose rates in air at 1 m above the ground from photon sources per unit concentration of a specific radionuclide in each soil layer. The dose-rate conversion factors for the surface source are also calculated in this code.

The MLSOIL and DFSOIL codes were originally designed to be applied to an undisturbed agricultural land. It is possible to apply the codes to an open area in the urban environment as well as an agricultural land. These two codes can estimate the external exposure from radionuclides in undisturbed areas, which would be the greatest contributor to the long-term dose rates in both the urban and rural environment. In the present work, therefore, MLSOIL and DFSOIL have been converted for a personal computer system to make the implementation of the codes easy. Some parts of the codes were modified at the conversion, but calculation models themselves remained unchanged. Input data files were also prepared for radionuclides important for the assessment of a nuclear accident.

This report describes calculation models used in the codes, conversions and modifications of the codes, and how to prepare input data files. The report also gives sample input and output data of the codes.

#### 2. Calculation models

#### 2.1 MLSOIL

## (1) Radionuclide migration in soil

The model of radionuclide transport through soil, implemented in the MLSOIL code, is a five-compartment linear transfer model. Figure 1 shows a schematic diagram of the model which could represent the migration through an undisturbed agricultural land such as a pasture ground or a fruit garden. The movement of radionuclides through the soil column is represented in the model by a series of transfers between compartments of various sizes. Within each compartment, the radionuclides are assumed to be uniformly mixed. It is noted that there is no upward transfer. The rates of transfer between the various compartments are determined by the transfer coefficients,  $k_{i,j}$ . The rate at which the migration takes place is dependent upon several factors, including the compartment thickness, the chemical form of radionuclides, soil composition, climate and rainfall.

The change rate of the radionuclide concentration is given by:

$$\frac{dC_i(t)}{dt} = Q_i(t) - \lambda_i C_i(t) - k_{i,1} C_i(t) + \sum_k b_{ki} \lambda_i C_k(t)$$
 (1)

where  $C_i(t)$  is the concentration of radionuclide i in layer 1 (Bq/m³),  $Q_i(t)$  is the rate at which radionuclide i enters layer 1 (Bq/m³/sec),  $\lambda_i$  is a radiological decay constant for radionuclide i (sec¹),  $k_{i,1}$  is the transfer coefficient for radionuclide i from layer 1 to layer 2 (sec¹), and  $b_{ki}$  is the branching ratio from radionuclide k to radionuclide i. Analogous equations can be written for the remaining layers of the model illustrated in Figure 1. The concentrations of all radionuclides in all layers at time t are obtained by solving the set of simultaneous equations represented by Equation (1).

#### (2) Transfer coefficients

The migration of radionuclides in soil has been studied only for a limited number of elements. As a result, there is only a very limited empirical data base to derive the values of the inter-layer transfer coefficients. Therefore, a model of migration removal rate constant is adopted to calculate the transfer coefficients in the MLSOIL code. This transfer coefficient is element-specific and is given by:

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The change rate of the radionuclide concentration is given by:

$$\frac{dC_{t}(t)}{dt} = Q_{t}(t) - \lambda_{t}C_{t}(t) - k_{t,1}C_{t}(t) + \sum_{k} b_{k,t}\lambda_{t}C_{k}(t)$$
 (1)

where  $C_i(t)$  is the concentration of radionuclide i in layer 1 (Bq/m³),  $Q_i(t)$  is the rate at which radionuclide i enters layer 1 (Bq/m³/sec),  $\lambda_i$  is a radiological decay constant for radionuclide i (sec⁻¹),  $k_{i,1}$  is the transfer coefficient for radionuclide i from layer 1 to layer 2 (sec⁻¹), and  $b_{ki}$  is the branching ratio from radionuclide k to radionuclide i. Analogous equations can be written for the remaining layers of the model illustrated in Figure 1. The concentrations of all radionuclides in all layers at time t are obtained by solving the set of simultaneous equations represented by Equation (1).

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$$k_{i,j} = \frac{P - E}{\theta d \left[ 1 + \frac{\rho}{\theta} k_d \right]}$$
 (2)

where  $k_{ij}$  is the transfer coefficient for radionuclide *i* between soil layers *j* and j+1 (sec<sup>-1</sup>), *P* is annual average precipitation (cm/sec), *E* is annual average evapotranspiration (cm/sec),  $\theta$  is the volumetric water content of soil (ml/cm<sup>3</sup>), *d* is the thickness of soil layer j (cm),  $\rho$  is the bulk density of soil (g/cm<sup>3</sup>), and  $k_d$  is the distribution coefficient of radionuclide i (ml/g).

In Equation (2), irrigation may be important in calculating the water balance. Irrigation, if any, is added to precipitation when irrigation water is not contaminated. Runoff will be also important not only for the water balance but also for the horizontal transfer of radionuclides. It lead to the movement towards low-lying points in a field or the removal to elsewhere. However the evaluation of radionuclide losses due to runoff is outside the scope of the present model, because they depend entirely on the local conditions. If the amount of runoff water is known, it is taken into account only in the calculation of the water balance: it is added to evapotranspiration. This assumption makes the external dose calculation conservative.

The values of the parameters which are used in the calculation of the transfer coefficients are very different from site to site. The user of the code should prepare site-specific values for all of the parameters. Unless the site-specific data are available for  $\rho$ ,  $\theta$  and  $k_d$ , the user can use default values provided in MLSOIL. However attention should be paid to the use of these default values because they are only the average for various types of soil.

# (3) Dose rates due to long-term external exposure

The MLSOIL code also computes the external dose rates from ground surface exposure and the effective ground surface concentrations for each radionuclide. It uses the radionuclide concentrations in soil computed in this code and the dose-rate conversion factors that are calculated by the DFSOIL code. The formulas used for each radionuclide are as follows:

$$H_L = \sum_{L=1}^5 C_L DCF_L \tag{3}$$

$$C_{ES} = \frac{H_L}{DCF_P} \tag{4}$$

where  $H_L$  is the dose rate in air from the layered soil model (Gy/sec),  $C_L$  is the radionuclide concentration in soil layer L (Bq/m³),  $DCF_L$  is the dose-rate conversion factor for soil layer L (Gy/sec per Bq/m³),  $C_{ES}$  is the effective ground surface concentration (Bq/m²), and  $DCF_P$  is the dose-rate conversion factor for the plane source (Gy/sec per Bq/m²).

#### 2.2 DFSOIL

# (1) Definition of dose-rate conversion factors

The DFSOIL code calculates the dose-rate conversion factors for photon sources in soil and for photon sources on the ground surface. The dose-rate conversion factors for soil layers are computed for specific soil layer thicknesses and specific radionuclides. These factors are intended to be used in environmental dose-rate assessments, particularly in the MLSOIL code.

The calculations for soil layers represent an extension of those for photon sources which are confined to the ground surface, namely, the source concentration at a given depth in soil is assumed to be uniform over an infinite plane surface parallel to the ground. With this assumption, the external dose rate, H(t) (Gy/sec), at any time t to an exposed individual can be expressed in the general form:

$$H(t) = C(t)DCF ag{5}$$

where C(t) is the radionuclide concentration at the location of the exposed individual (Bq/m<sup>3</sup>), and DCF denotes the dose-rate conversion factor which is defined as the dose rate per unit source concentration (Gy/sec per Bq/m<sup>3</sup>).

For the purposes of this computation, it is only noted that the dose-rate conversion factor for external exposure to photon emitters on the ground depends on the height of the receptor location above the ground. For photon emitters in soil, however, the dose-rate conversion factor is more sensitive to the depth in soil than the height of the receptor location above the soil surface. For an exposed individual standing on the ground, the height of the receptor position is usually assumed to be 1 m.

For electrons produced by radioactive decay, the electron range in soil is usually less than 2 cm never exceeds 4 cm. Therefore, a normal penetration of radionuclides into soil with time will provide more effective shielding against electrons than photons. The external dose rates from electron emitters in soil are not considered here but are transferred to other future research.

#### (2) Computation of dose-rate conversion factors

The following represents calculations of photon dose-rate conversion factors for monoenergetic sources at various depths in soil and on the ground surface. The calculations assume that the source concentration is uniform over a horizontal plane. An equation for the dose-rate conversion factor for monoenergetic photon sources which are confined to the ground surface can be expressed by:

$$DCF_{\gamma}^{a}(z, E_{\gamma}) = \frac{1}{2} K E_{\gamma}(\mu_{en}/\rho)_{a} \cdot \left[ F_{1}(\mu_{a}z) - \frac{C_{a}}{(D_{a}-1)} \exp[(D_{a}-1)\mu_{a}z] \right]$$
 (6)

where  $DCF_{\gamma}^{a}$  is the photon dose-rate conversion factor (Gy/sec per Bq/m²), z is the height of the receptor location above the ground (cm),  $E_{\gamma}$  is the photon energy (MeV), K is a constant equal to  $1.6 \times 10^{-14}$  (g·Gy·cm²/MeV/m²),  $(\mu_{er}/\rho)_a$  is the mass energy absorption coefficient in air (cm²/g),  $\mu_a$  is the linear attenuation coefficient in air (cm¹),  $C_a$  and  $D_a$  are the coefficients in the Berger form,  $B_{er}^{a}$ , of the energy absorption buildup factor in air given by:

$$B_{\sigma\sigma}^{a} = 1 + C_{\sigma}\mu_{\sigma}r \cdot \exp\left(D_{\sigma}\mu_{\sigma}r\right) \tag{7}$$

where r is the distance from any point in the source region to the receptor position (cm), and  $F_1$  is the first-order exponential integral:

$$F_1(\mu_a z) = \int_{\infty}^{\infty} \frac{1}{r} \exp(-\mu_a r) dr$$
 (8)

For an exposed individual standing on the ground, the dose-rate conversion factor is usually calculated for the single height z = 1 m above the ground.

The dose-rate conversion factors for monoenergetic sources are applied to radionuclides by assuming that the spectrum of photons from radioactive decay consists of  $\gamma$  and X rays of discrete energy. Therefore, the dose-rate conversion factor for ground surface exposure to a particular radionuclide,  $DCF_{\gamma}^{P}$ , is given by:

$$DCF_{\gamma}^{P}(z) = \sum_{i} f_{i\gamma} DCF_{\gamma}^{a}(z, E_{i\gamma})$$
 (9)

where  $f_{i\gamma}$  is the intensity of *i*-th photon of energy,  $E_{i\gamma}$ , per decay and the summation includes all photons in the decay spectrum.

The dose-rate conversion factor for monoenergetic sources in soil can be obtained by analogy with Equation (6) by calculating photon attenuation and buildup in soil rather than in air. The dose-rate conversion factor immediately above the soil layer as a function of depth x of the monoenergetic plane source in soil is given by:

$$DRF_{\gamma}^{a}(x,E_{\gamma}) = \frac{1}{2}KE_{\gamma}(\mu_{ex}/\rho)_{a} \cdot \left[F_{1}(\mu_{s}x) - \frac{C_{s}}{(D_{s}-1)}\exp\left[(D_{s}-1)\mu_{s}x\right]\right]$$
(10)

It is noted that even though the medium between the source and receptor positions is assumed to be in soil rather than in air, the dose-rate conversion factor at a receptor location in air is still calculated. Thus the dose-rate conversion factor itself and the mass energy absorption coefficient on the right-hand side of Equation (10) are values in air and not in soil.

In practice, Equation (10) is to be evaluated at 1 m above the ground, and not immediately above the ground. The effect of the layer of air between the soil surface and the receptor can be approximated by a layer of soil which would provide the same shielding as the layer of air. This equivalent depth of soil,  $x_a$ , may be calculated by setting Equation (10) equal to Equation (6) and solving the resulting transcendental equation for  $x_a$ . For z = 1 m, the resulting value of  $x_a$  is less than 1 mm for all photon energies. The dose-rate conversion factor for a receptor 1 m above the soil surface may be then calculated for a plane monoenergetic source at a depth x by evaluating Equation (10) at  $x+x_a$  rather than at x.

Radionuclides in soil will be usually distributed throughout a volume rather than confined to a plane surface. The dose rate in air above the ground from a volume source can be obtained by an integration of the plane-source dose-rate conversion factor and the radionuclide concentration over the source volume. From Equation (5), the dose rate in air,  $H_{\gamma}^{a}$ , for energy  $E_{\gamma}$  is given by:

$$H_{\gamma}^{a}(E_{\gamma}) = \int_{x_{1}}^{x_{2}} C_{s}(x) DCF_{\gamma}^{a}(x+x_{a}, E_{\gamma}) dx$$
 (11)

where  $C_s(x)$  is the source concentration at depth x (Bq/m³),  $x_1$  and  $x_2$  are the upper and lower boundaries of the source region, respectively (m), and  $x_a$  is the thickness of soil corresponding to 1 m of air (m).

For most distributions of sources with depth in soil, Equation (11) must be solved numerically. The dose-rate conversion factor for a layer source is obtained by integrating Equation (10) over the vertical extent of the layer. Using the relation for derivatives of exponential integral:

$$\frac{dF_n(\omega)}{d\omega} = -F_{n-1}(\omega) \tag{12}$$

The result is:

$$DCF_{\gamma}^{a}(x_{1}',x_{2}',E_{\gamma}) = \frac{1}{2}KE_{\gamma}(\mu_{ex}/\rho)_{a}\frac{1}{\mu_{s}}$$

$$\times \left\{ F_{2}(\mu_{s}x_{1}') - F_{2}(\mu_{s}x_{2}') + \frac{C_{s}}{(D_{s}-1)^{2}} \left\{ \exp\left[(D_{s}-1)\mu_{s}x_{1}'\right] - \exp\left[(D_{s}-1)\mu_{s}x_{2}'\right] \right\} \right\}$$
(13)

where the second-order exponential integral is given by:

$$F_2(\omega) = \exp(-\omega) - \omega F_1(\omega)$$
 (14)

The variables  $x_1$ ' and  $x_2$ ' are equal to  $x_1 + x_a$  and  $x_2 + x_a$ , respectively. The nuclide-specific dose-rate conversion factors for layer sources are computed by summing these monoenergetic conversion factors analogously to Equation (9) as:

$$DCF_{\gamma}^{P}(x_{1}',x_{2}') = \sum_{i} f_{i\gamma} DCF_{\gamma}^{a}(x_{1}',x_{2}',E_{i\gamma})$$
 (15)

#### 3. Conversion and modification

#### 3.1 Code conversion

The MLSOIL and DFSOIL codes were originally developed at ORNL in USA. Source listings of the two codes were given in appendixes of the user's manuals. Both of the original codes were implemented on IBM compatible computers and related FORTRAN compilers. MLSOIL and DFSOIL have been typed from the source listings and converted for the present computer system. The system consists of a personal computer (PC) named COMPAQ Deskpro 5/60m and a PC-FORTRAN compiler named Lahey F77L EM/32<sup>3)</sup>. Calculation models of the modified versions of both codes are the same as those of the original versions.

At the beginning, both codes did not run in the present PC system at all. Various kinds of errors were detected at compiling, linkage and implementation of the codes. These errors might be caused mainly by the difference between the compilers used here the original versions. Following error messages printed out, the two codes were carefully converted without changing the logic of the codes.

The biggest problem at the conversion was to interpolate energy-dependent parameters such as the mass energy absorption coefficient in air, the linear attenuation coefficient in air and soil, and the coefficients in the buildup factors in air and soil. In the DFSOIL code, the values of these parameters are given for discrete energy and are interpolated for energy values of interest. Although DFSOIL utilized the spline interpolation technique as an external function, the compiler used here did not support it. Therefore, a FORTRAN subroutine program for the spline interpolation was offered from the Computer Center in Risø and was incorporated into DFSOIL.

#### 3.2 Code modification

Some parts of the MLSOIL and DFSOIL codes have been also modified at the conversion. Main modifications of the codes are as follows:

where the second-order exponential integral is given by:

$$F_2(\omega) = \exp(-\omega) - \omega F_1(\omega) \tag{14}$$

The variables  $x_1$ ' and  $x_2$ ' are equal to  $x_1 + x_a$  and  $x_2 + x_a$ , respectively. The nuclide-specific dose-rate conversion factors for layer sources are computed by summing these monoenergetic conversion factors analogously to Equation (9) as:

$$DCF_{\gamma}^{P}(x_{1}',x_{2}') = \sum_{i} f_{i\gamma} DCF_{\gamma}^{a}(x_{1}',x_{2}',E_{i\gamma})$$
 (15)

#### 3. Conversion and modification

#### 3.1 Code conversion

The MLSOIL and DFSOIL codes were originally developed at ORNL in USA. Source listings of the two codes were given in appendixes of the user's manuals. Both of the original codes were implemented on IBM compatible computers and related FORTRAN compilers. MLSOIL and DFSOIL have been typed from the source listings and converted for the present computer system. The system consists of a personal computer (PC) named COMPAQ Deskpro 5/60m and a PC-FORTRAN compiler named Lahey F77L EM/32<sup>3)</sup>. Calculation models of the modified versions of both codes are the same as those of the original versions.

At the beginning, both codes did not run in the present PC system at all. Various kinds of errors were detected at compiling, linkage and implementation of the codes. These errors might be caused mainly by the difference between the compilers used here the original versions. Following error messages printed out, the two codes were carefully converted without changing the logic of the codes.

The biggest problem at the conversion was to interpolate energy-dependent parameters such as the mass energy absorption coefficient in air, the linear attenuation coefficient in air and soil, and the coefficients in the buildup factors in air and soil. In the DFSOIL code, the values of these parameters are given for discrete energy and are interpolated for energy values of interest. Although DFSOIL utilized the spline interpolation technique as an external function, the compiler used here did not support it. Therefore, a FORTRAN subroutine program for the spline interpolation was offered from the Computer Center in Risø and was incorporated into DFSOIL.

## 3.2 Code modification

Some parts of the MLSOIL and DFSOIL codes have been also modified at the conversion. Main modifications of the codes are as follows:

- (1) DFSOIL needs the radiation data for calculating the dose-rate conversion factors for soil layers and the ground surface. The radiation data means intensity, and average and maximum energies of each radiation which is emitted from a radionuclide. The original file of the radiation data was not available for the present work. The code have been modified to read the radiation data which are calculated by using the RADCAL code in the DOSDAC system<sup>5-6</sup>. This computer code system was developed at the Japan Atomic Energy Research Institute (JAERI).
- (2) In the original versions of both codes, the depths of five soil layers were fixed using a data initialization statement, that is, 0-1, 1-5, 5-15, 15-30 and 30-100 cm. These depths were determined by taking into account not only a shielding effect of the soil but also root zones of some plants of interest and a layer which contributes to resuspension. However the modified version of DFSOIL reads the soil depths from an input file, and the user can freely select the depths by changing input data. The depths are then read by the modified version of MLSOIL together with the dose-rate conversion factors.
- (3) The original versions of both codes assume that the soil is uniform over the depth to be assessed. The original codes provide single default values for the distribution coefficient (k<sub>d</sub>), bulk density of soil (ρ) and volumetric water content of soil (θ). However there is a possibility that the characteristics of soil change with depth. Among the above parameters, the dependence of ρ with depth will influence both the dose-rate conversion factors calculated in DFSOIL and the radionuclide migration into soil estimated in MLSOIL. In the modified versions of both codes, the user can input the site-specific data of ρ for each soil layer if such data are available. To take account of the effect of the depth dependence of ρ on the calculation of the dose-rate conversion factors, the modified version of DFSOIL calculates the average bulk density of soil:

$$\rho_{av}^{m} = \frac{\sum_{i=1}^{m} \rho_{i} d_{i}}{\sum_{i=1}^{m} d_{i}}$$

$$(16)$$

where  $\rho_{av}^{m}$  is the average bulk density of soil from the surface to a lower boundary of *m*-th layer (g/cm<sup>3</sup>),  $\rho_{i}$  is the bulk density of soil in *i*-th layer (g/cm<sup>3</sup>), and  $d_{i}$  is the thickness of *i*-th soil layer (cm).

(4) The dependence of  $k_d$  and  $\theta$  with depth may also have an effect on the estimation of the radionuclide migration into soil in MLSOIL. If the site-specific data of the parameters are available for each soil layer, the user can use these values in the modified version of MLSOIL. The dependence of  $k_d$  with depth are taken into account by preparing a correction factor:

$$k_d^m = FK^m k_d \tag{17}$$

where  $k_d^m$  is the distribution coefficient for *m*-th soil layer (ml/g),  $FK^m$  is a correction factor for *m*-th soil layer.

- (5) In the modified version of MLSOIL, the calculated results of the radionuclide concentrations in each soil layer are stored in an output file. The user can then use the results for drawing figures with a graphic software or for carrying out further analysis with another computer code.
- (6) The modified versions of both codes read all input data and calculate all results in the SI unit system for radiation dose and radioactivity. Namely they use the units of 'Gy' and 'Bq' instead of 'rad' and 'Ci'. Formats of input and output data are also changed in some parts of both codes.
- (7) The original version of DFSOIL had two serious mistakes. One was concerned with the conversion of units for several input parameters  $(K, (\mu_{en}/\rho)_a, \mu_a \text{ and } \mu_s)$  and for the calculated results of the dose-rate conversion factors. The other was involved in the value of the coefficient,  $D_s$ , in the buildup factor in soil. These errors were corrected in the modified version.
- (8) In the original versions of both codes, the default value for bulk density of soil ( $\rho$ ) prepared for MLSOIL was different from that for DFSOIL. The values were 1.35 and 1.4 g/cm<sup>3</sup>, respectively. The default value of  $\rho$  has been unified to be 1.4 g/cm<sup>3</sup> in the modified versions.

#### 4. Input and output data

4.1 Formats of input data

## (1) MLSOIL

Input data to be prepared for the MLSOIL code are:

- a) definition of input and output data files,
- b) user-defined options,
- c) decay chain information,
- d) distribution coefficients,
- e) dose-rate conversion factors, and
- f) site-specific data for the water balance.

These input data are read from different data files which have different logical units. Appendix 1 gives formats of the input data to be provided.

The user of the MLSOIL code defines logical units and names of seven files which are used in the code. They are:

$$k_d^m = FK^m k_d \tag{17}$$

where  $k_d^m$  is the distribution coefficient for *m*-th soil layer (ml/g),  $FK^m$  is a correction factor for *m*-th soil layer.

- (5) In the modified version of MLSOIL, the calculated results of the radionuclide concentrations in each soil layer are stored in an output file. The user can then use the results for drawing figures with a graphic software or for carrying out further analysis with another computer code.
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The user of the MLSOIL code defines logical units and names of seven files which are used in the code. They are:

- a) input file for user-defined options,
- b) input file for decay chain information,
- c) input file for distribution coefficients,
- d) input file for dose-rate conversion factors,
- e) input file for site-specific water balance data,
- f) output file of the MLSOIL code, and
- g) output file of radionuclide concentrations in soil layers.

Both of the two output files must be installed before the implementation of the code.

The file for user-defined options includes: options for calculation conditions, logical unit numbers of input and output data files, bulk density ( $\rho$ ) and volumetric water content ( $\theta$ ) of soil, time at which the assessment is performed and time for radionuclide deposition onto soil, longitude and latitude of a receptor point, and air concentrations and deposition rates of radionuclides to be assessed. The options for calculation conditions, the logical unit numbers, and the values of  $\rho$  and  $\theta$  are read via a NAMELIST format. Default values are provided for the logical unit numbers of all data files except INL. MLSOIL also prepares the default values for  $\rho$  and  $\theta$ , which are set to be 1.4 (g/cm³) and 0.49 (ml/cm³), respectively, for all soil layers. The user can input the site-specific data for each soil layer instead of the single default values.

The user of the MLSOIL code provides input data on radionuclides to be assessed and their decay chains. Main input data are: number of parent nuclides to be assessed, indexes for identifying the parent nuclides, number and indexes of all radionuclides including daughters, and information on decay chains of the radionuclides to be assessed (names and half lives of all radionuclides, and branching ratios from parents to daughters).

The distribution coefficient,  $k_d$ , is strongly dependent upon physical and chemical forms of deposited radionuclides and the characteristics of soil. It means that the value of  $k_d$  is very different from site to site. The user of the code, therefore, should provide the site-specific value of  $k_d$  for elements to be assessed. However it is difficult to obtain such data for  $k_d$  compared with other parameters. Unless the site-specific data are available, the user can use default values prepared in MLSOIL. Table 1 gives the default values of  $k_d$  for each element. These values are given for all elements except for hydrogen, carbon, oxygen, rare gases and actinides of larger atomic numbers.

The DFSOIL calculates the dose-rate conversion factors for five soil layers and the ground surface, and stores them in the data file. Boundaries of each soil layer are also determined by input data of DFSOIL. The dose-rate conversion factors used here have the units of Gy/year per Bq/m³ for soil layers and Gy/year per Bq/m² for the ground surface, respectively.

The site-specific data for the water balance are read via a NAMELIST format. The data include: annual average values for precipitation and evapotranspiration. These data are used to estimate transfer coefficients between a soil layer to another, together with the other site-specific data such as the distribution coefficients, and bulk density and volumetric water content of soil.

# (2) DFSOIL

The user of the DFSOIL code must prepare input data concerning:

- a) definition of input and output data files,
- b) boundaries of soil layers, and
- c) radiation data for each radionuclide.

These input data are stored in different data files and read from different logical units. Formats of input data to be provided are represented in Appendix 2.

Logical unit numbers and names of three files which are used in the DFSOIL code are defined by the user of this code. They are:

- a) input file for boundaries of soil layers,
- b) input file for radiation data, and
- c) output file of the DFSOIL code.

The user must also install the output file before the implementation of the code.

Six boundaries are necessary to define five soil layers without a break. The user gives the boundaries for each layer from the shallow part of soil to the deeper. When the doserate conversion factors calculated here are used in the MLSOIL code, the boundaries have to start from the ground surface to the deeper.

The DFSOIL code computes dose-rate conversion factors only for radionuclides, radiation data of which are included in the file. The file includes the name, half life, decay mode of a radionuclide as well as radiation data for the radionuclide. Radionuclides decay with emitting various kinds of radiation such as  $\gamma$  ray, X ray, annihilation radiation, positive and negative  $\beta$  particles, internal conversion electron, Auger electron,  $\alpha$  particle, neutron and other heavy particles. In calculating dose-rate conversion factors for soil layers, DFSOIL uses only the data for photons (i.e.  $\gamma$  ray, X ray and annihilation radiation) since the ranges of the other particles are usually short in soil. In spite of the long range of neutron in soil, the evaluation for neutron is out of the scope of this report.

# 4.2 Preparation of input data files

As explained in the above section, various kinds of input data are necessary for the implementation of the MLSOIL and DFSOIL codes. All of input data files have been prepared for the modified versions of both codes. Among the data provided, the distribution coefficients and the annual average data for water balance are the same as default values given for the original versions.

Appendix 3 shows sample input data for MLSOIL and Appendix 4 for DFSOIL. Concerning nuclide-dependent data, this sample shows the data for <sup>137</sup>Cs-<sup>137m</sup>Ba, <sup>134</sup>Cs and <sup>106</sup>Ru-<sup>106</sup>Rh, which are important radionuclides for the long-term external dose rates after an accident at a nuclear power plant. Only part of the data are listed for the distribution coefficients and the radiation data since the volume of these data is large.

Table 2 gives 54 radionuclides and their daughters for which nuclide-dependent input data were prepared for the codes. These radionuclides are considered to be important for a radiological consequence assessment of an accident at a nuclear power plant. Among these radionuclides, rare gases are assumed not to be deposited onto the ground. It is also assumed that rare gases produced in soil are removed from the soil immediately. These nuclide-dependent data are divided and stored into six files, which are shown in Table 3. There are two other files on nuclide-dependent data: RISOE for the main contributors to the long-term external dose rates, and TEST for testing the original versions of both codes.

The decay chain data are based on the 1987 version of the Evaluated Nuclear Structure Data File (ENSDF) decay data<sup>7</sup>. The radiation data are also calculated from the ENSDF by using the RADCAL code incorporated in the DOSDAC system<sup>5-6</sup>. This computer code system calculates systematically and consistently dose conversion factors for internal and external exposure using fundamental data such as nuclear structure, atomic, anatomical and metabolic data. Calculations of the internal dose conversion factors are done with the methodology described in ICRP Publication 30<sup>8</sup>. The method of Kocher<sup>9</sup> in ORNL is used for computing the external dose-rate conversion factors. The function of RADCAL for calculating the radiation data is equivalent to that of the EDISTR code<sup>10</sup> developed at ORNL.

# 4.3 Sample outputs

Appendix 5 gives a sample output of the MLSOIL code, which is written on the logical unit IOUT. This output was computed by using the sample input data given in Appendix 3. The sample shows the calculation for <sup>137</sup>Cs-<sup>137m</sup>Ba, <sup>134</sup>Cs and <sup>106</sup>Ru-<sup>106</sup>Rh, which are the main contributors to the long-term external dose rates at a nuclear accident. The output represents the radionuclide concentration in soil layers ten years after unit deposition on the ground. In the calculation, default values are used for all input parameters specific to site. The option for specifying the outputs is selected so that all outputs can be written (IWRITE=1). They include intermediate results useful for checking calculations, but not needed for assessments. Generally the output file contains:

- (1) Number and indexes of radionuclides to be assessed.
- (2) User-defined options for calculation conditions, including the number of receptor locations, and their longitude and latitude.
- (3) Values of nuclide-dependent parameters such as the distribution coefficient, a radiological decay constant, and dose-rate conversion factors for each of five soil layers and for the ground surface.
- (4) Input parameter values for correction factors for taking account of the dependence of  $k_d$  values with depth.
- (5) Input parameter values for time at which the assessment is done, time of radionuclide deposition onto soil, and bulk density and volumetric water content of soil for each of five soil layers.
- (6) Calculated results for radionuclide concentrations in each of five soil layers and on the ground surface, together with those for the effective concentrations on the ground surface, and the layer and plane dose rates.

(7) Site-specific data for the water balance, that is, annual average precipitation and evapotranspiration.

(8) Transfer coefficients from one soil layer to the deeper one, calculated for each

radionuclide.

(9) Input data for air concentrations and deposition rates, and calculated results of the effective concentration on the ground surface.

Among the outputs described above, the layer dose rate is defined by Equation (3). The plane dose rate is calculated by:

$$H_P = C_P DCF_P \tag{18}$$

where  $H_P$  is the dose rate in air from the plane source (Gy/sec),  $C_P$  is the radionuclide concentration in the ground surface (Bq/m<sup>2</sup>), and  $DCF_P$  is the dose-rate conversion factor for the plane source (Gy/sec per Bq/m<sup>2</sup>). The ground surface concentration is computed by using Equation (1), assuming that a migration removal rate from the surface is the same as that for layer 1.

In the modified version of MLSOIL, calculated results of radionuclide concentrations in each soil layer are stored in an output file which has the logical unit 60. The user can then use the results for drawing figures with a graphic software or for carrying out further analysis with another computer code. Figure 2 shows a sample figure drawn by a graphic software.

The outputs of the DFSOIL code are dose-rate conversion factors for radionuclides to be assessed. In turn they are used for input data of MLSOIL without any conversion. The data of dose-rate conversion factors read from the logical unit IDCF, which are shown in Appendix 3, give sample outputs of DFSOIL.

## 5. Verification

The MLSOIL and DFSOIL codes were converted for a personal computer system and were modified at the present work. It is necessary to verify the intended functions of the codes. The verification of the codes were carried out by comparing the calculated results of MLSOIL and DFSOIL to those of other computer codes.

The concentrations of <sup>137</sup>Cs and <sup>137m</sup>Ba in five soil layers were calculated with MLSOIL using default values for each input parameter. These results were compared to those of the GEARB code<sup>11-12)</sup>, in which the same parameter values were used as MLSOIL. GEARB is a computer tool for solving simultaneous first-order differential equations. Table 4 gives a comparison of the calculated results of the two codes, together with the parameter values used in the calculations. A fairly good agreement can be seen between the two results. The differences might be due to those in mathematical techniques for an integration used in the codes.

(7) Site-specific data for the water balance, that is, annual average precipitation and evapotranspiration.

(8) Transfer coefficients from one soil layer to the deeper one, calculated for each

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(9) Input data for air concentrations and deposition rates, and calculated results of the effective concentration on the ground surface.

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where  $H_p$  is the dose rate in air from the plane source (Gy/sec),  $C_p$  is the radionuclide concentration in the ground surface (Bq/m<sup>2</sup>), and  $DCF_p$  is the dose-rate conversion factor for the plane source (Gy/sec per Bq/m<sup>2</sup>). The ground surface concentration is computed by using Equation (1), assuming that a migration removal rate from the surface is the same as that for layer 1.

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The dose-rate conversion factors for <sup>137</sup>Cs and <sup>137m</sup>Ba were computed with DFSOIL for various depths of soil layers. A comparison was done between the calculated results of DFSOIL and those by Kocher *et al*<sup>13)</sup>. They computed the dose-rate conversion factors for the specified values of energy, using another computer code which adopts the same models as DFSOIL. The author of this report has obtained the factors for radionuclides of interest by linearly interpolating the results for the discrete values of energy. A comparison of the two results is given in Table 5. This table shows that the two results agree well. The differences might be caused mainly by those in the interpolation methods. In the calculations of DFSOIL, the spline technique was used to interpolate the values of energy-dependent parameters, whereas the calculated results themselves were interpolated linearly for the values of Kocher *et al*. The differences in the radiation data used for the calculations could also contribute to those in the results.

By the comparisons described above, the modified versions of MLSOIL and DFSOIL were verified to have the intended calculational functions. Calculation models used in the codes should be also validated before the results of the models are used for recommendatory purposes. The validation of the models, however, is out of the scope of this report and is transferred to other future research.

## 6. Concluding remarks

The MLSOIL and DFSOIL codes were developed at ORNL in USA to estimate the migration of radionuclides into soil and the resultant external dose rates. The original versions of both codes were designed to be applied to an undisturbed agricultural land, for example a pasture ground. It is possible to apply these codes to an open area such as a garden or a park in the urban environment as well. The two codes can estimate the external exposure from radionuclides in undisturbed areas, which would be the greatest contributor to the long-term dose rates in both the urban and rural environment.

In the present work, therefore, MLSOIL and DFSOIL have been converted for a PC system to make the implementation of the codes easy. Some parts of both codes were modified at the conversion, but calculation models themselves remained unchanged. Input data files were also prepared for both codes. These files include nuclide-dependent data for 54 radionuclides and their daughters, which are considered to be important for a radiological consequence assessment of an accident at a nuclear power plant. Finally the modified versions of both codes were verified to have the intended calculational functions.

The transfer of radionuclides in soil is very complicated and is influenced by various factors associated with deposited materials, soil characteristics and weather conditions. A simple model is used here to estimate the downward migration of radionuclides into soil: a five-compartment linear transfer model. This model simplifies the complex migration in soil by introducing the element-specific transfer coefficients as a function of the  $k_d$  values and the water balance parameters. The  $k_d$  value is strongly dependent upon physical and chemical forms of deposited radionuclides and the characteristics of soil. It means that the value of  $k_d$  is very different from site to site. Unless the site-specific data are available, the user can use default values provided in MLSOIL. However attention

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should be paid to the use of these default values because they are only the average for various types of soil.

Further research is necessary on the validation of models used in MLSOIL and DFSOIL. This could be achieved by comparing model predictions with measured data. The comparison will be done for the vertical distributions of radionuclides in soil and the resultant external dose rates. Such a comparison would reveal structural deficiencies and invalid assumptions in models, and wrong selection of input parameter values. We expect to recognize limitations on applications of the codes and to obtain prospects of modifying models to improve the accuracy of predictions.

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- 13) D.C. Kocher and A.L. Sjoreen: Dose-rate conversion factors for external exposure to photon emitters in soil, *Health Physics*, Vol.48, No.2, pp.193-205 (1985)

Table 1 Default values of distribution coefficients used in the MLSOIL code

element	k <sub>d</sub> (ml/g)	element	$k_d$ (ml/g)	element	$k_d$ (ml/g)
Ac	1.5E+03	Ge	2.5E+01	Pu	4.5E+03
Ag	4.5E+01	Hf	1.5E+03	Ra	4.5E+02
Al	1.5E+03	Hg	1.0E+01	Rb	6.0E+01
Am	7.0E+02	Но	6.5E+02	Re	7.5E+00
As	2.0E+02	I	6.0E+01	Rh	6.0E+01
At	1.0E+01	In	1.5E+03	Ru	3.5E+02
Au	2.5E+01	Ir	1.5E+02	s	7.5E+00
В	3.0E+00	ĸ	5.5E+00	Sb	4.5E+01
Ba	6.0E+01	La	6.5E+02	Sc	1.0E+03
Be	6.5E+02	Li	3.0E+02	Se	3.0E+02
Bi	2.0E+02	Lu	6.5E+02	Si	3.0E+01
Br	7.5E+00	Mg	4.5E+00	Sm	6.5E+02
Ca	4.0E+00	Mn	6.5E+01	Sn	2.5E+02
Cđ	6.5E+00	Mo	2.0E+01	Sr	3.5E+01
Ce	8.5E+02	N	5.0E-01	Ta	6.5E+02
Cl	2.5E-01	Na	1.0E+02	Tb	6.5E+02
Cm	2.0E+03	Nb	3.5E+02	Tc	1.5E+00
Co	4.5E+01	Nd	6.5E+02	Te	3.0E+02
Cr	8.5E+02	Ni	1.5E+02	Th	1.5E+05
Cs	1.0E+03	Nр	3.0E+01	Ti	1.0E+03
Cu	3.5E+01	Os	4.5E+02	Tl	1.5E+03
DΥ	6.5E+02	P	3.5E+00	Tm	6.5E+02
Er	6.5E+02	Pa	2.5E+03	υ	4.5E+02
Eu	6.5E+02	Pb	9.0E+02	v	1.0E+03
F	1.5E+02	Pd	6.0E+01	W	1.5E+02
Fe	2.5E+01	Pm	6.5E+02	Y	5.0E+02
Fr	2.5E+02	Po	5.0E+02	Yb	6.5E+02
Ga	1.5E+03	Pr	6.5E+02	Zn	4.0E+01
Gđ	6.5E+02	Pt	9.0E+01	Zr	3.0E+03

Table 2 Radionuclides for which input data have been prepared for the MLSOIL and DFSOIL codes

No.	Nuclide		Daughter nuclio	de
1 2 3 4 5 6 7 8 9	Co-58 Co-60 Kr-85(*) Kr-85m(*) Kr-87(*) Kr-88(*) Rb-86 Sr-89			
10 11 12	Sr-90 Sr-91 Y-90 Y-91	Y-90 Y-91m	Y-91	
13	Zr-95 Zr-97 Nb-95	Nb-95m Nb-97m	Nb-95 Nb-97	
15 16 17 18 19 20 21	Mo-99 Tc-99m Ru-103 Ru-105 Ru-106 Rh-105	Tc-99m Tc-99 Rh-103m Rh-105 Rh-106	Tc-99	
22 23 24	Sb-127 Sb-129 Te-127	Te-127m Te-129m	Te-127 Te-129	I-129
25 26 27 28 29 30	Te-127m Te-129 Te-129m Te-131m Te-132 I-131	Te-127 I-129 Te-129 Te-131 I-132 Xe-131m(+)	I-129 I-131	Xe-131m(+)
31 32 33	I-132   I-133	Xe-133m(+)	Xe-133(+)	
34 35 36 37	I-134 I-135 Xe-133(*) Xe-135(*) Cs-134	Xe-135m(+)	Xe-135(+)	Cs-135 (+)
38 39 40 41	Cs-136 Cs-137 Ba-140 La-140	Ba-137m La-140		
42 43	Ce-141 Ce-143	Pr-143 Pr-144m	Pr-144	
44 45 46 47 48	Ce-144 Pr-143 Nd-147 Np-239 Pu-238	Pm-147 Pu-239		
49	Pu-239 Pu-240	Am-241		
51 52 53 54	Pu-241 Am-241 Cm-242 Cm-244	Pu-238 Pu-240		

<sup>\*</sup> These rare gases are assumed not to be deposited onto the ground.
+ These radionuclides are assumed to be removed from the soil immediately after they are born.

Table 3 Nuclide-dependent input data files for the MLSOIL and DFSOIL codes

File	Name of radionuclide							
	8 nuclides + 5 daughters							
CHRON1	Co-58 Co-60 Sr-89 Sr-90 (Y-90) Zr-95 (Nb-95m, Nb-95) Nb-95 Ru-103 (Rh-103m) Ru-106 (Rh-106)							
	10 nuclides + 4 daughters							
CHRON2	Cs-134     Cs-136     Cs-137 (Ba-137m)     Pu-238       Pu-239     Pu-240     Pu-241 (Am-241)     Am-241       Cm-242 (Pu-238)     Cm-244 (Pu-240)							
	6 nuclides							
CHRON3	Kr-85 Kr-85m Kr-87 Kr-88 Xe-133 Xe-135							
·	9 nuclides + 8 daughters							
CHRON4	Rb-86 Sr-91 (Y-91m, Y-90) Y-90 Y-91 Zr-97 (Nb-97m, Nb-97) Mo-99 (Tc-99m, Tc-99) Tc-99m (Tc-99) Ru-105 (Rh-105) Rh-105							
	4 nuclides + 4 daughters							
CHRON5	Te-127 Te-127m (Te-127) Te-129 (I-129) Te-129m (Te-129, I-129)							
	10 nuclides + 11 daughters							
CHRON6	Sb-127 (Te-127m, Te-127) Sb-129 (Te-129m, Te-129, I-129) Ba-140 (La-140) La-140 Ce-141 Ce-143 (Pr-143) Ce-144 (Pr-144m, Pr-144) Pr-143 Nd-147 (Pm-147) Np-239 (Pu-239)							
	7 nuclides + 3 daughters							
CHRON7	Te-131m (Te-131, I-131) Te-132 (I-132) I-131 I-132 I-133 I-134 I-135							
DICOR	3 nuclides + 2 daughters							
RISOE	Cs-137 (Ba-137m) Cs-134 Ru-106 (Rh-106)							
	2 nuclides + 8 daughters							
TEST	Cs-137 (Ba-137m) Rn-222 (Po-218, Pb-214, Bi-218, Po-214, Pb-210, Bi-210, Po-210)							

<sup>\*</sup> The names of radionuclides in the parentheses represent those of daughters.

Table 4 A comparison of radionuclide concentrations in five soil layers calculated with the MLSOIL and GEARB codes

Nuclide	Soil layer	Concentration*) (Bq/m³)					
Nucriae	(cm)	MLSOIL	GEARB				
	0 - 1	6.42 × 10 <sup>1</sup>	6.41 × 10 <sup>1</sup>				
	1 - 2	1.36 × 10 <sup>1</sup>	1.36 × 10 <sup>1</sup>				
Cs-137	2 - 3	1.44 × 10°	1.44 × 10°				
	3 - 4	1.02 × 10 <sup>-1</sup>	1.02 × 10 <sup>-1</sup>				
	4 - 5	5.41 × 10 <sup>-3</sup>	$5.40 \times 10^{-3}$				
	0 - 1	6.08 × 10 <sup>1</sup>	6.07 × 10 <sup>1</sup>				
	1 - 2	1.29 × 10 <sup>1</sup>	1.29 × 10 <sup>1</sup>				
Ba-137m	2 - 3	1.37 × 10°	1.36 × 10°				
	3 - 4	$9.66 \times 10^{-2}$	9.64 × 10 <sup>-2</sup>				
	4 - 5	$5.12 \times 10^{-3}$	5.11 × 10 <sup>-3</sup>				

## \*) Parameter values used in the calculations

Annual average precipitation (P): 109 (cm)

Annual average evapotranspiration (E): 79.3 (cm)

Volumetric water content of soil ( $\theta$ ): 0.49 (ml/cm<sup>3</sup>)

Bulk density of soil ( $\rho$ ): 1.4 (g/cm<sup>3</sup>)

Distribution coefficient (k<sub>d</sub>): 1000 (ml/g) for caesium

60 (ml/g) for barium

Deposition rate of radionuclides (D<sub>s</sub>): 1 (Bq/m<sup>2</sup>/hour)

Time for radionuclide deposition onto soil: 1 (hour)

Time at which the assessment is performed: 10 (year)

Table 5 A comparison of dose-rate conversion factors for various depths of soil layers calculated with the DFSOIL code and by Kocher et al.

Soil layer	Dose-rate conversion factor for Ba-137m*) (Gy/year per Bq/cm³)					
(cm)	DFSOIL	Kocher et al.				
0 - 1	1.70 × 10 <sup>-4</sup>	1.52 × 10 <sup>-4</sup>				
1 - 2	1.16 × 10 <sup>-4</sup>	1.18 × 10 <sup>-4</sup>				
2 - 3	9.29 × 10 <sup>-5</sup>	9.43 × 10 <sup>-5</sup>				
3 - 4	$7.74 \times 10^{-5}$	7.79 × 10 <sup>-5</sup>				
4 - 5	6.59 × 10 <sup>-5</sup>	6.62 × 10 <sup>-5</sup>				
1 - 5	3.53 × 10 <sup>-4</sup>	3.56 × 10 <sup>-4</sup>				
5 - 15	3.40 × 10 <sup>-4</sup>	3.43 × 10 <sup>-4</sup>				
15 - 30	1.28 × 10 <sup>-4</sup>	1.27 × 10 <sup>-4</sup>				
30 - 100	3.21 × 10 <sup>-5</sup>	3.48 × 10 <sup>-5</sup>				
0 - 5	5.22 × 10 <sup>-4</sup>	5.09 × 10 <sup>-4</sup>				
0 - 15	8.62 × 10 <sup>-4</sup>	$8.52 \times 10^{-4}$				
0 - 30	9.90 × 10 <sup>-4</sup>	9.79 × 10 <sup>-4</sup>				
0 - 100	1.02 × 10 <sup>-3</sup>	1.01 × 10 <sup>-3</sup>				

<sup>\*)</sup> All of the dose-rate conversion factors for Cs-137 are zero since this radionuclide emits no photon.

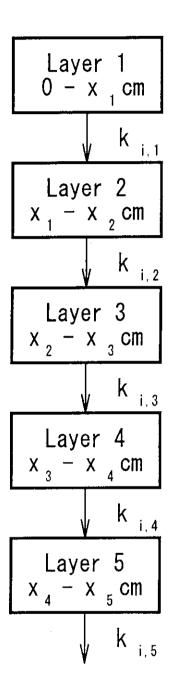


Figure 1 A five-compartment linear transfer model used in the MLSOIL code

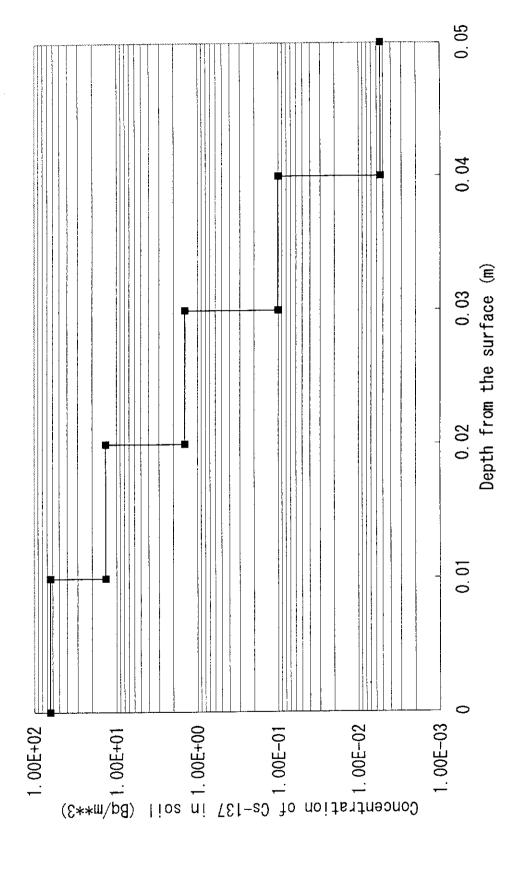


Figure 2 An example of the calculated result by MLSOIL code (Concentration of Cs-137 in soil ten years after the deposition)

## Appendix 1 Formats of input data for the MLSOIL code

## Logical unit 3

Definition of input and output data files

The card #1 is repeated 7 times.

#1 FNUM, FILEN

(A6,4X,A40)

FNUM: logical unit of an input or output data file

='INC' : input file for user-defined options ='NPRIME' : input file for decay chain information ='INE' : input file for distribution coefficients

='IDCF' : input file for dose-rate conversion factors ='INL' : input file for site-specific data

='IOUT' : output file of the MLSOIL code

='60' : output file of radionuclide concentrations in soil layers

FILEN: name of the file

## Logical unit INC

User-defined options for calculation conditions

#1 DAT (NAMELIST format)

#2 TA,TB (2E10.3)

The card #3 is repeated NRECP times.

#3 XLONG, YLAT (2F10.0) #4 (CONAI(I), I=1, NPACK) (8F10.0) #5 (DEPRR(I), I=1, NPACK) (8F10.0)

DAT

: options and logical unit numbers

**IOPT** 

: option for specifying the source of the location and deposition data The user should input IOUT=3 in the current version of the code. It means that the user enters a list of longitudes and latitudes of locations of interest, and air concentrations and deposition rates for each radionuclide.

**IWRITE** 

: option for specifying the written outputs on logical unit IOUT

=0 : SITE parameters and radionuclide concentrations are written for each location of interest.

=1: All outputs are written, including intermediate results useful for checking calculations, but not needed for assessments.

=2 : Constants, a summary table and radionuclide concentrations for each location are written, but SITE parameters and intermediate results are not written.

: option for reading SITE data **ISTORE** The user should input ISTORE=3 in the current version of the code. It means that SITE data are read via NAMELIST format on logical unit INL for each location. : number of user-defined receptor locations of interest **NRECP** The user should input NRECP=1 in the current version of the code. : logical unit from which decay chain information is read NPRIME default value=11 : logical unit from which distribution coefficients are read **INE** default value=12 : logical unit from which dose-rate conversion factors are read **IDCF** default value=15 : logical unit from which SITE data are read in NAMELIST format INL : logical unit on which the listing of the MLSOIL code is written **IOUT** default value=6 : bulk density of soil for each of five soil layers (g/cm³) RHO(M) default value=1.4 for all soil layers THETA(M): volumetric water content of soil for each of five soil layers (ml/cm³) default value=0.49 for all soil layers : time at which the assessment is performed (year) TA : time for radionuclide deposition onto soil (year) TB XLONG: longitude of a receptor location : latitude of a receptor location YLAT : concentration of the radionuclide in the air (Bq/m³) CONAL : deposition rate of the radionuclide to the ground (Bq/m²/sec) DEPRR

# Logical unit NPRIME

Decay chain information for radionuclides to be assessed

#1	NUMCHA,NPACK	(215)
#2	(IC(I),I=1,NPACK)	(1615)
#3	(JC(I),I=1,NPACK)	(1615)
	NREL,NEXP	(215)
#5	(N1(I),I=1,NREL)	(8110)
#6	(N2(I),I=1,NEXP)	(8I10)
The c	ards from #7 to #9 are repea	ited NUMCHA times.
#7		(I5)
The c	ard #8 is repeated L times.	•
#8	NAME, HLF, NNIT, NBRA,	(IBRA(K), K=1,5), (BRAT(K), K=1,5),
	(FKD1(M), M=1,5)	
		(A6,E10.3,A1,I2,5I2,5F5.2,1X,5F5.2)
#9	DUM	(A10)

#### JAERI-Data/Code 95-009

NUMCHA: number of parent nuclides to be assessed

NPACK : number of all radionuclides including daughters

IC : index of the radionuclide

JC : index for presenting in which decay chain the radionuclide is included

NREL: The user should input NREL=NUMCHA in the current version of the

code.

NEXP : The user should input NEXP=NPACK in the current version of the

code.

N1 : indexes for identifying parent nuclides to be assessed

(atomic number, mass number and the state of isomer)

N2 : indexes for identifying all radionuclides including daughters

(atomic number, mass number and the state of isomer)

L : number of radionuclides included in this decay chain

NAME: name of the radionuclide
HLF: half life of the radionuclide

NNIT : unit of the half life

='Y' : year ='D' : day ='H' : hour ='M' : minute ='S' : second

NBRA: number of radionuclides in the decay chain which have this nuclide

as an immediate daughter (NBRA≤5)

IBRA: index for radionuclides in the decay chain which have this nuclide as

an immediate daughter

BRAT : branching ratio from the parent nuclides to this nuclide

FKD1 : correction factor for taking account of the dependence of distribution

coefficients with depth

All the correction factors are set to be 1.0 when FKD1(1)=0.0.

DUM: dummy parameter which is not used in the code.

#### Logical unit INE

Distribution coefficients of elements

The card #1 is repeated as many as the number of elements.

#1 ATNO,DUM,KD

(I2,1X,A2,3X,E8.1)

ATNO: atomic number of an element

DUM: symbol of the element, which is not used in the code

KD : distribution coefficient of the element (ml/g)

#### JAERI-Data/Code 95-009

#### Logical unit IDCF

Dose-rate conversion factors

#1 (SLAY(M), M=2,6), IDOPT

(20X.5F10.3,I10)

The card #2 is necessary when IDOPT=1.

#2 (SD(M), M=1,5)

(20X,5F10.3)

The card #3 is repeated as many as the number of radionuclides.

#3 DZAS,DUM,(DCF(M),M=1,6)

(I10,2X,A8,6E10.3)

SLAY

: lower boundary for each soil layer (m)

SLAY(1)=0.0 is set in the MLSOIL code.

**IDOPT** 

: option for preparing the bulk density of soil in the DFSOIL code

=0 : The default value (1.4 g/cm<sup>3</sup>) is used for all soil layers.

=1 : The site-specific data for each soil layer is provided by the user.

SD(M)

: bulk density of soil for each soil layer (g/cm<sup>3</sup>), which is prepared by the

user in the DFSOIL code

This parameter is needed only when IDOPT=1.

SD(M) must be equal to RHO(M) for all soil layers. The MLSOIL

code stops if  $SD(M) \neq RHO(M)$ .

**DZAS** 

: index for identifying a radionuclide

(atomic number, mass number and the state of isomer)

DUM

: name of the radionuclide, which is not used in the code.

DCF(M)

: dose-rate conversion factors

1≤M≤5: factors for each soil layer (Gy/year per Bq/m³)

: factor for the ground surface (Gy/year per Bq/m²)

## Logical unit INL

Site-specific data at receptor locations

#1 SITE

(NAMELIST format)

SITE: annual average data for water balance

: annual average precipitation (mm/year)

ET

: annual average evapotranspiration (mm/year)

# Appendix 2 Formats of input data for the DFSOIL code

Logical unit 1

Definition of input and output data files

The card #1 is repeated 3 times.

#1 IFNUM, FILEN

(I2,3X,A40)

IFNUM: logical unit of an input or output data file

: input file for boundaries of soil layers

: input file for radiation data

: output file of the DFSOIL code =8

FILEN: name of the file

Logical unit 10

Boundaries of soil layers

#1 (X(M),M=1,6),IDOPT

(6E10.3,I10)

The card #2 is necessary when IDOPT=1.

#2 (SD(M), M=1,5)

(5F10.3)

X

: boundaries of five soil layers (m)

IDOPT: option for preparing the bulk density of soil

=0 : The default value (1.4 g/cm<sup>3</sup>) is used for all soil layers.

=1 : The site-specific data for each soil layer is provided by the user.

SD

: bulk density of soil for each soil layer (g/cm<sup>3</sup>)

This parameter is needed only when IDOPT=1.

Logical unit 14

Radiation data for each radionuclide

#1 ANUM, EXCH, RADNAM, ZNUM, THALF, UNIT, NO, NRTYP1, NRTYP2

(F4.0,A1,1X,A12,F4.0,1X,E10.4,3X,A1,T43,I4,1X,A2,2X,A2)

The card #2 is repeated NO times.

#2 ID,PIRAD,AVE,AMAX

(I2,T6,3(E12.4,1X))

ANUM

: mass number of a radionuclide

**EXCH** 

: index for identifying the state of isomer

='M'

: meta-stable

=blank : stable

RADNAM: name of the radionuclide

ZNUM

: atomic number of the radionuclide

THALF

: half life of the radionuclide

UNIT : unit of the half life

='Y' : year

='D' : day ='H' : hour

='M' : minute

='S' : second

NO : total number of the radiation which are emitted from the radionuclide

NRTYP1 : decay mode of the radionuclide

NRTYP2 : another decay mode of the radionuclide, if any.

ID : identification of the sort of radiation

=1 : γ ray =2 : X ray

=3 : annihilation radiation
=4 : positive β particle
=5 : negative β particle

=6: internal conversion electron

=7 : Auger electron =8 : α particle

=9 : spontaneous fission

PIRAD : intensity of the radiation per decay

AVE : average energy of the radiation (MeV)
AMAX : maximum energy of the radiation (MeV)

# Appendix 3 Sample input data for the MLSOIL code

# Logical unit 3

Definition of input and output data files

INC	C:\MLSOIL\DATA\MLOPT\RISOE.DAT
NPRIME	C:\MLSOIL\DATA\MLCHN\RISOE.DAT
INE	C:\MLSOIL\DATA\MLKD\DEFAULT.DAT
IDCF	C:\MLSOIL\DATA\MLDFRADR\RISOE.DAT
INL	C:\MLSOIL\DATA\MLSITE\TEST.DAT
IOUT	C:\MLSOIL\MLOUT\ORG\RISOE.DAT
60	C:\MLSOIL\MLOUT\ORGCN\RISOE.DAT

# Logical unit INC

User-defined options for calculation conditions

```
&DAT NRECP=1,IOPT=3,IWRITE=1,ISTORE=3,IMERGE=0,INL=50 &END

1.000E+01 1.141E-04

101. 41.

2.778E-02 0.0 2.778E-02 0.0

2.778E-04 0.0 2.778E-04 0.0
```

# Logical unit NPRIME

Decay chain information for radionuclides to be assessed

```
3
          5
          2
                          5
    1
               3
                     3
                          3
    1
          1
    3
          5
    551370
               551340
                          441060
                                                 451060
               561371
                          551340
                                     441060
    551370
    2
CS137
         30.0
          2.552
                                .946
BA137M
                 M 1 1
       0
FILE
    1
          2.062 Y
CS134
       0
FILE
    2
RU106
       368.2
                                1.0
        29.9
                  s 1 1
RH106
FILE
```

# Logical unit INE

Distribution coefficients of elements

44	RU	3.5E+02
45	RH	6.0E+01
46	PD	6.0E+01
47	AG	4.5E+01
48	CD	6.5E+00
49	IN	1.5E+03
50	SN	2.5E+02
51	SB	4.5E+01
52	TE	3.0E+02
53	I	6.0E+01
55	CS	1.0E+03
56	BA	6.0E+01

# Logical unit IDCF

Dose-rate conversion factors

```
        441060. RUTHENIU
        0.010
        0.020
        0.030
        0.040
        0.050

        451060. RHODIUM
        5.833E-11
        4.001E-11
        3.193E-11
        2.657E-11
        2.257E-11
        8.670E-09

        551340. CESIUM
        4.360E-10
        2.996E-10
        2.396E-10
        2.000E-10
        1.705E-10
        6.459E-08

        551370. CESIUM
        0.000E+00
        0.000E+00
        0.000E+00
        0.000E+00
        0.000E+00
        0.000E+00

        561371. BARIUM
        1.698E-10
        1.163E-10
        9.291E-11
        7.743E-11
        6.592E-11
        2.532E-08
```

# Logical unit INL

Site-specific data at receptor locations

&SITE ET=7.93E2, PRECIP=1.09E3 &END

# Appendix 4 Sample input data for the DFSOIL code

# Logical unit 1

Definition of input and output data files

- 10 C:\MLSOIL\DATA\LAYER\RISOE.DAT
- 14 C:\MLSOIL\DATA\RADTN\RISOE.DAT
- 8 C:\MLSOIL\DATA\MLDFRADR\RISOE.DAT

# Logical unit 10

Boundaries of soil layers

0,D-00 1.0D-02 2.0D-02 3.0D-02 4.0D-02 5.0D-02

# Logical unit 14

Radiation data for each radionuclide

137.	CESIUM	55. 3.0000D+01	Y	2	В-	137.0	cs	55.	
5	5.5700D+00		.1732D+00	-	_	2N137.0			1
5	9.4430D+01		.1154D-01			10137.0			2
_	BARIUM	56. 2.5513D+00	M	15	IT	137.1			_
	3.9376D+00		.2194D-02	4.5		137.1			1
2 2	2.1381D+00		.1817D-02			137.1			2
2	2.7012D-04		.1454D-02			137.1			3
2	7.6390D-01		.6378D-02			137.1			4
	2.7564D-01		.7188D-02			137.1			5
2	3.9376D-01		.6304D-02			137.1			6
2 2	9.6079D-03		.6652D-02			137.1			7
	3.7775D-01		.4660D-03			137.1			8
2			.4510D-03			137.1			9
	4.1930D-02 2.4597D-01		.8280D-03			137.1			
2 2			.1555D-03			137.1			
	7.8193D-02		. 9240D-03			137.1			
2 2	4.7190D-02		.8500D-03			137.5			
2	2.8078D-02 3.1315D-03		.9940D-03			137.1			
2	3.1315D-03 3.5666D-02		.5310D-03			137.E			
2	6.9842D-03		.8070D-03			137.1			
2	1.1326D-02		.8070D-03			137.5			
2	7.0103D-03		.3310D-03			137.E			
2	1.2466D-04		.9540D-03			137.E			
2 7	6.0301D-02		.5316D-02			137.E			
7	8.5203D-02		.5696D-02			137.E			
7	7.6308D-02		6059D-02			137.E			
7	1.6664D-02		6032D-02			137.E			
7	2.0760D-01		6416D-02			137.E			
7	9.0996D-02		6800D-02			137.E			
7	8.2708D-02		1111D-02			137.E			
7	6.3911D-02		1474D-02			137.E			
7	1.0741D-01		1851D-02			137.E			
7	3.5070D-02		6035D-02			137.E			
7	3.3298D-01		0298D~03			137.E			
7	2.3142D-01		2060D-03			137.E			
7	3.7626D-02		8940D-03			137.E			
7	1.3697D+00		6668D-03			137.E			
7	7.2455D-01		8430D-03			137.E			
7	1.1779D-01	*	.5310D-03			137.E			
7	3.0732D+00		2898D-03			137.E			
7	1.8316D+00		4660D-03			137.E			
	2.9319D-01		1540D-03			137.E			
7 7	1.4591D+01		9275D-04			137.E			
7	3.3715D+00		5709D-05			137.E			
1	9.0114D+01		6166D-01			137.E			
6	8.3451D+00		2422D-01			137.E			
	1.1946D+00		5567D-01			137.E			
6 6	1.1946D+00 1.6980D-01		5604D-01			137.E			
			5641D-01			137.E			
6	1.3919D-01	0.30410-01 0.	20470-07			131,1		~ · ·	•••

# Appendix 5 A sample output of the MLSOIL code

CASE: MLSOIL OUTPUT
SOURCE LOCATION: LONGITUDE= 100.0000 LATITUDE= 40.0000
RADIOLOGICAL UNITS = BQ
NO. OF LOCATIONS= 1

OPTIONS USED:

GRDOPT = 3 MEANS (R, THETA) POINTS

ANEMOS RUN-OPTIONS-POINT

NRECP= 1 IOPT= 3 IWRITE= 1 ISTORE= 3 ITRNS= 0 IMERGE= 0 ISOIL= 0

IOPT = 3 MEANS DAIA FROM UNIT INC AND CONCENTRATIONS ARE FOR THE WHOLE CELL THAT CONTAINS USER-SELECTED LOCATION(S)

IWRITE = 1 MEANS TOTAL WRITTEN OUTPUT GIVEN

NUCLIDE AIR CONCENTRATIONS AND DEPOSITION RATES ARE SUPPLIED BY THE USER.

THE USER HAS CHOSEN OPTION # 3 AND HAS DEFINED 1 POINT(S) OF INTEREST

LONGITUDE LATITUDE 101.0

THE FOLLOWING PARAMETERS WERE USED IN ALL CALCULATIONS:

	NE .	GY/SEC PER BQ/M**2		E+00	5E-16	7E-15	E+00	3E-16
	PLANE	EC PER		0.000	8.025	2 047	0.000	2 748
ECK:	LAYER 5	GX/SI	0.04-0.05	7.322E-10 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	4.527E-03 5.382E-18 3.686E-18 2.945E-18 2.454E-18 2.089E-18 8.025E-16	1.065E-08 1.382E-17 9.496E-18 7.594E-18 6.339E-18 5.404E-18 2.047E-15	2.179E-08 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00	2.318E-02 1.849E-18 1.268E-18 1.012E-18 8.422E-19 7.154E-19 2.748E-16
ON FACTORS	LAYER 2 LAYER 3 LAYER 4 LAYER 5	E**	0.03-0.04	0.000E+00	2.454E-18	6.339E-18	0.000E+00	8.422E-19
DOSE-KATE CONVERSION FACTORS FOR:	LAYER 3	GY/SEC PER BQ/M**3	0.02-0.03	0.000E+00	2:945E-18	7.594E-18	0.000E+00	1.012E-18
	LAYER 2		0.00-0.01 0.01-0.02 0.02-0.03 0.03-0.04 0.04-0.05	0.000E+00	3.686E-18	9.496E-18	0.000E+00	1.268E-18
	LAYER 1		0.00-0.01	0.000E+00	5.382E-18	1.382E-17	0.000E+00	1.849E-18
RADIOLOGIC	DECAY	CONSTANT		7.322E-10	4.527E-03	1.065E-08	2.179E-08	2.318E-02
SOIL/WATER	DIST. COEFF.	Q		1.000E+03	6.000E+01	1.000E+03	3.500E+02	6.000E+01
NUCLIDE				CS-137	BA-137M	CS-134	RU-106	RH-106
Z				-	2	m	4	ß.

	LAYER 5	0.04-0.05	1.000	1.000	1.000	1.000	1.000
FOR KD	LAYER 4	0.03-0.04	1.000	1.000	1.000	1.000	1.000
ION FACTORS	AYER 2 LAYER 3 LAYER 4	0.01-0.02 0.02-0.03 0	1.000	1.000	1.000	1.000	1.000
CORRECT	LAYER 2	0.01-0.02	1.000	1.000	1.000	1.000	1.000
	LAYER 1	0.00-0.01	1.000	1.000	1.000	1.000	1.000
	NUCLIDE		CS-137	BA-137M	CS-134	RU-106	RH-106
	N.		н	8	ო	4	ហ

TA = TIME (YEARS) AT WHICH ASSESSMENT IS DONE = 1.000E+01 TB = TIME (YEARS) OF LONGTERM BUILDUP IN SOIL = 1.141E-04

RHO(1) = BULK DENSITY OF SOIL (G/CM\*\*3) = 1.400
RHO(2) = BULK DENSITY OF SOIL (G/CM\*\*3) = 1.400
RHO(3) = BULK DENSITY OF SOIL (G/CM\*\*3) = 1.400
RHO(4) = BULK DENSITY OF SOIL (G/CM\*\*3) = 1.400
RHO(5) = BULK DENSITY OF SOIL (G/CM\*\*3) = 1.400

THETA(1) = VOLUMETRIC WATER CONTENT OF SOIL (ML/CM\*\*3) = 0.490
THETA(2) = VOLUMETRIC WATER CONTENT OF SOIL (ML/CM\*\*3) = 0.490
THETA(3) = VOLUMETRIC WATER CONTENT OF SOIL (ML/CM\*\*3) = 0.490
THETA(4) = VOLUMETRIC WATER CONTENT OF SOIL (ML/CM\*\*3) = 0.490
THETA(5) = VOLUMETRIC WATER CONTENT OF SOIL (ML/CM\*\*3) = 0.490

- ACTIVITIES BQ/M\*\*2 IN PLANE 0.04 - 0.05S 0,00-0.01 0.01-0.02 0.02-0.03 0.03-0.04 -ACTIVITIES IN LAYERS-2 BQ/M\*\*3 PLANE DOSE GY/SEC LAYER DOSE GY/SEC BQ/M\*+2 EFF. ZAS NO.

551340 2.195E-02 4.494E-17 5.745E-17 2.806E+00 5.951E-01 6.310E-02 4.461E-03 2.365E-04 2.806E-02 551370 0.000E+00 0.000E+00 0.000E+00 6.422E+01 1.362E+01 1.444E+00 1.021E-01 5.412E-03 6.422E-01 561371 4.719E-01 3.787E-16 4.876E-16 6.075E+01 1.288E+01 1.366E+00 9.657E-02 5.120E-03 6.075E-01 551370 0.000E+00 0.000E+00 0.000E+00 6.422E+01 1.362E+01 1.444E+00 1.021E-01

441060 0.000E+00 0.000E+00 0.000E+00 5.637E-02 3.413E-02 1.033E-02 2.086E-03 3.157E-04 5.637E-04 451060 5.820E-04 1.599E-19 1.549E-19 5.637E-02 3.413E-02 1.033E-02 2.086E-03 3.157E-04 5.637E-04

THE FOLLOWING SITE DATA IS USED FOR LOCATION #

ET = EVAPOTRANSPIRATION (MM/Y) = 793.0 PRECIP = PRECIPITATION (MM/Y) = 1090.0

FOR LOCATION # 1 THE FOLLOWING LEACHING CONSTANTS (/SEC) HAVE BEEN CALCULATED:

S	0.04-0.05	6.720E-10	1.114E-08	6.720E-10	1.919E-09	1.114E-08
4	0.03-0.04	6.720E-10	1.114E-08	6.720E-10	1.919E-09	1.114E-08
m	0.00-0.01 0.01-0.02 0.02-0.03 0.03-0.04 0.04-0.05	6.720E-10	1.114E-08	6.720E-10	1.919E-09 1.919E-09 1.919E-09 1.919E-09 1.919E-09	1.114E-08
7	0.01-0.02	6.720E-10	1.114E-08	6.720E-10	1.919E-09	1.114E-08
-	0.00-0.01	6.720E-10 6.720E-10 6.720E-10 6.720E-10 6.720E-10	1.114E-08 1.114E-08 1.114E-08 1.114E-08 1.114E-08	6.720E-10 6.720E-10 6.720E-10 6.720E-10 6.720E-10	1.919E-09	RH-106 1,114E-08 1,114E-08 1,114E-08 1,114E-08
NUCLIDE		CS-137	BA-137M	CS-134	RU-106	RH-106
Z		Ħ	2	m	4	LC)

FOR LOCATION WITH LONGITUDE = 101.0000 AND LATITUDE = 41.0000 THE FOLLOWING CONCENTRATIONS WERE CALCULATED:

SURFACE SOIL	EFF. CONC. (BQ/M**2)	0.000E+00	4.719E-01	2.195E-02	0.000E+00	5.820E-04
ION	RATE (BQ/M**2/SEC)	2.77BE-04	0.000E+00	2.778E-04	2.778E-04	0.0005+00
	AIR CONC. (BQ/M**3)	2.77BE-02	0.000E+00	2.778E-02	2.778E-02	0.0008+00
NUCLIDE		CS-137	BA-137M	CS-134	RU-106	RH-106
N.		Ħ	N	m	4	Ľ