AN ASSESSMENT OF SELECTED ATMOSPHERIC EXPOSURE PATHWAY COMPUTER CODES FOR USE BY OCRWM*

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ABSTRACT

This work is part of the ongoing Systems Modeling Program at Oak Ridge National Laboratory, which is assisting the DOE Office of Civilian Radioactive Waste Management in selecting appropriate computer codes for the process of licensing a high-level radioactive waste repository or a monitored retrievable storage facility. A study of codes for predicting dose to man following airborne releases of radionuclides is described. These codes use models for estimating atmospheric dispersion of activity and deposition onto the ground surface; exposures via external irradiation, inhalation of airborne activity, and ingestion following transport through terrestrial food chains; and the dose per unit exposure for each exposure mode. A set of criteria is given for use in choosing codes for further examination. From a list of over 150 computer codes, five were selected for review. In the area of atmospheric dispersion, AIRDOS-EPA, MESORAD, and MATHEW/ADPIC are described. Under the heading of food-chain transport, AIRDOS-EPA and RAGTIME are discussed. AIRDOS-EPA and MESORAD are reviewed in the area of dose-to-man. Pending a more complete assessment, AIRDOS-EPA is recommended for use by OCRWM for calculating doses from the atmospheric and food-chain pathways, largely because it is mandated by the Environmental Protection Agency for demonstrating compliance with 40 CFR Part 61.

INTRODUCTION

The work described here is part of the Systems Modeling Program (SMP) underway at Oak Ridge National Laboratory. The purpose of the SMP is to assist the Office of Civilian Radioactive Waste Management (OCRWM) in selecting appropriate computer codes for the process of licensing a high-level radioactive waste repository, or a monitored retrievable storage (MRS) facility, should one be authorized. These codes should produce desired results in usable form, produce results that are sufficiently accurate, and have been judged against an adequate quality assurance plan such that they will withstand licensing scrutiny. Previous computer code assessments have been performed in the areas of thermal analysis, shielding, criticality, and radionuclide generation and depletion. This work is concerned with codes for predicting dose to man following airborne releases of radionuclides. They consider models and data bases for estimating atmospheric dispersion of activity and deposition onto the ground surface; exposures via external irradiation, inhalation of airborne activity, and ingestion following transport through terrestrial food chains; and the dose per unit exposure for each exposure mode.

The first step was to identify codes which fall in these categories and which are presently being used in OCRWM programs by subcontractors, national laboratories, and field offices. In addition, codes which are not presently being used, but which show good capabilities for certain OCRWM applications, will be discussed. To accomplish this task, a draft compendium of technical computer codes (1) completed for OCRWM in July 1987, was used to determine codes in present use, and a literature search was undertaken to identify other promising codes. This step resulted in a list of over 150 computer codes.

The next step was to develop a set of criteria to be used in choosing codes for more detailed inspection. Of particular importance was the ability of the code to deal with postulated airborne release scenarios for operations at a geologic repository or MRS facility. In addition, the code should be nonproprietary and have thorough documentation. Other criteria included the relevance of the mathematical model used for calculation and whether the code input parameters or data libraries were up-to-date. Emphasis has been placed on code capabilities as they relate to OCRWM needs.

Using these criteria, two or three codes in each group were chosen for more thorough investigation. Since some codes fell in more than one area, they are discussed more than once. Preliminary recommendations were made based on the outcome of those evaluations.

ATMOSPHERIC DISPERSION CODES

One code presently in use within the OCRWM program, AIRDOS-EPA, will be examined along with MESORAD and MATHEW/ADPIC, which are representative of other dispersion models. AIRDOS-EPA utilizes the familiar Gaussian plume model, while MESORAD represents the Gaussian puff model and MATHEW/ADPIC represents the particle-in-cell (PIC) model. These codes were chosen because they are all nonproprietary and well-documented. They also will run on generally available computer systems, although some revisions may be necessary in order to switch between systems. They are also suitable for the release scenarios postulated for a geologic repository. AIRDOS-EPA and MESORAD follow through with a calculation of dose-to-man, which is desirable but not necessary since the air

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concentration values from ADPIC may be used as input to a dose calculation code.

AIRDOS-EPA

The AIRDOS-EPA code was developed at Oak Ridge National Laboratory for use by the U. S. Environmental Protection Agency(2). It employs a modified Gaussian plume model for air dispersion, and follows the calculation through various exposure pathways to dose to man. Annual average ground-level air concentrations at various distances from a continuous source are estimated and are averaged over sixteen 22.5-degree sectors. As an option, the data may be displayed on a 20 X 20 Cartesian grid. As many as 36 radionuclides may be traced simultaneously from up to six stacks or area sources. This code has been used widely for many years, and has the approval of the U. S. Environmental Protection Agency and the Nuclear Regulatory Commission.

One of the main strengths of AIRDOS-EPA is its relatively long history of use. This has resulted in extensive documentation and validation studies. The fact that AIRDOS-EPA is well-documented and widely used is an important factor in favor of its use in the OCRWM facility licensing process. This code has been used many times to generate data in support of NRC license applications and other environmental impact statements, and so is generally accepted as suitable for these purposes. The Environmental Protection Agency (EPA) also mandates the use of AIRDOS-EPA in 40 CFR Part 61 (3) for determining compliance with emission standards, unless an alternative code is approved by the EPA.

Most of the limitations associated with AIRDOS-EPA as an atmospheric dispersion code are due to the constraints of the Gaussian plume model. These include the assumptions of constant wind speed, no wind shear, flat topography, and no chemical or physical interactions during plume travel. These ideal conditions are rarely satisfied in real situations, since instantaneous changes in wind direction or speed and terrain features often are encountered. However, many of these variations will average out if long-term, steady-state concentrations are desired.

MESORAD

The MESORAD code was developed at Pacific Northwest Laboratory (PNL) for use by the Nuclear Regulatory Commission in responding to emergency situations and accidental releases(4). It uses the Gaussian puff model for calculating atmospheric dispersion, and also calculates external and inhalation doses. Food-chain transport is not included as an exposure pathway. MESORAD can trace up to 50 radionuclides during each run. Since it is designed for emergency response applications, the time frame that is modeled is on the scale of hours, rather than days or weeks.

MESORAD, although relatively recent, is the result of the progression of MESODIF and related codes, which began in 1974. Therefore, there is adequate documentation of the theoretical basis and practical applications of the code.

The puff model incorporated in MESORAD has the advantage of being able to represent meteorological variations more accurately than plume models. This is important for modeling accident scenarios and short-term air concentrations. However, several locations for sampling of meteorological data are needed to obtain accuracy that is better than that of the straight-line Gaussian plume codes.

Some compromises were made in order to keep the computer run time for MESORAD low, which is important for accident response applications. These compromises are related to the resolution of the output grid and to the interval used in the time-integration. These factors may be changed by the user if run time is not a major consideration.

MATHEW/ADPIC

The codes MATHEW and ADPIC were developed at Lawrence Livermore National Laboratory (LLNL) (5,6), and have been coupled because of their complimentary capabilities. MATHEW produces a mass-adjusted, three-dimensional wind field which is used as input for ADPIC, which calculates time-dependent air concentrations by the particle-in-cell (PIC) model. Dose calculations are not performed by these codes. MATHEW/ADPIC is particularly suited for dispersion in areas of complex terrain, since the wind field is determined for each specific site to include terrain influences.

Even though MATHEW/ADPIC has a sophisticated method of dealing with complex terrain, there are practical limitations to the accuracy of the method. These limitations arise from a lack of accurate representative data and from the need for more work on the theory involved with terrain modelling. MATHEW/ADPIC also requires extensive computer memory capabilities and, depending on the computer, may require long run times. However, with sufficient site-specific meteorological data and a well-tuned advection field, it could provide useful information for a facility license application. In order to "tune" a code to a specific site, one must have substantial data on wind, turbulence, and measured air concentrations. This will require multiple measuring towers, higher altitude measuring devices, and tracer releases.

Recommendations

All three of the codes discussed above may be very useful, provided the application is appropriate for the model. In comparing the two Gaussian model codes, AIRDOS-EPA is generally applied to emergency planning, while MESORAD is used for emergency response. In emergency planning, simplifying assumptions concerning the stability of atmospheric conditions may be made, which are necessary for a plume model. These assumptions are often chosen in the interest of worst-case scenario planning. Emergency response requires the use of real-time atmospheric data, for which the puff-type model is better suited. The particle-in-cell model in MATHEW/ADPIC may be useful if a large quantity of meteorological data is available for determining the three-dimensional wind field. This is not generally the case at present, but such data could result from site-characterization activities to be performed at the repository location.

Many feel that the most suitable model is the simplest model which can be acceptably validated (7). This criterion would seem to point to codes which use the Gaussian plume model, but this may not be the case for situations in which validation studies show that plume models are not appropriate, such as in regions of complex terrain. The user must decide, using all available resources, which code or codes to use.

FOOD-CHAIN TRANSPORT CODES

The terrestrial food-chain exposure pathway to man via airborne contamination is an important part of the calculation of dose. Most of the computer codes which are currently in use for the estimation of terrestrial food-chain transport utilize models which are given in the U. S. Nuclear Regulatory Commission's Regulatory Guide 1.109 (8), which assume chronic release and equilibrium exposure conditions. Since all of the current OCRWM codes use this model, the calculations used in AIRDOS-EPA will be examined in this report in the interest of continuity. In addition, there are models which accommodate time-dependent transport and accumulation of radionuclides in the food chain and which are therefore useful under accident release conditions. These models are used in the RAGTIME code, which will also be reviewed.

AIRDOS-EPA

As mentioned above, AIRDOS-EPA is a radiological assessment code that performs atmospheric dispersion, food-chain transport, and dose-to-man calculations. For estimating radionuclide concentrations in meat, milk, and vegetables, AIRDOS-EPA uses the models contained in the Nuclear Regulatory Commission's Regulatory Guide 1.109(8). The models and equations given in this Regulatory Guide are designed to be used to calculate annual doses from routine releases from nuclear reactors. Equations are given to calculate external, inhalation, and ingestion doses from releases to the atmosphere or to water. To support the calculation of ingestion doses, models are given for the estimation of steady-state equilibrium radionuclide concentrations in meat, milk, and vegetables. The Regulatory Guide also lists suggested values of input parameters for these equations. Separate models are given for ^{14}C and ^{3}H, since they behave quite differently from other radionuclides.

The use of NRC models for food-chain transport is an important point in favor of the use of AIRDOS-EPA for OCRWM applications. However, these NRC models have some shortcomings of which the user should be aware. The use of annual average deposition rates to calculate crop concentrations does not account for seasonal factors, such as the length of the growing season and the feeding of non-pasture grass to livestock during the winter. There may also exist some positive correlations that could have a significant effect on food-chain concentrations. An example is the possible correlation between deposition rates and crop assimilation when the relationship between rainfall and crop growth is considered. In this case, the use of annual average deposition rates may lead to a non-conservative estimate of radionuclide concentrations. Another limitation of the NRC equilibrium models is the inability to simulate daughter-product ingrowth during transport through food chains. Equilibrium concentration factors are used to distribute radionuclides between food-chain levels or compartments, and so the dynamic nature of radioactive decay may not be directly incorporated(9). AIRDOS-EPA attempts to correct this problem by adding the daughter isotopes to the source term at the point of deposition.

As with the use of most models, the selection of input parameter values is a large source of uncertainty. The values chosen for a specific application will depend on the needs, interests, and considerations of the user. Someone who is attempting to determine compliance with regulations may choose very conservative values, while someone who is interested in more representative results may choose values closer to the geometric mean of the given range(9). The user should be aware of these uncertainties and present them clearly with the results. A helpful discussion of statistical distributions associated with food-chain transport parameters is given in Ref. 10.

RAGTIME

The time-dependent food-chain transport code RAGTIME (11) was developed at Oak Ridge National Laboratory. The model uses first-order linear differential equations, with time as the independent variable. This method attempts to account for seasonal and other variations that occur in real agricultural situations. However, the model is still in development, and so is presented here mainly as a comparison to the historical equilibrium approach and as an important possible improvement that merits further study.

The main advantage of the RAGTIME code, over codes which use an equilibrium model, is the increased ability to represent dynamic seasonal factors and ingrowth of radioactive daughters during transport through food-chain compartments. The use of differential equations as opposed to normal algebraic equations allows these variations to be described explicitly. These capabilities are not yet utilized fully due to a lack of appropriate parameter values. However, the option is available for these values to be utilized once they have been determined experimentally.

Recommendations

Of the models currently available for representing radionuclide food-chain transport, the ones contained in NRC Regulatory Guide 1.109 are most often used for generating dose estimates in support of license applications and environmental impact statements. Since there are few data at present to define the parameters used in the time-dependent model, the equilibrium concept seems to be the most suitable one for use in the OCRWM site characterization and licensing effort. There are many available codes from which to choose that use essentially the same equilibrium models as given in NRC Regulatory Guide 1.109. The selection of a particular code will depend on the needs of the user. AIRDOS-EPA may be an appropriate choice, especially if atmospheric dispersion and dose calculations are also desired, since it is well-documented and widely accepted.

DOSE-TO-MAN CODES

As with the previous two sets of computer codes, there are quite a few codes which calculate dose to man, but the number of different models represented is limited. Most codes calculate external dose from immersion in contaminated air by the semi-infinite cloud model and the dose from exposure to a contaminated ground surface by the infinite plane model. Internal dose models are based on recommendations of the International Commission on Radiological Protection (ICRP). These recommendations are updated periodically to reflect advances in internal dose calculations.

After applying the general selection criteria, two codes were selected for study. AIRDOS-EPA (2) is already in use within the OCRWM program, and represents the standard models described above. MESORAD (4) is distinct in using a finite-cloud external dose model, although it does not include a method for calculating an ingestion dose.

AIRDOS-EPA

AIRDOS-EPA calculates doses for eleven organs, including the total body, from exposure to radionuclides via immersion in air or water, external exposure to contaminated ground surfaces, inhalation, and ingestion of contaminated food. Atmospheric dispersion of up to 36 radionuclides may be performed within the code, or values of air concentration per unit release rate (X/Q) and deposition rate per unit release rate (D/Q) may be input by the user. AIRDOS-EPA uses ICRP models and dose conversion factors for internal exposures. It will calculate either the population dose or the dose to the maximally exposed individual. Population doses assume average individual intakes, while maximally exposed individual doses are based on maximum intakes. These doses may be displayed on a 20 X 20 Cartesian grid or a sixteen-sector polar grid.

There are some limitations involved with the use of the semi-infinite cloud approximation for calculating external gamma dose. In cases where the plume has not reached ground level, the air concentration and the external dose are assumed to be zero, even though there may be a significant dose from the elevated plume. In these cases, the AIRDOS-EPA documentation (2) advises that this dose be calculated separately and added to the immersion dose calculated by the code. In cases of a ground-level release where the plume does not have much of a vertical extent, the semi-infinite cloud model may overestimate the external immersion dose, since there is actually less radioactivity above the individual than the model assumes.

MESORAD

MESORAD uses a combination of the semi-infinite cloud and the finite puff model for calculating external dose. The dose from contaminated ground assumes a uniform concentration on a flat infinite plane. Inhalation doses are estimated using dose conversion factors from three different models, depending on the nature of the inhaled radionuclide. The ingestion pathway is not included. MESORAD dose calculations concentrate on a maximally exposed individual, since the code is designed for accident response applications. The whole body dose to a maximally exposed individual is used in an accident scenario to determine what protective measures may be needed. MESORAD also calculates lung and thyroid doses. The total-body and lung doses are calculated for a standard adult; but the thyroid doses use parameters for a child, since the child's thyroid dose is higher than an adult's under similar exposure conditions.

One of the most important strengths of the MESORAD code for dose calculations is the use of the finite puff model for external doses. This model is somewhat more realistic than the semi-infinite cloud model, particularly for estimating doses close to an elevated release, when an elevated plume may contribute significantly to the dose. The use of the finite puff model is supported by MESORAD's Gaussian puff atmospheric dispersion model, which gives time-dependent air concentrations of radionuclides in each puff. Both of these models are especially useful for describing accident scenarios.

Recommendations

In comparing the dose components of AIRDOS-EPA and MESORAD, AIRDOS-EPA has the advantage of handling all of the major atmospheric exposure pathways, including food-chain transport. MESORAD's major strength is the implementation of the finite-cloud external dose model, which includes dose from an elevated plume.

FINAL RECOMMENDATIONS

Due to the complexities associated with atmospheric modeling and the many models available for dealing with different scenarios, it is unlikely that any one atmospheric dispersion code could be determined to be the best for all applications. The selection of a code will need to be done by experts familiar with the peculiarities of the site to be modeled. In some cases, it may be beneficial to use more than one code and compare their outputs.

The areas of food-chain transport and dose-to-man are somewhat easier to resolve. Until time-dependent values for food-chain variables are better determined, the model of choice seems to be the equilibrium model given in U. S. Nuclear Regulatory Commission Regulatory Guide 1.109 (8). The fact that it is recommended by the Nuclear Regulatory Commission makes it a particularly good selection for OCRWM activities. The internal dose models given by the ICRP in their Publications 26 (12) and 30 (13) and in the report of the Task Group on Lung Dynamics (14) are most often used to calculate dose conversion factors. External dose factors derived from the semi-infinite cloud immersion model and the finite-plane ground contamination model also are chosen most frequently.

Pending a more complete assessment, the present code of choice for calculating dose-to-man from atmospheric and food-chain pathways would seem to be AIRDOS-EPA. This code has a large body of documentation already in place that shows its usefulness and applicability for many release scenarios. AIRDOS-EPA is mandated for use by the Environmental Protection Agency in 40 CFR Part 61, Subpart I,(3) for demonstrating compliance with the regulations in that document. It also has the endorsement of the Department of Energy, and it has been accepted many times for use in Nuclear Regulatory Commission licensing applications. There are many limitations associated with AIRDOS-EPA, some of which are highlighted in this report. Potential users must be aware of these limitations and how they might affect the usefulness of the code output in their specific situation. For example, in cases where the external dose from an overhead plume may be important, the writers of AIRDOS-EPA recommend that this dose be calculated separately and added to the overall external dose estimate.

It is important to keep in mind the developing nature of models and codes. Research involving complex terrain modeling and age-dependent dose conversion factors will soon allow models to be improved even further, and these newer models will be incorporated into new and existing codes. Therefore, code assessment should be an on-going effort, and new codes should not be overlooked in the selection process.

In order for a code to withstand licensing scrutiny, it must be very well-documented. In researching the codes in present use within the OCRWM system, many were found to be lacking in this area. If these codes are to continue in use, this problem must be remedied. Thorough documentation is essential for quality assurance and for general code usability.

Quality assurance has recently become a very important part of any work related to the OCRWM program. Therefore, any codes used in the OCRWM program will need to be brought into compliance with all relevant quality assurance guidelines (15). In order to insure this compliance, it may be advantageous to organize a code distribution center, where codes with the proper quality assurance and configuration control can be distributed for use by OCRWM contractors.

On-site validation studies should be performed to help determine the applicability of a code for the site in question. A large body of data from the Nevada Test Site area already exists, which will be a valuable resource if the Yucca Mountain site remains as the one chosen for the high-level waste repository. These data include lengthy meteorological measurement records and tracer release studies (16).

It is important that ample meteorological data be gathered carefully and thoroughly during site-characterization. Output from a code can be no more accurate than the input values used. Meteorological experts should be involved in this data collection, to help insure that it is done properly. Quality assurance is also an important consideration during this process.

This preliminary study should be followed by a more thorough assessment of these code categories. This assessment will need to cover such topics as uncertainty analysis and sensitivity analysis, and it should discuss the practicalities involved with actually running the codes.

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