RECENT IMPROVEMENTS TO THE SOURCE1 AND SOURCE2 COMPUTER CODES

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ABSTRACT

Performance assessments of low-level radioactive waste (LLW) disposal facilities often involve the use of computer codes to describe radionuclide releases from a waste form and the subsequent transport of radionuclides through the environment. The SOURCE1 and SOURCE2 computer codes are used to calculate radionuclide release rates (i.e., source terms) for LLW disposal facilities. These codes have been used to evaluate the source terms for Oak Ridge National Laboratory performance assessments. SOURCE1 is applicable to tumulus-type facilities, while SOURCE2 can be applied to silo, well-in-silo, well, and trench-type facilities. In addition to the calculation of radionuclide release rates, both SOURCE1 and SOURCE2 calculate the degradation of engineered barriers. This paper provides an overview of these codes and a description of recent improvements to the codes. Major improvements include incorporation of a new advective transport model into SOURCE1 and SOURCE2, development of a new model for SOURCE1 that calculates the degradation and failure of the tumulus pad and leachate collection system, improvement of routines for controlling water infiltration inputs, expansion of options for obtaining output summaries, and restructuring of SOURCE1 and SOURCE2 for sensitivity and uncertainty analyses. The status of code verification efforts is also presented.

INTRODUCTION

Performance assessments of low-level radioactive waste (LLW) disposal facilities often involve the use of computer codes to describe radionuclide releases from a waste form and the subsequent transport of radionuclides through the environment. The SOURCE1 and SOURCE2 computer codes calculate radionuclide release rates (i.e., source terms) for LLW disposal facilities.[1] These codes have been used to evaluate the source terms for Oak Ridge National Laboratory (ORNL) performance assessments. SOURCE1 is applicable to tumulus-type facilities, while SOURCE2 can be applied to silo, well-in-silo, well, and trench-type facilities. In addition to the calculation of radionuclide release rates, both SOURCE1 and SOURCE2 calculate the degradation of engineered barriers. This paper provides an overview of these codes and a description of recent improvements to the codes. Major improvements include incorporation of a new advective transport model into SOURCE1 and SOURCE2, development of a new model for SOURCE1 that calculates the degradation and failure of a tumulus-type concrete pad and leachate collection system, improvement of routines for controlling water infiltration inputs, and expansion of options for obtaining output summaries. In addition, summarized results from sensitivity analyses as well as the status of code verification efforts are presented.

OVERVIEW OF SOURCE1 AND SOURCE2 COMPUTER CODES

The SOURCE1 and SOURCE2 computer codes, collectively called the SOURCE computer codes, are used to estimate the source term (i.e., radionuclide release rate) for various types of waste disposal facilities. SOURCE1 simulates radionuclide releases from tumulus-type disposal facilities. SOURCE2 simulates radionuclide releases from silo, well, well-in-silo, and trench-type disposal facilities. Both codes simulate the degradation of engineered barriers (e.g., concrete and metal containers) as a function of time. The estimated degradation is incorporated into the calculation of the radionuclide release rate.

Radionuclide release rates from waste disposal facilities are a function of the integrity of the waste (or waste form) and the engineered barriers used in construction of the facility. When intact, these barriers minimize the contact of water with the waste, thereby minimizing releases of radionuclides. As the barriers deteriorate, over time, water can more readily contact the waste and mobilize radionuclides, thereby accelerating releases to the environment. The SOURCE codes simulate the long-term performance of engineered barriers currently in place at waste disposal facilities. Changes in the material properties of the barriers caused by chemical attack and physical stress are modeled. Specifically, concrete barriers are simulated to degrade as a result of sulfate attack, calcium hydroxide leaching, and corrosion of steel reinforcement. Linear corrosion models are used to simulate the degradation of metal barriers. Projected material properties are considered in structural and cracking analysis of a disposal facility. These analyses are performed to assess the ability of a disposal facility to bear the loads placed upon it. As the ability to bear design loads is compromised and structures crack or fail, rates of infiltration of water through the waste are increased.

The SOURCE computer codes consider two mechanisms through which waste radionuclides are released into the environment: advection (bulk flow driven by hydraulic pressure differences) and diffusion (nuclide movement driven by concentration differences). The calculated total release rate resulting from advection and diffusion is compared with the rate of release dictated by the solubility limit of the nuclide in water. If the solubility limit is exceeded, the release rate is adjusted to the solubility-limited rate. As a disposal facility degrades, the percolation rate of water through the waste increases. Thus, except for cases constrained by solubility, advective releases will increase with degradation and, in general, dominate the total release.

The output of the SOURCE codes includes summaries, as a function of time, of the (a) results from the barrier degradation and failure analyses and (b) calculated contaminant release rates. The generation of a source term with these codes requires more than 100 input parameters to describe the physical and chemical characteristics of the disposal facility and waste type under consideration.

A detailed discussion of the SOURCE computer codes (including a description of the types of facilities modeled, engineered barrier degradation, radionuclide transport models, and input data requirements) can be found in refs. 1 and 2.

NEW ADVECTIVE TRANSPORT MODEL

A new advective transport model was incorporated into the SOURCE codes to better simulate the time dependence of the radionuclide inventory in the disposal facility. This analytical model was developed based on work presented in ref. 3. A detailed derivation of the model can be found in ref. 2.

The total radionuclide release during a time step is calculated by the following formula:

$$L = \frac{\lambda_L}{\lambda_L + \lambda_d} Q_o \left[e^{-(\lambda_L + \lambda_d)t_1} - e^{-(\lambda_L + \lambda_d)t_2} \right] \quad , \tag{1}$$

where

L = mass of radionuclide leached because of advection (g),

λ_L = leach rate constant (s^{-1}),

λ_d = radioactive decay constant (s^{-1}),

Q_o = initial mass of radionuclide in the waste (g), and

t_1, t_2 = the bounds of the time period of interest (s).

The leach rate constant, λ_L, is given by

$$\lambda_L = \frac{q}{W \theta R_d} \quad , \tag{2}$$

where

q = water infiltration rate (cm/s),

W = waste thickness (cm),

θ = relative saturation (i.e., volume of water in waste/volume of waste) (dimensionless),

R_d = retardation factor (dimensionless).

Finally, the retardation factor, R_d, can be calculated by the following equation:

$$R_d = 1 + \frac{\rho_b}{\theta} K_d \quad , \tag{3}$$

where

ρ_b = bulk density of waste (g/cm^3) and

K_d = distribution coefficient (mL/g).

In ref. 2, comparisons were made between the new advective transport model and the original model in the SOURCE codes. To perform these comparisons, a number of simulations were conducted using the SOURCE1 and SOURCE2 codes. These simulations allowed for examination of various radionuclides, half-lives, distribution coefficients, radionuclide inventories, and types of disposal. In general, the two advective models produced similar results with the original model predicting a slightly higher cumulative radionuclide release than the new model. A detailed description of the advective model comparisons can be found in ref. 2.

DEGRADATION MODELS FOR CONCRETE PAD AND LEACHATE COLLECTION SYSTEM

The tumulus-type disposal facility in use at ORNL has both a steel-reinforced pad on which disposal vaults are placed and a leachate collection system. The leachate collection system collects water that infiltrates through the waste and reaches the concrete pad. Hence, as long as the pad and collection system are intact and perform correctly, any radionuclide releases from the waste should be captured and not released to the environment. Routines that simulate the degradation and failure of the concrete pad and the leachate collection system have been developed and incorporated into the SOURCE1 code.

Concrete Pad Degradation Model

The SOURCE1 code predicts the performance of concrete vaults in a tumulus-type disposal facility. However, the original version of SOURCE1 did not account for the presence of a reinforced concrete pad under the vaults. This pad, while intact, should divert water to the leachate collection system. To incorporate the performance of the concrete pad into SOURCE1, a compressive failure model was assumed. Failure was estimated by calculating the reinforcement ratio.[4] The reinforcement ratio is defined by

$$\rho = \left(\frac{A}{b}\right)\frac{1}{d} \quad , \tag{4}$$

where

ρ = reinforcement ratio (dimensionless),

$\frac{A}{b}$ = cross-sectional area of steel reinforcement per unit width of slab (m), and d = effective depth of steel (distance from the top of the slab to the center of the steel reinforcement) (m).

The reinforcement ratio at which compressive failure may occur is called the *limiting reinforcement ratio* and is given by[4]

$$\rho_{lim} = \frac{\epsilon_c'}{\epsilon_c' + \epsilon_y} 0.85 \beta_1 \frac{f_c'}{f_y} \quad , \tag{5}$$

where

ρ_{lim} = limiting reinforcement ratio (dimensionless),

ϵ_c' = ultimate concrete strain (for this application, taken as 0.003) (dimensionless),

ϵ_y = yield strain of steel (dimensionless),

β_1 = a factor used in the equivalent rectangular stress diagram for concrete at the ultimate load (dimensionless),

f_c' = specified compressive strength of concrete (MPa), and

f_y = specified yield strength of steel reinforcement (MPa).

The yield strain of the steel reinforcement can be calculated by

$$\epsilon_y = \frac{f_y}{E_s} \quad , \tag{6}$$

where

E_s = modulus of elasticity of steel (for this application, taken as 200,000 MPa) (MPa).

The value of β_1 is determined as follows:[4]

$$\beta_1 = 0.85 \text{ for } f_c' \leq 30 \text{ MPa or}$$

$$\beta_1 = 0.85 - 0.08 \left(\frac{f_c' - 30}{10} \right) \text{ for } f_c' > 30 \text{ MPa} .$$

The values of the reinforcement ratio and the limiting reinforcement ratio are evaluated at annual time steps in SOURCE1. These two values are compared, and when the reinforcement ratio exceeds the limiting value, the pad is said to have failed hydraulically. Failure of the pad will allow leachate to pass through it. Values of both ρ and ρ_{lim} will change because of the degradation of the concrete. The concrete is simulated to degrade by using the sulfate attack and calcium hydroxide leaching subroutines in SOURCE1. Corrosion of reinforcing steel was not considered because the rates of sulfate attack and calcium hydroxide leaching was judged to greatly exceed the rate of degradation resulting from corrosion. Sulfate attack results in the spalling off of the concrete cover on the reinforcing steel. Hence, as the effective depth of the steel decreases, the reinforcement ratio increases. Leaching of calcium hydroxide from the concrete pad results in reduced concrete strength. Therefore, as the compressive strength of the concrete decreases, the limiting reinforcement ratio decreases. Both of the concrete degradation mechanisms result in a decrease of the margin between the reinforcement ratio and the limiting reinforcement ratio, ultimately resulting in pad failure.

Leachate Collection System Degradation Model

Water that reaches an intact concrete pad of a tumulus-type facility will be diverted to a leachate collection system. This system consists of piping, valves, collection sumps, and monitoring equipment. Ideally, with a properly functioning system, all leachate will be collected, and no release of radionuclides to the environment will occur.

As with the concrete pad, the original version of the SOURCE1 code did not simulate the performance and degradation of the leachate collection system. A model has subsequently been developed that describes the functionality fraction of the collection system as a function of time. The functionality fraction is defined as the ratio of the amount of radionuclide in the collected leachate to the total radionuclide release from the disposal vaults and can vary from 0 to 1. With a value of 1, the leachate collection system is fully functional, and no radionuclides are released to the environment. A zero value indicates a fully degraded system which allows all leached radionuclides to be released to the environment.

The initial functionality fraction and the length of the institutional control period are input parameters to the SOURCE1 code. The functionality fraction degrades linearly to zero from the beginning of the simulation until the end of the institutional control period. The degradation of the collection system is assumed to result from piping and valve leaks or failures, flow obstructions within the system, leakage or overflow of collection sumps, degraded monitoring equipment, etc. At the end of the institutional control period, no maintenance of the collection system is assumed to occur. Hence, no credit is taken for the collection system after the end of institutional control. Additionally, if the concrete pad is predicted to fail hydraulically before the end of institutional control, the functionality fraction is set to zero at the time of pad failure.

VARIATION OF WATER INFILTRATION INPUT

In the original version of the SOURCE codes, only one set of water infiltration values could be input. This set consisted of 12 values of water infiltration data (1 value for each month in the year) that were used for each year of the simulation. Because simulations are typically performed for 1000-year or greater periods, water infiltration would certainly vary with time. The SOURCE codes were modified to allow for variation of water infiltration data. The one set of infiltration values in the input data file was replaced with the name of a file which contains multiple sets of infiltration data. Each set corresponds to a defined time period during the disposal facility performance simulation. For example, six such periods have been defined by ORNL for tumulus-type disposal facilities: (1) the active-use period during which vaults are placed on the tumulus pad, (2) the capping period during which the facility is covered with an engineered cap, (3) the cap decline period during which the cap weathers and degrades, (4) the grass cover period during which the facility is covered with grass and vegetation, (5) the forest succession period during which small trees and bushes begin to grow on top of the facility, and (6) the forest cover period during which the disposal facility is completely covered by trees. Representative water infiltration values can be developed for each of these periods, and with the modifications to the SOURCE codes, these values can be applied during the appropriate time period.

ADDITION OF OUTPUT FILES

The original version of the SOURCE codes contained three output files. One file provided a summary of input data and of engineered barrier degradation. Another file provided, as a function of time, calculated radionuclide releases that recharge to groundwater. The third file provided, also as a function of time, calculated radionuclide releases that flow laterally in the shallow storm-flow region. To provide more information from each simulation, five new output files were created for SOURCE1, and three new output files were created for SOURCE2. A summary of the input and output file structure for SOURCE1 and SOURCE2 is presented in Tables 1 and 2, respectively. These tables list the filename extension, function of the file, and output control variables. The output control variables are used to select which, and at what frequency, output files are written during a simulation.

The output files now available for the SOURCE codes provide a wide variety of data for a source term simulation. Additionally, the output files have been structured to allow for use of the output data by both spreadsheet and graphing software. These types of software applications aid in quality assurance checks and interpretation of simulation results.

SENSITIVITY ANALYSES

To provide more insight into input data needs, extensive sensitivity analyses have been performed on the SOURCE codes. These analyses were conducted for a variety of radionuclides and disposal facilities to cover the spectrum of situations expected to be encountered in a performance assessment. Sensitivity analyses were performed on the SOURCE codes using the Latin Hypercube method. The PRISM computer code[5] was used to implement this random sampling technique. A summary of the results of the sensitivity analyses is presented in Table 3, with a more detailed description of the sensitivity analyses provided in refs. 2 and 6. The sensitive parameters and their rank of importance varied by disposal technology, radionuclide, and year of simulation.

Once sensitive parameters are identified, input data collection efforts can be focused on selecting the most probable values of these parameters and the information required to describe their statistical distribution. These efforts result in a range of uncertainty for each sensitive parameter. Then, through an uncertainty analysis, the overall uncertainty in simulation results can be established.

Table 1. File structure for SOURCE1

Name[a]	Function	Output control variables[b]
filename.inp	Input: Model parameters	
Specified in *filename*.inp Example: water_tum1.dat	Input: Water infiltration values	
filename.con	Output: Summary of input information and concrete analysis	iprint, iprn3, ifrq3
filename.h2o	Output: Beginning year, ending year, monthly water infiltration values	iprint
filename.rch	Output: Year, water flow rate, recharge component of radionuclide release	iprn1, ifrql
filename.1at	Output: Year, water flow rate, lateral component of radionuclide release	iprn2, ifrq2
filename.sum	Output: Year, radionuclide inventory, total leach rate, cumulative leached	iprn4, ifrq4
filename.lch	Output: year, advection component, diffusion component, total leach rate	iprn5, ifrq5
filename.vt1	Output for intact vaults: Year, radionuclide inventory, advection component, diffusion component	iprn6, ifrq6
filename.vt2	Output for cracked vaults: Year, radionuclide inventory, advection component, diffusion component	iprn7, ifrq7

[a]The filename selected by the code user is common to input and output files. The type of file and its contents are identified by the three-character extension.

[b]The output control values determine if data are written to a particular file and at what frequency:

iprint = 0: input data written to file
iprint = 1: input data not written to file
iprn1 through iprn7 = 0: data written to file
iprn1 through iprn7 = 1: data not written to file

The values of ifrq1 through ifrq7 determine how often data are written to a file. Example: For iprn1 = 0 and ifrql = 50, data are written to *filename*.rch every 50 years of the simulation.

Table 2. File structure for SOURCE2

Name[a]	Function	Output control variables[b]
filename.inp	Input: Model parameters	
Specified in *filename*.inp Example: water_th.dat	Input: Water infiltration values	
filename.con	Output: Summary of input information and concrete analysis	iprint, iprn3, ifrq3
filename.h2o	Output: Beginning year, ending year, monthly water infiltration values	iprint
filename.rch	Output: Year, water flow rate, recharge component of radionuclide release	iprn1, ifrq1
filename.1at	Output: Year, water flow rate, lateral component of radionuclide release	iprn2, ifrq2
filename.sum	Output: Year, radionuclide inventory, total leach rate, cumulative leached	iprn4, ifrq4
filename.lch	Output: year, advection component, diffusion component, total leach rate	iprn5, ifrq5

[a]The filename selected by the code user is common to input and output files. The type of file and its contents are identified by the three-character extension.

[b]The output control values determine if data are written to a particular file and at what frequency:

iprint = 0: input data written to file
iprint = 1: input data not written to file
iprn1 through iprn5 = 0: data written to file
iprn1 through iprn5 = 1: data not written to file

The values of ifrq1 through ifrq5 determine how often data are written to a file. Example: For iprn1 = 0 and ifrq1 = 50, data are written to *filename*.rch every 50 years of the simulation.

Table 3. Summary of SOURCE1 and SOURCE2 sensitive parameters

Sensitive parameters[a]	Source term code[b]	
	SOURCE1	SOURCE2
Density of earthen cover (g/cm^3)	X	
Density of waste (g/cm^3)	X	X
Moisture content of waste (unitless)		X
Sulfate diffusion coefficient in concrete (m^2/s)	X	X
Time for complete corrosion of metal waste containers (year)	X	
Saturated hydraulic conductivity of the soil under the disposal facility (cm/s)	X	X
Saturated hydraulic conductivity of concrete (cm/s)	X	X
Radionuclide distribution coefficient in waste (mL/g)	X	X
Radionuclide inventory[c] (g/disposal unit)	X	X
Radionuclide diffusion coefficient in concrete (m^2/s)	X	X
Concentration of sulfate inside vault (mol/L)	X	X
Concentration of sulfate in groundwater (mol/L)	X	X
Containment area per unit (m^2)	X	X
Initial functionality fraction of leachate collection system (unitless)	X	
Time for complete corrosion of corrugated steel liners (year)		X
Time for complete corrosion of cast iron pipe (year)		X

[a]Sensitive parameters are those which contribute at least 3%, during a simulation, to the release rate calculation.

[b]Items marked with an "X" indicate that the item is a sensitive parameter for the computer code.

[c]For SOURCE1, inventory units are expressed as grams per tumulus vault. For SOURCE2, inventory units are expressed as grams per silo, well, or trench, as appropriate.

SUMMARY

The SOURCE1 and SOURCE2 codes are used to calculate the source term for performance assessments of ORNL LLW disposal facilities. These codes simulate the degradation of engineered barriers and the release of radionuclides. Recent major improvements and modifications to the SOURCE codes including incorporation of a new advective model, development of SOURCE1 models for degradation of a tumulus-type concrete pad and leachate collection system, addition of a water infiltration input-data file, and expanded output files and output options have been effected. Additionally, sensitive parameters for both SOURCE1 and SOURCE2 have been summarized.

In parallel with the SOURCE code improvements, an effort was undertaken to verify the computer codes. This effort involved the development and execution of a verification plan for both SOURCE1 and SOURCE2. This plan consisted of a detailed review of the algorithms used in the codes, a review of code structure and programming, and a comparison of different advective models. In addition, tools such as sensitivity analyses and graphical representation of output were used to evaluate the performance of the SOURCE codes. Improvements and revisions to the SOURCE1 and SOURCE2 codes, as well as summary of verification efforts, will be incorporated into a revision of the SOURCE code user's manual.[7]

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