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October 1980 – September 1981**

**Multimedia Radionuclide
Exposure Assessment Modeling**

December 1982

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OCTOBER 1980 - SEPTEMBER 1981

MULTIMEDIA RADIONUCLIDE EXPOSURE
ASSESSMENT MODELING

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EXECUTIVE SUMMARY

Pacific Northwest Laboratory (PNL) and Los Alamos National Laboratory (LANL) are jointly developing a methodology for assessing exposures of the air, water, and plants to radionuclides as part of an overall development effort of a radionuclide disposal site evaluation methodology. The assessment methodology will predict radionuclide exposure levels in the environment by simulating dominant mechanisms of radionuclide migration and fate. The methodology is more sophisticated than those for a basic worst-case scenario analysis, but less sophisticated than a full-scale, extremely detailed, and expensive and time-consuming onsite survey. The methodology encompasses five different environments (i.e., atmospheric, terrestrial, overland, groundwater, and surface water) and combines them into a highly flexible tool. The purpose of the work in FY-1981 was to continue the development of the Multimedia Contaminant Environmental Exposure Assessment (MCEA) methodology and to initiate an assessment of radionuclide migration in Los Alamos and Pueblo Canyons, New Mexico, using the methodology.

The scope of the work performed in FY-1981 consisted of four elements. The first involved the atmospheric component in which the AIRTRAN model was completed for its development, briefly tested, and documented. In addition, a literature search for existing validation data for AIRTRAN was performed. The second element involved the terrestrial and groundwater components of the methodology. This study was performed to assess the feasibility and advisability of including the UNSAT moisture flow model as a submodel of the of the terrestrial code BIOTRAN. The third element discussed a preliminary application of the proposed MCEA methodology, as it related to the Mortandad-South Mortandad Canyon site in New Mexico. This preliminary application represented a scaled-down version of the methodology in which only the terrestrial, overland, and surface water components were used. Lastly, an update describing the progress in the assessment of radionuclide migration in Los Alamos and Pueblo Canyons is presented. The overland and surface water components of the methodology will be used to simulate the migration and fate of radionuclides in these two canyons in Los Alamos, New Mexico.

This study is a part of a long-term effort to define and develop an assessment tool for describing the migration and fate of radionuclides in multimedia environment. The study revealed (1) that a significant amount of atmospheric information exists at the DOE Rocky Flats Plant in Colorado, which has been identified as a promising site for validation of AIRTRAN; (2) that UNSAT in its present form should not be included directly as a subprogram of BIOTRAN; (3) that the scaled-down version of the MCEA methodology, as related to the Mortandad-South Mortandad Canyon site, demonstrated its usefulness for providing a reasonably accurate assessment of the ability of radioactive waste sites to confine the release of radionuclides.

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1.0 INTRODUCTION

Legislators and private citizens are very concerned about the release of radionuclides from radioactive waste disposal sites into the environment and the danger that these releases present to humans and the environment. Radionuclides released from the disposal site undergoes complex interactions in the atmosphere, hydrosphere, and biosphere. These complex interactions and the scenario depicting the release of radionuclides into the environment are presented in Figure 1.1. Since mathematical models can integrate these complex, interactive mechanisms into a single system, they must be an integral part of a site-evaluation methodology.

Currently, Los Alamos National Laboratory (LANL) and Pacific Northwest Laboratory (PNL) are jointly developing a site-evaluation methodology. The overall effort encompasses the development of: 1) a usable and credible site-evaluation methodology for present and future land use around disposal sites; 2) long-term scenarios; and 3) a multimedia radionuclide exposure assessment methodology.

The Multimedia Contaminant Environmental Exposure Assessment (MCEA) methodology consists of integrating several mathematical models, which depict various environments, at common interfaces so an exposure assessment can be performed on the possible migration of radionuclides. These models should consider site specific conditions and characteristics and simulate realistic environmental transport mechanisms. The environments under consideration include atmospheric, terrestrial, overland, subsurface (groundwater), and surface water. In order to fulfill the above criteria, a composite multimedia modeling approach has been presented (as opposed to a fully coupled approach). In a fully coupled multimedia modeling approach, the various pathway models generally become oversimplified in order to achieve understandable input data streams, a reasonable core size, and reasonable run times for these models. In the composite multimedia modeling approach, more realistic individual pathway models can be retained as required. The composite modeling approach also allows updating or replacing individual pathway model easily if it is desired in the future. Coupling between these individual pathway models is achieved

FIGURE 1.1. Multimedia Contaminant Environmental Exposure Assessment Methodology

via transferring the output file from one pathway model to the input file of the next pathway model. Feedback between the various media pathways, which is the justification for the generally less flexible, completely coupled multi-media models, is handled by analysis of the problem in terms of primary pathways for each media and the appropriate compositing of the results of the separate analyses.

The purpose of this study was to continue the development of the MCEA methodology and to perform an assessment of radionuclide migration in Los Alamos and Pueblo Canyons, New Mexico. Specifically, the work was divided into four categories:

1. The developmental work initiated in FY-1980 on the computer code AIRTRAN, which simulates atmospheric transport and location of contaminants through processes of resuspension, atmospheric dispersion and deposition, was completed and tested. Transport matrices for the Los Alamos area were to have been computed in FY-1981, but appropriate meteorological data were not available in time to accomplish this portion of the task. The DOE Rocky Flats Plant in Colorado had been identified as a promising site for validation of AIRTRAN. Extensive measurements of airborne and soil contamination have been made at the site, particularly since 1969, and concurrent on-site meteorological data were available. The proposed validation of AIRTRAN was discussed, along with a description of the data available at the Rocky Flats Plant.
2. The work related to the second category was performed to assess the feasibility and advisability of including the UNSAT moisture flow model as a submodel of the terrestrial code BIOTRAN. UNSAT's relationship with BIOTRAN was discussed as well as the developmental progress of UNSAT. Also presented was a methodology for developing an alternate version of a water flow submodel for BIOTRAN.
3. The results of the modeling of radionuclide transport by overland and in-stream water flow in the watershed of Mortandad and South Mortandad Canyons were presented. This represents a preliminary (scaled-down version) application of the proposed MCEA methodology.

4. The modeling of radionuclide transport in Los Alamos and Pueblo Canyons by snowmelt and precipitation-generated runoff events was discussed. The numerical codes used in the modeling scenario, the interfacing methodology employed between the various codes, and the radionuclide pathway and modeling methodology were also discussed. This task represents a progress report on the Los Alamos - Pueblo Canyon modeling scenario.

This report mainly discusses the work performed by PNL. Chapter 2 presents the conclusions and recommendations of this composite study. Chapter 3 discusses the atmospheric transport modeling as related to the atmospheric code AIRTRAN. It also provides a brief evaluation of the atmospheric information available at the Rocky Flats site. Chapter 4 describes the applicability of coupling UNSAT and BIOTRAN. It also presents alternatives for developing a moisture flow model for BIOTRAN. Chapter 5 discusses the radionuclide multimedia modeling results at the Mortandad-South Mortandad Canyon site. The last chapter presents the progress on the multimedia radionuclide exposure assessment modeling for Los Alamos and Pueblo Canyons, New Mexico.

2.0 CONCLUSIONS AND RECOMMENDATIONS

The migration and fate of radionuclides in a given environment are controlled by a complex set of mechanisms. Models used to simulate natural events must themselves be complex enough to simulate the major mechanisms affecting the movement of radionuclides in a given environment. In order to comprehend the movement of radionuclides in various media, a standardized approach was developed for examining the complex and interdependent processes of radionuclide transport. The MCEA methodology encompasses five media (atmospheric, terrestrial, overland, subsurface, and surface water) for describing the continuous migration of radionuclides from one medium to the next. Numerical models representing the five environs are compositely coupled to retain scenario flexibility in the modeling approach.

This study was instituted to continue the development of the multimedia modeling concepts developed in previous years. The work herein was divided into four areas representing various environments: 1) continue development of the atmospheric transport component, 2) investigate the feasibility of combining the unsaturated moisture flow model UNSAT with the terrestrial model BIOTRAN, 3) discuss the application of the scaled down version of the MCEA methodology in which only the terrestrial, overland, and in-stream components were considered, and 4) present the progress of employing the methodology in simulating the migration of significant amounts of radionuclides in Los Alamos and Pueblo Canyons, New Mexico.

The following recommendations and conclusions have been developed for the various tasks associated with this composite study:

1. Atmospheric Transport Modeling

- Information obtained at the Rocky Flats Plant in Colorado looks promising as validation data for the atmospheric transport model AIRTRAN.
- Simulating the migration of contaminants in the atmosphere based on Rocky Flats information is recommended for verification of AIRTRAN.

2. Unsaturated Flow – Groundwater Modeling

- The unsaturated moisture flow model UNSAT in its present form should not be included directly as a subprogram of BIOTRAN.
- The present methodology employed by UNSAT should be used to develop a more simplified moisture flow model, which is more consistent with the level of conceptualization of other sub-models now comprising BIOTRAN.
- A more suitable flow model should be found intermediate to the mathematical approaches taken by BIOTRAN (WTRFLX) and UNSAT: a simplified implicit finite difference scheme dealing directly with water content changes.
- If a detailed unsaturated moisture distribution is required by BIOTRAN, the UNSAT code can be applied in a quasi-coupled mode that does not attempt to include the code as a permanent part.

3. Simplified Multimedia Contaminant Environmental Exposure Assessment Methodology and Its Application to Mortandad Canyon in Los Alamos, New Mexico

- The MCEA methodology discussed here has demonstrated its usefulness for evaluating how specific sites curtail radionuclide migration.
- The methodology could be used as 1) a scientific decision-making tool for regulating the management of radioactive wastes; 2) a research tool for evaluating the relative effectiveness of natural and man-made features at the site in curtailing radionuclide migration to the biosphere; 3) a research tool for estimating the relative significance of environmental pathways and radionuclide transport and fate mechanisms; and 4) a means of providing a rational base for analyzing field sampling data.
- Although their sophistication, time frames and land-surface areas of the models BIOTRAN, ARM, DKWAV, and TODAM under consideration differ, these models were reasonably coupled (via output-input data files) in the MCEA methodology. Since the

methodology is currently being expanded to include atmospheric and groundwater compartments, the framework for coupling the models must be farther improved. It is also recommend that TODAM be combined with an appropriate hydrodynamic model to include feedback of sediment-contaminant transport results to flow conditions, thus enabling TODAM to handle longer morphological changes of a stream system in an analysis.

- Limited data were used to partially test the methodology's validity. Additional tests are strongly recommended.

4. Progress Report: Multimedia Radionuclide Exposure Assessment Modeling of Los Alamos - Pueblo Canyon, New Mexico

- Because a significant amount of the radionuclide inventory in Los Alamos and Pueblo Canyons is ^{239}Pu , the migration and fate of ^{239}Pu was selected to be simulated in this study.
- There are several possible modeling scenarios examining the transport of potentially significant amounts of radionuclides downstream, as discussed below. Each scenario depends upon the size of the resulting storm event and its potential consequence on radionuclide migration. For simulating large storm events: 1) in-stream contaminant concentration levels could be diluted due to an excess volume of water below significant levels, and 2) contaminated sediment and water could be swept through the watershed system to the Rio Grande where radionuclide concentration levels would be insignificant. For simulating small storm events: 1) because the bulk of the contaminant inventory is associated with large sediment sizes thereby reducing the resuspension capabilities of the flow (median sediment diameter $D_{50} > 0.43 \text{ mm}$), a significant amount of radionuclides may not be transported significant distances downstream, 2) if seepage and infiltration are major factors on the watershed, flow velocities, discharges, and depths may be reduced, decreasing the chance for entrainment of contaminated sediment into the flow for movement downstream. An alternate scenario is one in

which the runoff events are large enough to transport the radionuclides downstream but small enough to deposit them at one location, which would produce a significant build-up of contamination downstream.

- The modeling scenario of the transport of radionuclides in Los Alamos and Pueblo Canyons will tentatively consist of the following codes: ARM (overland water-sediment-contaminant transport), MODSEEP (in-stream hydrodynamics), and TODAM (in-stream sediment and contaminant transport).

3.0 ATMOSPHERIC TRANSPORT MODELING

This chapter presents the research performed with regard to the atmospheric component of the multimedia modeling effort. It includes a summary of the progress in the preceeding fiscal year (FY-1981), a description of the atmospheric contaminant transport code AIRTRAN, and validation requirements for AIRTRAN.

3.1 INTRODUCTION

AIRTRAN is a set of Fortran computer programs which are being developed to estimate the atmospheric transport in a multimedia contaminant transport model. Other pathways in the model include botanical, overland, subsurface, and surface water transport. Following the release of a contaminant to the atmosphere or the suspension of surface contamination by wind, AIRTRAN estimates airborne contaminant concentration downwind of a source and contaminant deposition to the surface. The deposition provides input to other pathways, as well as increasing the surface contamination which is a source for resuspension and continued atmospheric transport.

AIRTRAN has been developed specifically to simulate the movement of surface contamination by the repeated process of suspension by the wind, downwind transport and diffusion, and dry deposition. Most contemporary models use the resuspension factor to predict resuspended contamination directly from local surface contamination. This has been shown to be unrealistic (Horst 1981) and is incapable of describing the horizontal transport of surface contamination. In contrast, AIRTRAN predicts the resuspended contamination by using a resuspension rate to calculate the source term in a diffusion-deposition model. Thus, AIRTRAN can interact with other elements of the MCEA methodology to predict the temporal and spatial distribution of surface contamination.

The interaction of atmospheric, botanical, and water transport models is complicated by differences in the space and time scales appropriate for each model. It would be inefficient for all models to be run on the time and space

scales of the model requiring the finest resolution. This is solved in AIRTRAN by initially computing atmospheric transport on appropriate scales, e.g. one hour and 500 m, and then averaging the results over larger scales, e.g., one year and 5 km, prior to interaction with other media. The output of AIRTRAN is an annual-average matrix of atmospheric transport rates among large subdivisions of the total area of concern. This allows efficient interaction with the botanical and water transport models despite differences in scales.

3.2 SUMMARY OF PROGRESS IN FY-1981

The development of AIRTRAN began in FY-1980 and has continued in FY-1981. The AIRTRAN resuspension-diffusion-deposition model has been completed and tested. It is described below, along with the proposed interaction of AIRTRAN with other elements of the MCEA Methodology. Transport matrices for the Los Alamos area were to have been computed in FY-1981, but appropriate meteorological data were not available in time to accomplish this task.

THE DOE Rocky Flats Plant in Colorado has been identified as a promising site for validation of AIRTRAN. Extensive measurements of airborne and soil contamination have been made at the site, particularly since 1969, and concurrent on-site meteorological data is available. The proposed validation of AIRTRAN is discussed below, along with a description of the data available at Rocky Flats.

3.3 AIRTRAN DESCRIPTION

This section describes the general computational structure of AIRTRAN, as well as the specific models and subroutines used in AIRTRAN to simulate atmospheric transport.

3.3.1 Computational Structure

AIRTRAN is designed to accommodate the large difference in time scales of the various transport models. Atmospheric transport varies on an hourly basis with changes in the wind speed, wind direction, and thermal stability. Water transport can vary on a shorter time scale due to precipitation events, and

botanical transport varies on a much longer time scale as plants grow, die, and decay. The major interface between the various media, however, occurs within the overland surface modeling environ where soil and botanical contamination are considered. The rates of exchange between the surface contamination and each of the transport pathways are generally small compared to the rate-of-change of the weather. Therefore, after an initial period following the original release of contamination to the environment, significant changes in the soil contamination will be on a time scale which is large compared to the time scale of weather changes, and the soil contamination will act as a buffer between the models. That is, rapid changes in atmospheric transport will not cause similar changes in botanical or water transport. As a consequence, the change of radionuclide concentrations on the land surface due to air can be adequately simulated by calculating atmospheric transport on a longer time frame such as monthly- or annual-average basis.

AIRTRAN calculates the annual-average atmospheric transport by summing over a joint probability distribution of wind speed, wind direction, and atmospheric stability. This distribution is computed from site-specific meteorological data, such as hourly values of wind speed, wind direction, and temperature at two levels, over a period of one to ten years. Since resuspension would be unlikely during precipitation, these periods are excluded from the computation. The details of this probability distribution calculation, in particular the determination of atmospheric stability, depend on the particular meteorological data available at each site; hence, this distribution is determined prior to application of the AIRTRAN model.

AIRTRAN is structured to interact with other transport models which deal with area-averaged surface contamination. For each combination of wind speed, wind direction, and stability, the computer routine WXAVG averages the airborne contamination and dry deposition over the area of each element of a rectangular array, assuming resuspension of unit surface contamination within the central element. This calculation is made on a dense, fine-resolution grid, e.g., 40 x 40 elements with dimensions of 500 m, oriented N-S and E-W. The results are summed over all meteorological conditions, weighted by their probability of occurrence, to produce arrays of the annual-average transport as a function of distance and direction between area elements.

The annual-average transport arrays output by WXAVG, one for airborne contamination and one for dry deposition, are then used to calculate matrices for atmospheric transport among large subdivisions of the total area of concern. The boundaries of these areas are selected on the basis of uniformity in transport properties. Examples would be an area with approximately uniform vegetation or the drainage area of a single stream. Each subdivision is treated as a source area and the average transport to each of the other areas is calculated by integrating the predictions of the WXAVG array over the areas of the source and receptor subdivisions. The resulting matrices provide mean atmospheric transport rates of surface contamination among the subdivisions.

These atmospheric transport matrices are then used in combination with transport models for the other media to predict the annual-average airborne contamination and to simulate the movement of the soil contamination. For each subdivision, BIOTRAN would predict the net change of surface contamination due to biological processes; there would be a loss of contamination due to resuspension; and the atmospheric transport matrix would predict the gain or reduction of surface contamination due to resuspension, transport, and deposition from the other subdivisions.

3.3.2 AIRTRAN Atmospheric Transport Models

The transport, diffusion, deposition, and resuspension of airborne contamination is affected by a variety of physical processes. A model which includes all of these mechanisms becomes quite complex and expensive to use. Simpler models can be developed for restricted situations by including only those mechanisms which are important for the situation of interest. This simplification is often achieved by investigating only a limited domain in space and time. This philosophy has been followed in selecting the models used in AIRTRAN.

AIRTRAN estimates atmospheric transport and diffusion in subroutine CAV with a straight-line Gaussian diffusion model. This assumes that the

contaminant is transported at the speed and in the direction of a horizontally homogeneous wind field. In the absence of deposition, the contaminant has a normal distribution in the vertical direction with a standard deviation σ_z which is calculated as a function of downwind distance and atmospheric stability from the empirical formulas of Briggs (1973). The horizontal contaminant distribution is identical to the distribution of wind direction. With the common resolution of observed wind direction to a 16 point compass, the horizontal distribution for each wind direction is a top hat distribution of width $\pi r/8$, where r is distance from the source. This model is inexpensive to run, requires only modest input data, and is fairly realistic through the use of empirical plume spread parameters. It is best applied at downwind distances less than 10 km due to spatial variability of the mean wind field and limited knowledge of σ_z beyond that distance.

The flux of contaminant to the ground due to dry deposition is parameterized as a deposition velocity multiplied by the ground-level airborne contamination. The deposition and settling velocities are estimated by subroutine VDVS as a function of particle size and density, wind speed, and surface roughness using the empirical formula of Sehmel and Hodgson (1976). Therefore, the WXAVG transport arrays are calculated separately for each particle size.

The airborne contamination calculated in CAV is reduced as a function of distance from the source to account for deposition. Subroutine DAIRXI computes a standard source-depletion integral to account for the loss of material from the atmosphere, and DEPRFL computes a profile factor to account for the alteration of the vertical profile of contamination from that assumed by the Gaussian plume model (Horst 1980). This alteration is caused by deposition removing more contamination near ground level than at greater heights.

The suspension or resuspension rate RR of surface contamination is calculated in WXAVG from the empirical formula

$$RR = \begin{cases} A (u_* / u_r)^n & , u_* > u_t \\ 0 & , u_* < u_t \end{cases} \quad (3.1)$$

This equation expresses the general observation that resuspension is proportional to some power n (often $n = 3$) of the friction velocity u_* and is zero when u_* is less than a threshold value u_t . However, data are currently not available to specify general values of n , u_t , A or u_r , and these must be determined from site-specific data or estimated with a high degree of uncertainty from the limited data available for other sites (Healy 1977, 1980 and Sehmel 1981). Although these data support the above formula, the values of the parameters are highly variable and their dependence on soil structure, history, vegetative cover, etc. is poorly known.

3.4 VALIDATION OF AIRTRAN

This section describes the data required to validate AIRTRAN and the data available at one potential test site: Rocky Flats plant in Colorado.

3.4.1 Validation Requirements

During the development of AIRTRAN, the operation of each routine has been tested by comparing its output to the known results for special cases. Thus, we are confident that the code performs as it was designed. However, AIRTRAN has not been validated by comparing to simulated results to observed data. Given a distribution of surface contamination and a sequence of meteorological events, AIRTRAN predicts the airborne contamination and the movement of surface contamination. Hence, for validation, concurrent data are required on surface contamination, airborne contamination, and diffusion meteorology.

The most complete test of AIRTRAN would be a comparison of predicted and observed changes in the amount and distribution of surface contamination. The site-specific resuspension rate model requires data for two periods: one to estimate the resuspension rate and a second to test the model. However, due to the small transport rates, the length of data record required for a detectable change in soil contamination may not be available. The next best test of AIRTRAN would be a comparison of predicted and observed airborne contamination, which would require concurrent data over a much shorter period.

The most complete record of the movement of surface contamination by the wind is thought to be found at the DOE Rocky Flats site near Denver, Colorado.

The extent of the data was investigated by means of a literature review during FY-1981, and the results are described below. The data appear adequate for a test of the model, but a definite conclusion can only follow acquisition of the data in FY-1982.

3.4.2 History of the Rocky Flats Site

The Rocky Flats Plant site is used primarily for producing components for nuclear weapons to assist in fulfilling U.S. nuclear weapons production requirements. The prime operating contractor of the facility from 1952 until June 30, 1975, was Dow Chemical, U.S.A. Beginning July 1, 1975, Rockwell International assumed responsibility for operating the plant. The plant is operated under the direction of the DOE Albuquerque Operations Office.

The Rocky Flats Plant is located about 12 km northwest of the Denver metropolitan area and directly east of the Front Range of the Rocky Mountains (Figure 3.1). DOE controls approximately 30 km² of land, most of which is used as a buffer zone to separate the public from plant production operations.

FIGURE 3.1. Rocky Flats Plant Environmental Air-Sampling Off-Site Network (Boss and Stewart 1971)

The topography of the plant site is characterized by a series of sloping and relatively flat, wind-scoured plateaus divided by five separate water-courses running roughly west to east (Figures 3.1 and 3.2). The climate is typified by strong and often gusty winds (mean: 3 to 7 ms⁻¹) and moderate rainfall (mean: 40 cm yr⁻¹). Typically, the stronger winds blow from the west and northwest. Vegetation within and surrounding the installation is modified grassland. Except for a new buffer zone purchased in 1975, Rocky Flats land has not been significantly disturbed by man for over 25 years.

FIGURE 3.2. Rocky Flats Plant Site Including Buffer Zone (Hunt and Hurley 1981)

Operation of the Rocky Flats Plant started around 1952 and, since that time, a number of accidental explosions, fires, and spills have occurred at the plant site. A costly fire at Rocky Flats in 1969 and later detection of off-site ^{239}Pu in soil samples by Martell,^[1](a) Poet and Martell,^[12] and DOE's Health and Safety Laboratory (HASL)^[2] spurred discussion of the environmental contamination problems and safety implications of the Rocky Flats installation.^[6] These investigations indicated that the primary contaminating event was leakage from drums containing plutonium-laden cutting oil that had been stored outdoors in the southeast corner of the plant. Wind suspension of the contaminated soil and subsequent transport to the east-southeast of the plant occurred mostly during 1967 to 1969 period. The spill area was covered by asphalt in 1969 which terminated the main source but subsequent mechanical disturbances of the nearby soil and strong wind events have continued the suspension and transport of minor amounts of contaminated soil to the east and southeast.

The plant's prime contractor conducts an environmental monitoring program for radioactivity and chemical and biological pollutants. Stack emissions, ambient air, water, and soil are sampled on the plant site and in the surrounding region. The environmental monitoring program has intensified since the 1970s. In addition, outside agencies conduct independent environmental surveys, both on and off the plant site. The Colorado Department of Health conducts air, water, and soil sampling programs around the Rocky Flats site,^[9] the DOE Environmental Measurements Laboratory (EML) of New York (formerly HASL) maintains air sampling stations in the vicinity of the Rocky Flats Plant and periodically performs soil sampling and analysis,^[2] and the Jefferson County Health Department and U.S. EPA sample air and liquid effluents. Other laboratories (such as PNL) and groups have also conducted various independent studies on meteorology, soil and vegetation sampling, and ambient-air sampling. Figures 3.1 and 3.3 indicate the locations of several onsite and offsite air sampling stations.

(a) Refer to Rocky Flats Bibliography.

FIGURE 3.3. On-Site Air Sampling Locations
(Boss and Stewart 1971)

Figure 3.4 indicates the general history of Rocky Flats accidents and soil, air, and meteorological sampling. Further details are given in the following sections.

3.4.3 Soil Sampling

Prior to 1969, soil sampling was done on a limited basis and did not include plutonium analysis. Since 1969, soil samples have been collected annually at alternate intersections of a 152.4 m grid in the exclusion area of the plant and also from about 60 locations on the circumference of three circles having radii of 1.6, 3.2, and 8.0 kilometers from the center of the plant. The soil samples are analyzed for plutonium.

During the investigation of plutonium contamination that resulted from oil-drum leakage, the contractor collected soil samples semi-annually from 75

FIGURE 3.4. History of Contaminant Release, Contaminant Sampling, and Meteorological Measurements at DOE Rocky Flats Plant. (Special studies are indicated by bibliographic references. Circled references are of particular interest for AIRTRAN validation and refer to the Rocky Flats Bibliography.)

off-site locations within a 815.8 km^2 area around the plant. In addition, spot samples were taken from areas in which plutonium contamination was known to exist.

Every year the Colorado Department of Health samples soil in the Rocky Flats Plant area, in addition to making an annual determination of plutonium in Colorado soil from worldwide fallout. Independent soil surveys have been made by DOE/EML and Jefferson County Health Department.

3.4.4 Ambient Air Monitoring

Ambient air is presently monitored for airborne particulate matter by a network of 73 air sampling stations located both on and off the Rocky Flats Plant site. The number of sampling stations have varied with time, the number increasing after 1969.

There are 23 continuously running, high-volume air samplers located on the plant site inside (or just outside) the security-fenced area. Samples are collected weekly, analyzed for total long-lived alpha (TLL α) activity, composited biweekly, and analyzed for plutonium.

Airborne particulate samples are collected from 14 continuously running, high-volume air samplers at the plant perimeter at distances ranging from three to seven kilometers. These samples are collected weekly, analyzed for TLL α activity, and composited monthly. Following chemical separation by ion exchange, the samples are analyzed radiochemically for plutonium.

The Colorado Department of Health operates five, on-site continuous air sampling stations, one of which is operated jointly with the Jefferson County Health Department. The samples are collected on alternate days and analyzed for long-lived alpha and beta radionuclides.

Samples in which the total alpha activity exceeds $4 \times 10^{-14} \mu \text{Ci/ml}$ are analyzed specifically for plutonium. A regional air-sampling system of 16 stations provides additional surveillance in the vicinity of Rocky Flats and in the metropolitan Denver area.

The DOE/EML of New York City operates three air-sampling stations, one at the east security fence (S-8), one at the original east perimeter (cattle)

fence, and one at the intersection of the east access road and Indiana Street (Figures 3.2 and 3.3). Samples from these stations are collected every week and analyzed radiochemically for plutonium.

In addition to these routine air-sampling measurements, a number of special studies have been conducted by other groups. These studies are listed numerically in Figure 3.4 and in the bibliography.

3.4.5 Meteorological Monitoring

Meteorological data have been collected at Rocky Flats since the plant became operational in 1952. These data have included wind direction and speed, pressure, humidity, and daily precipitation. Wind data have been collected about 12.2 m above the ground from an anemometer on a building. These data are normally presented in a monthly summary.

In the first quarter of 1975, a 61.0-m meteorological monitoring tower was installed in the southwest quadrant of the Rocky Flats Plant site. The system became operational in May of 1975. Data are recorded digitally at 10-min intervals onto a 9-track magnetic tape. The following data are collected and recorded by the system:

1. Julian days	6. Solar radiation
2. Hours and minutes	7. Wind direction (61.0 m, 6.1 m) ^(a)
3. Temperature (61.0 m, 30.5 m, 6.1 m) ^(a)	8. Average and peak wind speed (61.0 m, 6.1 m) ^(a)
4. Temperature difference ($T_{61.0}$ to $T_{6.1}$) ^(a)	9. Barometric pressure
5. Dewpoint temperature	10. Precipitation.

In addition to the 61.0-m tower, the Wind Energy Test Facility has three or more towers located in the northwest corner of the plant site for collecting meteorological data, and there is a 36.6-m portable meteorological tower presently located on Woman Creek, 1.6 km west of Indiana Street.

Reports on the climatic characteristics, meteorology (winds, etc.), and diffusion meteorology of the Rocky Flats site are presented in the Rocky Flats Plant Site Environmental Impact Statement (EIS).^[34,35]

(a) Refers to vertical distance from ground level in meters.

3.4.6 Special Studies

Reference 1

This article discusses the first off-site soil sampling at Rocky Flats which identified ^{239}Pu concentration. Twenty off-site soil samples and a few reservoir water and sediment samples were included in the report.

Reference 2

Soil samples were collected by the HASL group to a depth of 20 cm at 33 sites extending as far as 64.4 km from the Rocky Flats Plant site. The contamination pattern extends eastward from the plant in the direction of the resultant wind vectors and has virtually no westward component.

Reference 3

Two microsorban filter papers with particles sampled with a high-volume air sampler located at the east Rocky Flats security fence at a height of about 0.9 m were analyzed for ^{239}Pu and particle distribution. Distribution is lognormal with median diameters around 10 μm .

Reference 4

Continuous, high-volume airborne particulate sampling has been maintained for over a year, close to, and downwind from, the Rocky Flats plant. Concentrations have averaged about 2 fCi m^{-3} , 10 to 100 times higher than fallout. Results indicate a correlation between wind velocity and ^{239}Pu concentration in the air. Results also suggest a resuspension factor of between 10^{-7} and 10^{-9} .

Reference 6

Science "News and Comment" article addresses the Rocky Flats off-site contamination problem.

Reference 7

This report is similar to Reference 3: dealing with analysis of ^{239}Pu particles.

Reference 8

This reference is an example of a Dow Chemical Semiannual Report. Air, soil, and other samples are reported on a monthly basis. Location of sampling stations are presented on maps.

Reference 9

This reference is an example of the Colorado Department of Health's Environmental Surveillance Summary Report on Rocky Flats. Soil and air sampling results are presented, as well as location of samplers.

Reference 10

HASL-249 contains two articles, "Plutonium Levels in the Rocky Flats Environs," by M. R. Boss (Dow Chemical), and "Plutonium Isotopic Ratios at Rocky Flats," by P. W. Krey and B. T. Krajerski (HASL).

The first article is a semiannual report on soil, air, and water sampling at Rocky Flats. The second article addresses the plutonium isotopic ratios at Rocky Flats (mostly ^{239}Pu) and the total inventory of Plutonium off-site of the plant (~3.6 Ci).

Reference 12

This reference presents a discussion on the soil-sampling results from over 35 different locations off-site of the Rocky Flats Plant. The analysis includes ^{239}Pu , ^{241}Am , and ^{90}Sr samples from surface waters and sediments. A more detailed report on the soil sample is mentioned in Reference 1.

Reference 13

This report discusses the respirable fraction of resuspended ^{239}Pu close to the Rocky Flats Plant. The results indicate that in this area, with concentrations in excess of 1 fCi m^{-3} , the respirable fraction is about 0.2 to 0.4. Very steep vertical gradients of Pu concentration may be present in the air in this vicinity.

Reference 15

Monthly airborne concentrations at six sampling stations near the east Rocky Flats security fence and downwind from the oil spill pad are correlated with summarized wind data at Rocky Flats from May 1970 to August 1972. In addition, weekly airborne concentrations $\bar{X}$ at sampling station S-8 (HASL) were related to wind speed $\bar{u}$ from July 1970 to January 1971. A general model is developed and is

$$\bar{X} = 0.45 (\bar{u})^{2.1} \quad (3.2)$$

Reference 16

Measured concentrations of plutonium in air and soil, and wind data are used to compute the fraction of the soil inventory which became re-entrained during a 14-month period at Rocky Flats Plant. This computation was performed by a plutonium resuspension model.

Reference 17

The plutonium resuspension model developed in Reference 15 becomes invalid for predicting Pu levels, due to a source change as the result of mechanical disturbance of soil near the oil spill pad. Measured plutonium levels are much greater than levels predicted by the model.

Reference 19

A critique on soil sampling results is discussed by P. W. Krey (HASL) and S. E. Poet and E. A. Martell (NCAR).

Reference 20

This reference is an extension of Reference 18. It discusses a PNL field experiment at Rocky Flats during July 1973. Vertical airborne plutonium concentrations were determined as a function of respirable particle size and wind-speed. A 30.5-m meteorological tower was used at one site. Three sites were instrumented downwind from the oil spill pad. Concentrations decreased with height below the 10-m level. From 10 m to 30 m the airborne concentrations increased suggesting that an elevated upwind source could be contributing to

the movement of the contaminant. The maximum airborne concentration measured was 3.7 fCi m^{-3} . The maximum concentration per gram of gross airborne soil was 50 pCi g^{-1} .

Reference 21

This reference discusses a 3-week field study at Rocky Flats during the summer of 1973 which included three air-sampling sites extending from the security fence to past the cattle fence, one upwind (west) sampler, and twenty-one soil samples taken east of the plant and one taken to the west of the plant.

It was shown that resuspended total mass and plutonium concentrations were inversely related to precipitation and soil moisture. Respirable fraction of both mass and activity concentrations in surface air averaged about 49%. Only 2.5% of the respirable mass was derived from local soil surfaces. The resuspension factor during this time period (generally wet) was $3 \times 10^{-9} \text{ m}^{-1}$.

Reference 25

This reference discusses more results from July 1973 PNL field experiment at Rocky Flats. It also discusses ^{239}Pu and ^{238}Pu concentrations on 13 non-respirable particle diameter sizes (10 to $210 \mu\text{m}$). Both ^{238}Pu and ^{239}Pu were found in all particle diameter size ranges. Airborne plutonium fluxes on non-respirable particles decreased with both height and distance. Airborne $^{238}\text{Pu}/^{239}\text{Pu}$ ratios were always equal to or greater than similar ratios measured on the ground surface. The ratios indicate that ^{238}Pu is more readily resuspended at greater distances from the eastern security fence than at distances near the eastern security fence.

Reference 26

HASL-304 is an update on HASL-235. Soil and vegetation sampling are reported on in the text. Twenty-six soil sample sites are used. The plutonium mass isotopic analysis and the ^{241}Am analyses of soil samples from Rocky Flats identify the contamination as plutonium which was processed in

1958. Nuclide ratios indicate that current operations at Rocky Flats contribute little to the airborne plutonium concentrations which are due to resuspension of the contaminated soil.

Reference 30

This reference is evidently an article written from HASL-315 "Pu-239 Concentrations in Air Near Rocky Flats, Colorado" by H. L. Volchok, M. Schonberg, and L. Toonkel. The article shows that the mean annual $^{239+240}\text{Pu}$ concentrations at three sites downwind from the contaminated area have generally decreased with time (1971 to 1975). The authors suggest that the results reflect the decreasing availability of resuspendible plutonium-bearing particles. This was probably the result of contaminated particle penetration into the soil and a change in particle size.

Reference 31

This article examines data from a study, begun in late 1971, of the patterns of plutonium contamination in the Rocky Flats soil. It provides data on Pu concentrations in the soil, a relationship of concentrations to location, depth, and soil particle size, and a description of likely contaminating mechanisms. Two main sampling plots were used in the study: one, just east of the security fence and the oil spill pad, and the other, directly south of the oil spill pad (~1 km). This article also references a Ph.D. thesis, "Plutonium in Grassland at Rocky Flats," (1976).

References 34 and 35

DOE/EIS-0064, Final Environmental Impact Statement for the Rocky Flats Plant Site, Vol. 1 and 2, 1980. The following sections may be of interest:

Volume 1, Section 2,3,6, Meteorology, and others, pp. 2-57 to 2-94. Section 2.10, Environmental Monitoring Programs, and others, pp. 2-200 to 2-230.

Volume 2, Appendix A-2, Radioecology of Natural Systems, pp. A-2-1 to A-1-12.

Appendix B, Meteorology, pp. B-i to B-2-6.

Appendix E-2, Natural Hazards that may Trigger a Radiological Release from a Plutonium Processing Facility, pp. E-2-1 to E-2-19.

Appendix F, Dose Calculation Methodology, pp. F-i to F-112.
Appendix G-4, Rocky Flats Facility/Technical Assessment Document
B. Inhalation Pathway, pp. 1 to 24 (has discussion on Wind
Resuspension.

Reference 37

This reference is another example of the Rocky Flats Plant Annual Environmental Monitoring Report. It discusses (briefly) meteorology, air, soil, and liquid sampling and provides the location of sampling sites.

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4.0 UNSATURATED FLOW - GROUNDWATER MODELING

This chapter presents a detailed review of soil moisture movement as related to the UNSAT (Gupta et al. 1978) and BIOTRAN (Gallegos et al. 1980) models.

4.1 INTRODUCTION

This study was performed to assess the feasibility and advisability of including the UNSAT moisture flow model as a submodel of the BIOTRAN code. This study is part of the overall effort to develop the MCEA methodology.

The BIOTRAN model was constructed to describe the movement of trans-uranics (TRU) through ecosystems within a study area. A design based on a compartmental representation of an ecosystem is employed. The compartments represent the atmosphere, hydrosphere (groundwater and surface water systems), and biosphere (plants and animals). Flows of water, biomass, and TRU between compartments are estimated by the model, based on many simple interrelated analytical equations. The interrelations are determined by common parameters in the flow equations, and the coupling of fundamental transport processes are described by those interrelations. Most of the flow equations represent a simplified summary of empirical observation, averaged in some particular way over both space and time. Thus, detailed physical mechanisms driving flows between compartments are not necessarily described explicitly in the model. Such a compartmental approach on an ecosystem level is often required because mechanistic theories may not exist or are incomplete. The BIOTRAN model maintains an exact account of accumulation of flows through all compartments: a mass balance is kept for all flows. All flows are ultimately driven in the model by the external forces of solar energy and precipitation (water input). As a dynamical model for transport of TRU, BIOTRAN is probably best suited to predict the long-term, environmental fate of TRU.

This particular study concerned only the relationship between the soil and plant compartments. An improvement in the description of plant-water uptake was the purpose of this effort to combine UNSAT with BIOTRAN. In as

much as transuranics (TRU) are believed to be transported into plants by soil-water used for growth and transpiration, a more accurate description of plant-water uptake was expected to yield improved estimates for the possible fate of TRU in the environment. By applying the UNSAT model to all aspects of water flow, an improved description of TRU movement is expected.

At the beginning of this study, the BIOTRAN code had a very simplified model for describing water movement. A soil profile was conceptualized as a sequence of 25 cm levels or layers with a special 2 cm layer at the surface. Moisture flow, however, was only calculated in the top 25 cm layer with all deeper layers taken as a single soil block. Infiltration of precipitation was determined by the holding capacity in the top 25 cm layer; excess water was lost to runoff without being allowed to re-enter the profile. The possibility for drainage was not accounted for in the code. Moreover, a simple linear relationship based on the available soil-water between the wilting point and field capacity limits described plant-water uptake. Potential evapotranspiration was not divided into soil surface and transpiration components. All evaporation appeared to pass through the plant. Thus, as realized by the LANL research group, improvements in the BIOTRAN water flow model were needed.

As this study to incorporate the UNSAT code proceeded, LANL simultaneously developed a more advanced version of a compartmental water flow based on explicit finite difference techniques. However, LANL found that their model, called WATFLX, had numerical difficulties typical of such mathematical techniques. To assist the developers of BIOTRAN, we have included an additional investigation of such a model.

In this report, we will first give preliminary conclusions and recommendations for development of an improved version of a water flow submodel for BIOTRAN. The general features of the UNSAT model will then be reviewed, since this model is believed to represent a "state of the art" one-dimensional, unsaturated zone flow model. Specific progress in preparing UNSAT for application with BIOTRAN in a quasi-uncoupled mode will then follow. The suggested revisions would be advisable in order to make effective use of the additional soil-water flow provided by UNSAT. Since it was found in this study that

BIOTRAN should undergo some revisions, which exceeded the project's present work scope, no specific simulations joining both models were performed. Finally, a discussion describing a methodology for testing a simple, explicit finite difference model for moisture flow (WTRFLX) will be offered. Although it was determined that such a method should not be used as a general-purpose simulation tool, nevertheless, the model serves to exemplify mechanistic aspects that should be taken into account. A summary of conclusions and recommendations is provided at the end of this reporting chapter.

4.2 CONCLUSIONS AND RECOMMENDATIONS

Preliminary conclusions of this study are that the UNSAT model in its present formulation should not be included directly as a subprogram of BIOTRAN. Instead, the present methodology employed by UNSAT should be used to develop a more simplified moisture flow submodel, which is more consistent with the level of conceptualization of other submodels now composing BIOTRAN. This suggested approach is consistent with that now being taken by LANL to construct a simplified compartmental flow submodel. In order to assist LANL, we have developed a flow model based on an explicit finite difference scheme for approximating solutions of the unsaturated flow equation. We have named this model WTRFLX (a name similar to that used by the LANL group).

After developing WTRFLX and examining its performance, our belief is that a model suitable for BIOTRAN should be found intermediate to the mathematical approaches taken in WTRFLX and UNSAT. That is, a simplified implicit finite difference scheme dealing directly with water content changes rather than hydraulic potential might be more appropriate. The model would be kept simple by applying it only to a few representative soil blocks or compartments. An implicit scheme, instead of a direct explicit one, is needed in order to impose the stability and regularity required for predicting moisture movement. In particular, we have found that the explicit approach used in WTRFLX can produce unpredictable oscillatory behavior unless simulation time steps are made inefficiently small.

It is possible to make an explicit scheme match accurate moisture flow simulations while utilizing relatively large spatial and time steps. This can be done by using effective conductivities and weighted hydraulic gradients. The matching can be done with simulations of basic moisture movement behavior similar to those described by Hillel (1977). Hillel has separately simulated the behavior of infiltration, drainage, redistribution, and evaporation. Explicit finite difference models written in the CSMP computer language were used by that author. However, accuracy was achieved using that numerical method only by applying arbitrarily small time steps and intrinsic integration algorithm built into CSMP. Matching a difference scheme with fixed spatial and time steps would amount to a regression representation of the basic flow behavior. Such an approach, however, cannot be recommended because it must be restricted to only the special cases on which matching was accomplished. Moreover, that approach gives a false impression that the Darcy flow equation is being solved properly. Proper design of an explicit finite difference scheme is discussed further in Section 4.5.

One of the most difficult aspects of a dynamical simulation of moisture movement is encountered during infiltration. The difficulty arises when simulating the advance of a wetting front. This difficulty, however, can be overcome by applying Philip's analytical infiltration equation. Simple analytical equations for drainage conditions can also be obtained. In fact, models based on the application of analytical equations have already been suggested by Eagleson (1978). (See also Cordova and Bras 1981.) Such an approach is well suited for stochastic simulation of rainfall and evapotranspiration as applied in BIOTRAN. Use of analytical equations has the advantage of avoiding the need to control spatial and time steps, and the approach is most consistent with that already adopted for other submodels in BIOTRAN. A detailed design for a water flow model like Eagleson's, however, was not developed in this study.

4.2.1 Coupling UNSAT with BIOTRAN

The final conclusion, which appears to have the greatest potential for the advanced development of BIOTRAN, is to apply UNSAT in a quasi-uncoupled mode. In such a mode, both codes could be run at different times, but various flows would still be coupled through a data (output) file generated by UNSAT

and read by BIOTRAN. A quasi-uncoupling mode could be achieved by placing all water flow aspects into UNSAT where a detailed dynamical simulation can be performed. All aspects of plant-water uptake would be transferred to UNSAT, and stochastic generation of rainfall and potential evapotranspiration would be duplicated in UNSAT. Moisture content and flux varying on a daily basis and integrated over selected soil levels could be transferred to BIOTRAN on a yearly simulation basis (or any other appropriate period). The transferred moisture flows would then be used to determine plant growth and TRU flow. Since plant-water uptake depends on the dynamics of plant growth, these aspects must also be duplicated in UNSAT. The UNSAT code has a subprogram design that allows easy modification of the plant-sink model. General capabilities of the UNSAT model, which make it adaptable to many problems, are discussed in Sections 4.3 and 4.4.

The interface between BIOTRAN and UNSAT is conceptually very simple and feasible (Figure 4.1). Parameters simulated by BIOTRAN would be transferred to UNSAT, and flow results returned to BIOTRAN as shown in Figure 4.1. In BIOTRAN, stochastic methods for generating the climatic parameters such as rainfall and temperature are used. BIOTRAN also uses simplified mathematical descriptions of biomass production, root growth and decay. All of these aspects are considered external parameters in UNSAT. Figure 4.2 illustrates a general schematic diagram of the functional relationships required to interface BIOTRAN and UNSAT. Before the UNSAT model can be applied effectively, certain suggestions for modification of BIOTRAN must be made.

4.2.2 Modification of BIOTRAN

The following is a list of aspects of BIOTRAN that may require modification to achieve a better coupling capability with UNSAT. Some of these suggested modifications are currently being implemented to BIOTRAN.

Precipitation

Water input is perhaps the most important controlling factor in a dynamic simulation model such as UNSAT. Storm intensity (specific duration of rainfall) is an important factor. The possibility of runoff will depend entirely on the storm intensity and the soil surface conductivity. Soil conductivity depends sensitively on soil type, i.e., clay, loam, or sand. In an unsaturated

FIGURE 4.1. Diagram Depicting Proposed Interface Between BIOTRAN and UNSAT

FIGURE 4.2. Schematic Representation of Functional Relationships Between BIOTRAN and UNSAT

flow simulation, the profile need not attain field capacity for runoff to occur. A saturated surface layer can build up and reject continued infiltration and thus increase runoff. Moreover, ponding of runoff may return water to the profile after an intense rainfall event. It may also be necessary to better represent the uncorrelated rainfall events simulated in BIOTRAN. The studies of Cordova and Bras (1981) may provide some useful methods for constructing an improved simulation of stochastic rainfall. An alternative approach is to apply actual rainfall patterns for a specific site. Yearly rainfall could be randomly sampled from a set of preselected "typical" yearly climatic records.

Temperature

The connection between a stochastic rainfall event and temperature is not clearly defined in BIOTRAN. Evapotranspiration usually occurs at reduced rates during rainfall events. Temperature is the main driving stochastic parameter in BIOTRAN, but rainfall does not appear to be explicitly related to temperature. Thus, high rainfall and potential evapotranspiration may occur simultaneously in BIOTRAN. On a monthly simulation period, this lack of correlation between rainfall and temperature (associated evapotranspiration and plant growth) may be adequate; but detailed dynamic daily simulations may be inaccurate. Because the unsaturated soil-water balance is a highly non-linear process, yearly simulations may not be correct if the current formulation of climate were applied to the UNSAT model.

Evapotranspiration

Potential evapotranspiration (PET) depends essentially on a stochastic temperature in BIOTRAN. PET is known to depend on relative humidity, cloud cover, and wind speed as well. A modified Penman equation is often employed to estimate PET (e.g., Feddes et al. 1978).

A partitioning of PET into evaporation and transpiration is required. This is usually based on plant growth (leaf cover), which will depend on temperature. It is seldom possible that entire PET will be extracted from a soil profile. Thus, a method for limiting PET to its actual value is required. BIOTRAN reviewed in this study uses a simplified approach based on a fraction of the holding capacity in the root zone. Rooting depth and actual detailed

soil-water availability to roots should be used to control estimation of transpiration. Currently BIOTRAN is implementing this mechanism. The detailed description of TRU movement now used in BIOTRAN could be applied to soil-water as well. Currently, the transport of TRU does not seem to reflect soil-water flow as a proportionality. That is, the same plant growth aspects controlling TRU should be applied to plant-water use.

Plant Growth and Root Sink

The plant root sink must be designed to depend on plant growth, which is reflected in photosynthesis and biomass accumulation models. Actual transpiration and plant growth activity need to be coupled to soil-water availability. The plant sink should respond directly to available solar energy, soil-water distribution, and a time dependent root distribution. Most of these aspects are already treated in BIOTRAN, but a unified set of relationships is needed.

4.3 RELATIONSHIP BETWEEN UNSAT AND BIOTRAN

This section includes comments on the appropriateness of the UNSAT model. The model could be applied in conjunction with BIOTRAN, although we do not recommend including it as a subprogram. The design of UNSAT has been discussed in detail elsewhere in readily available reports (Simmons and Gee 1981). UNSAT is a one-dimensional unsaturated moisture flow model having a numerical algorithm commonly reported in the literature (e.g., Feddes et al. 1978). It is not a solute transport code, however, but can be used to predict soil water fluxes for input into most typical convective-dispersive transport codes. The UNSAT model was designed with site specific applications in mind and includes the following aspects.

1. UNSAT describes the movement of water through a one-dimensional soil profile in which several types of surface and bottom boundary conditions can be described. The surface condition allows for rainfall, ponding, runoff, and evaporation. Conditions at the profile base can be a water table, unit hydraulic gradient drainage, or an impervious layer. A dynamic water table with flow into the profile can also be described. All of these boundary conditions can vary with time.

2. Detailed representations of soil hydraulic properties (soil-water characteristic and hydraulic conductivity) for each soil layer are employed. An auxillary program called HYDRAK, which is based on various capillary flow models, is used to estimate hydraulic conductivity from its saturated value when direct measurements are unavailable.
3. UNSAT utilizes hourly climatic data that includes rainfall, air temperature, relative humidity, wind speed, and solar insolation. These latter four variables are used to estimate a location specific potential evapotranspiration based on modifications of Penman's equation. The auxillary program FAOPET is used to calculate potential evapotranspiration (PET).
4. A hypothetical plant-water extraction term (plant sink) is an additional model component of UNSAT. The sink models of Hanks (1973) and Feddes (1976) have been coded. [See Moly 1981 for a review of plant-water uptake.] These submodels require rooting depth and root density distributions during a specified growing season. Various equations can be used to partition potential evapotranspiration into its components of evaporation and transpiration demand. An equation based on leaf cover (leaf area index) is usually used to estimate transpiration. Actual transpiration is determined by the UNSAT model as a result of the dynamic interaction between available soil water and climatic transpiration demand.

The UNSAT model currently does not attempt to describe the interaction between plant growth (respiration, photosynthesis, and biomass accumulation) and plant-water uptake. Plant growth activity is viewed as an externally driven process which is predetermined by its environment. The model, however, is structured so that inclusion of feed-back growth models would not be difficult.

A similar modeling objective is approached in the BIOTRAN code. Modeling of biological aspects is emphasized, whereas the original version (before efforts to include WATFLX) had a very simplified soil-water flow model.

In BIOTRAN, fundamental processes are conceptualized as averaged over a daily time step. On the other hand, experience with UNSAT simulations has shown that results are very sensitive to hourly climatic details. This holds especially true for intense rainfall on sandy soils. The detailed simulation of dynamics by the model causes the sensitivity. Thus, the application of UNSAT to averaged input variables may produce inaccurate and misleading results. Such behavior does not imply that the mathematical algorithms used in UNSAT do not apply to coarse spatial and time increments. It only indicates that interpretation of the results becomes more difficult. As a consequence, BIOTRAN in its present formulation would not make effective use of the additional computational detail provided by UNSAT. Improved estimates of runoff, however, might be an exception.

The very fact that UNSAT and BIOTRAN have many common aspects suggests that UNSAT would need to be reduced in order to avoid unnecessary duplications if it was inserted as a subprogram. Because BIOTRAN and UNSAT have common aspects, we suggest that a more effective and flexible approach would be to reproduce the missing coupling elements of plant growth in UNSAT. The simulation results for water flow including effects of plant growth duplicated in UNSAT could be provided as control input for BIOTRAN. Certain aspects of plant growth might require repeated calculation in BIOTRAN, but the advantage is in an external calculation of water flow done on a time scale relevant to UNSAT. Moreover, by running UNSAT and BIOTRAN in a sequential mode, site specific climate data can be easily incorporated, since UNSAT is prepared to accept such information. The output from UNSAT could then be accumulated and averaged on a spatial and temporal scale compatible with BIOTRAN. Although the two models would appear uncoupled by being physically separate during a computer run, they would actually be coupled through an output file from UNSAT, which would include the modeling results on plant growth. The output file would also depend on soil-water availability and climate. This approach is possible, essentially because the movement of plant biomass containing TRU and plant-water can be viewed as driven concurrently by external climatic conditions. The approach amounts to making BIOTRAN into a strictly biomass and TRU transport model and to relegating water flow aspects to UNSAT. Such an approach is similar to that generally taken in groundwater transport

simulations, which view a flow field as the vector for solute movement. Currently, the BIOTRAN model uses a highly simplified form to handle water flow as a vector for TRU movement. We believe this is a conceptual deficiency of BIOTRAN that can be corrected with the suggested sequential coupling approach. Then, in order to fully utilize details of unsaturated flow, the BIOTRAN model should include a convective-dispersive transport component. This would be compatible with the idea of making BIOTRAN into a model exclusively concerned with TRU transport.

4.4 UNSAT DEVELOPMENTAL PROGRESS

In view of the difficulties of inserting UNSAT into BIOTRAN as a soil-water flow model, the conclusion of this study was that LANL research objectives would be best satisfied by preparing UNSAT as a flexible, applications oriented model. UNSAT could then be applied to establish the importance of various plant-water uptake aspects. For applications to environmental transport problems, the need for a validated set of standard moisture-flow cases was also realized. The book by Hillel (1977) titled "Computer Simulation of Soil-Water Dynamics: A Compendium of Recent Work" appears to satisfy this need.

Hillel's book discusses in detail most aspects of one-dimensional unsaturated flow, including relationships to soil type and plant-water uptake. Moreover, the general philosophy of computer simulation of soil-plant-water systems is discussed. Hillel's three basic soil types (sand, loam, and clay) were adopted as generic representations of soil properties that might be encountered under different field conditions. These soil types were used to simulate the basic unsaturated moisture flow behavior that would be expected under dynamic conditions. Basic flow behavior includes drainage, infiltration, redistribution, and evaporation. A properly operating dynamic, unsaturated flow model should be able to reproduce Hillel's simulations of basic flow behavior. Tests of the UNSAT model on some of these cases are demonstrated in this section. Deviations in numerical results, however, were expected since UNSAT utilizes a more efficient and accurate implicit finite

difference scheme, whereas Hillel used an explicit scheme. Moreover, the smoothness of the curves represented in Hillel's figures depicting his results is believed to be obtained from the use of certain numerical integration methods, intrinsic in the CSMP computer language. Nevertheless, Hillel's example cases are ideal references that establish basic behavior, at least in correct qualitative terms. In the UNSAT simulations, curves are displayed without smoothing. We believe this is the least biased way to report simulation results.

Each of the basic test cases was programmed by Hillel as a separate model. The UNSAT model, however, can treat all test cases and perform simulations of unsaturated moisture flow under natural environmental conditions. Different applications can be accomplished simply by providing the proper input control parameters. A number of models similar to UNSAT have been developed. But, UNSAT is uniquely flexible in its applicability and has well-developed associated analysis and plotting programs to assist in the interpretation of results. The theoretical and mathematical development of UNSAT has been discussed in other studies (Simmons and Gee 1981) and a complete user's manual has been written (Bond et al. 1982). This manual describes the current state of development, but a few key features will be reviewed in this section. The effect of plants on a water balance has also been demonstrated with the model (Mayer et al. 1981). Implementation of a plant-sink submodel based instead on concepts included in BIOTRAN would follow a similar plan. A plant model was also discussed by Hillel (1977) and could be employed as a reference case. However, there does not appear to be a "best" plant model accepted by most research, since mechanisms of plant-water extraction are still under fundamental investigation (Moly 1981).

4.4.1 Improvements in UNSAT

Many improvements have been made to the original version of UNSAT (Gupta et al. 1978). A need for additional program features was recognized from past experience with simulating field problems. The current version of UNSAT can be applied to a variety of field problems with relatively little user experience. The following describes some of the improvements.

1. Interactive Input Preparation (UNSATINP): The new supportive program UNSATINP reduces the time and labor required for preparing input files. For a given problem, a user is prompted on an interactive terminal for the required input. As a user answers questions about a specific problem, UNSATINP constructs an input data file that controls a simulation by the main UNSAT program.
2. Data Input (DATAIN): This is a separate program which reads the input data, interpolates the watertable depth for each day from given values, and estimates potential evapotranspiration from climatic and plant growth data. It provides an opportunity to critically examine the input file prior to simulation of a problem.
3. Subdividing the Time Step Remainder: In the original version, if the mass balance or change in moisture content was not within prescribed limits during an hourly simulation, the results were discarded and the simulation was restarted from the beginning of the hour using a smaller time step. In the current version, the simulation is continued by subdividing the remaining period rather than restarting. This method reduces computation time considerably and still maintains mass balance.
4. Adjustment of Time Steps: Selection of an appropriate time step is very important for simulating unsaturated flow. Based on the boundary conditions and antecedent moisture conditions, the program adjusts the time step. Following each time step, appropriate checks are made to determine if it needs reduction. Similarly, if changes occurring in the system are less than 50% of prescribed limits, the time step is again increased. Through this automatic time step control, mass balance is achieved and computation time is reduced.
5. Time Steps Greater Than 1 hr: In the original version, a maximum time step of 1 hr was used during periods without water application, and a step of 0.1 hr was used during applications. Considering the needs of LANL, the code can now increase the time step up to one day.

For those systems that are not too dynamic, or where the input data are for daily values rather than hourly, the current version can simulate a system in considerably less computation time.

6. Restart Capabilities: In the event that a simulation has stopped before completion, for any reason, the new version permits restarting of a problem from the last day or any intermediate day of the simulation. This feature allows long periods to be simulated in segments.
7. Subdivision of Hydraulic Property Curves: The original version of UNSAT allowed for only two subdivisions of hydraulic property curves, whereas the current version allows five. The regression coefficients for representation of curves are also stored in a single dimensioned array for improved computational efficiency.

The HYDRAK program was developed for estimating hydraulic conductivity from the moisture retention curve. A user can also review interactively the results from plots generated automatically by the program.

Another program, POLYFIT, generates the polynomial fit for each subdivision needed to describe the hydraulic property curves. Tabulated values calculated from the polynomials are also plotted for review by the user.

8. Plotting of Results: The programs THPLT and FLXPLT allow a user to see the results for any simulated period. THPLT plots the moisture content versus depth for selected days. FLXPLT plots the daily or cumulative flux at a given depth.

By including the above capabilities, the current UNSAT package has become an effective tool for preparing input data (including hydraulic property estimation), simulating various problems, and plotting the results.

4.4.2 Basic Test Examples

Following suggestions by LANL, UNSAT was demonstrated by applying the code to test examples given by Hillel and van Bavel (1976). These examples are very exhaustive tests of unsaturated flow simulation. Each problem is solved for three basic soil textural classes: clay, loam, and sand. The

problems include 1a) initially saturated soil profile with drainage only, or 1b) evaporation only, or 1c) both drainage and evaporation. A second set includes 2a) initially dry soil with continual wetting, or 2b) cyclic wetting and drying. In actual field problems, many combinations of these soil properties and moisture conditions are encountered. The soil profile considered is 1.16 m deep. Eighteen subdivisions of the soil profile were used, and simulations were carried out for 10 days. A detailed discussion of each case can be found in Hillel (1978).

Case 1a: Initially Saturated Soil Profile with Gravity Drainage at Base and No Surface Evaporation

The downward flux through the bottom boundary of depth 1.16 m was specified as equaling the hydraulic conductivity of the lower layer (10 cm thick). With a decrease in water content, the transient rate of drainage diminishes in time. Figure 4.3 illustrates the soil moisture distribution on different days.

Case 1b: Initially Saturated Profile with Diurnally-Cyclic Surface Evaporativity without Drainage

The diurnal evaporation was described by a sine function during the daytime:

$$E = E_{\max} \sin (2\pi t/86400)$$

where $E_{\max}$ is the maximal midday evaporation rate taken to be 5.0×10^{-7} m/sec (1.8 mm/hr), and t is the time in seconds from sunrise. Nighttime evaporation was assumed to be steady at the rate of 1% of $E_{\max}$. The total daily evaporation was 13.7 mm. Figure 4.4 illustrates the soil moisture distribution.

Case 1c: Initially Saturated Profile with Simultaneous Drainage and Evaporation

Figure 4.5 shows the soil moisture distributions on different days, and Figure 4.6 illustrates the cumulative drainage with surface evaporation and drainage. Figure 4.7 illustrates the cumulative surface evaporation. Figure 4.8 compares the moisture content at 41 cm as a function of time with

FIGURE 4.3. Changing Soil Moisture Distribution during Drainage from Initially Saturated Uniform Profiles of Clay, Loam, and Sand

FIGURE 4.4. Changing Soil Moisture Distribution during Cyclic Evaporation from Initially Saturated Uniform Profiles of Clay, Loam, and Sand without Drainage

FIGURE 4.5. Changing Soil Moisture Distribution during Simultaneous Drainage and Evaporation from Initially Saturated Uniform Profiles of Clay, Loam, and Sand

FIGURE 4.6. Cumulative Drainage from Initially Saturated Uniform Profiles of Clay, Loam, and Sand (Solid lines: drainage without evaporation; Dashed lines: simultaneous drainage and evaporation)

FIGURE 4.7. Cumulative Evaporation during Simultaneous Drainage and Evaporation from Initially Saturated Uniform Profiles of Clay, Loam, and Sand

FIGURE 4.8. Volumetric Wetness at Depth of 41 cm as a Function of Time in Initially Saturated Uniform Profiles of Clay, Loam, and Sand (Dashed lines: simultaneous drainage and evaporation; Solid lines: drainage without evaporation)

drainage only and drainage combined with evaporation. Since the curves are based on daily cumulatives, the detailed pattern associated with the sine wave evaporativity is not displayed as shown by Hillel. Moreover, because the evaporation rate was limited to a one-hour resolution, the cumulatives differ from Hillel's values.

Case 2a: Initially Dry Soil Profile with Shallow Ponding

To simulate infiltrability under ponding conditions, the initial moisture profile was prescribed with a uniform suction of 3.3 m, and the surface hydraulic head was set equal to zero.

Figure 4.9 illustrates wetting front movements in hours for various soils. The wetting front advance for sand differs considerably from Hillel's as a result of the different computational schemes employed. Hillel's curves display a rather imaginative smoothness for such a coarse node separation. This shows the influence of the CSMP integration routine.

FIGURE 4.9. Successive Distributions of Soil Moisture during Infiltration into Uniform Profiles of Clay, Loam, and Sand (all at an initial matric suction of 1/3 bar)

Case 2b: Initially Dry Soil Profile with Cyclic Rain and Evaporation

The initial soil-moisture profile was set at 30 m of suction. Each rainfall period lasted 6 hr with the following rates:

<u>Period, hr</u>	<u>Amount, mm</u>
0-1	6
1-2	12
2-4	36
4-5	12
5-6	6

During precipitation events, evaporation was neglected. The simulation was carried out with such rainfall on alternate days. To compare the results with that of Hillel, simulated results of one day with one storm are plotted in Figure 4.10.

4.4.3 Discussion of Simulation Test Examples

UNSAT adjusted the time steps according to the moisture flow conditions. The results compare qualitatively with Hillel's, except for some differences during evaporation and infiltration. These differences can be attributed to the following:

- Hillel assumed potential evaporation to occur until the driest moisture content is reached at the surface. After that driest value was reached, Hillel approximated the surface evaporation by the hydraulic conductivity of the second layer. In UNSAT, this problem is considered in more detail. UNSAT adjusts the surface contents, and if the driest conditions are reached, the simulation is conducted with a held potential rather than a flux boundary condition.
- Similarly, UNSAT prescribes infiltration as a function of current surface moisture conditions, whereas Hillel used the saturated conductivity.
- Hillel used the explicit finite difference method with very small time steps, whereas UNSAT used the implicit method with larger time steps.

FIGURE 4.10. Successive Distributions of Soil Moisture during Infiltration with Subsequent Redistribution and Evaporation in Uniform Profiles of Clay, Loam, and Sand (These moisture distributions represent a single rainstorm of 72.2 mm lasting 6 hr.)

In brief, these examples provided an effective test of the new version of UNSAT with varied textured soils under dynamic moisture flow conditions. If the UNSAT algorithm were built into BIOTRAN, soil moisture movement, nuclide transport, and plant-uptake could be simulated effectively.

4.5 THE WTRFLX MODEL

Following the lead efforts of the LANL group to design and include a simplified moisture flow model (WATFLX) in BIOTRAN, we have devised a similar flow model called WTRFLX (Water and Flux). The objective was to develop a conceptually simple compartmental model that could be included immediately in BIOTRAN, with a minimum of mathematical complexity. We found that Hillel (1977) had already studied such models, but because they were coded in the CSMP language, re-working of his models in FORTRAN was necessary. As it turned out, the WTRFLX code did not adequately represent the unsaturated moisture flow theory contained in UNSAT. The WTRFLX development is presented herein to demonstrate the algorithms required if LANL decides to proceed with the development of the simplified moisture flow model.

In a sense, all finite difference or finite element representations of a spatially continuous physical process are compartmental. The node system used in a model defines the centers of its compartments. Perhaps the most important aspect of a dynamic model, however, is how processes are integrated over time, regardless of how a system is compartmentalized over space. Indeed, compartmentalizing space amounts to an a priori assumption about the spatial resolution required to represent a particular physical process. On the other hand, the integration of processes over time appears to be strictly a mathematical problem. If the physical variables of a system vary greatly over short times, then there appears to be no recourse but to integrate or simulate for the same times.

Explicit finite difference methods for solving Richard's equation appear to have become synonymous with compartmental water flow models. In an explicit solution scheme, the change in water content of a compartment during a single time step is effected only by flow from or into adjacent compartments. In contrast, with an implicit scheme all compartments are effected by the others simultaneously. The non-linearity of the unsaturated moisture flow equation

tends to make an explicit scheme unstable in the sense that irregular oscillations occur in the moisture distribution as time passes. These oscillations are a consequence of over and under shoots in moisture contents caused by fluxes acting independently over the profile during each time step. In principle, however, an explicit scheme can be made accurate by reducing the time step sufficiently. Unfortunately, this makes such schemes computationally inefficient. The obvious lack of such models in the literature suggests their inherent difficulties. Realizing the limitations of an explicit scheme, but wanting to emphasize a simple mathematical approach, we have developed the simplified WTRFLX code, nevertheless.

The main features of WTRFLX are a time step size control and an iterative procedure to reduce these oscillations. With an explicit scheme, water mass balance is automatically achieved, whereas with an implicit scheme it must be controlled by solution accuracy. Absolute mass balance is an important attribute for long simulations. It now appears obvious that time step control is an absolute necessity for an accurate simulation of detailed flow dynamics. Thus, use of a smaller time step in WTRFLX is unavoidable, and cannot be conveniently set at the one day step used by BIOTRAN. Perhaps the only alternative for eliminating the time step disparity is to relinquish detailed simulation of infiltration and redistribution events. Analytic solutions for approximate conditions, such as Philips' $\sqrt{t}$ rule for infiltration, might be adequate for BIOTRAN. However, we did not attempt this approach. For more information on models based on analytical equations see Eagleson (1978).

Although a mathematically detailed description of WTRFLX is provided in this section, the discussion has only an illustrative purpose of clarifying basic phenomena that should be taken into account in any unsaturated flow model, and an explicit scheme is not generally recommendable. Through a study of the explicit scheme, however, an appreciation of the difficulties and subtleties involved in solving the non-linear moisture flow problem is gained. It is also suggested that the limitations of the method should just be accepted, and imaginative programming should not be used to reach beyond those limitations, at least not without rigorous justification. Indeed, the implicit solution scheme currently used in UNSAT was designed to overcome those limitations.

In the following subsections, the finite difference equation formulation of moisture flow will be given, and the discussion will point out the specific implementation in the WTRFLX model. The reader is warned that the model is not fully functional or completely tested. Section 4.5.17 presents a summary of the operational steps included in the WTRFLX code, while Appendix A presents the corresponding FORTRAN listing.

4.5.1 Governing Flow Equation

The objective of the water flow model is to approximately solve the vertical flow equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} [K(\theta) \left(\frac{\partial h}{\partial z} + 1 \right)] - S(\theta, z) \quad (4.1)$$

where

- t = time (days)
- z = depth (cm) positive downward
- θ = soil water content (cm^3/cm^3)
- h = matric suction potential (cm)
- K = hydraulic conductivity (cm/day)
- S = plant root sink (cm/cm/day)

Equation (4.1) must be solved subject to certain initial and boundary condition, which will be specified in the model's construction.

4.5.2 Soil Profile

The soil profile consists of a sequence of layers or compartments. Water content in each layer will be identified with its average value at the midpoint of each compartment. Figure 4.11 presents the nodal representation of the system. In Figure 4.11, the depths z_i ($i=1, \dots, N+1$) identify the midpoints of N soil layers or compartments. The nodes z_1 and z_{N+2} are auxiliary, and are used to locate the application of boundary conditions. The width of each layer will be denoted by W_i , and node locations will be:

FIGURE 4.11. Node System for Soil Profile

$$z_1 = -(w_2)/2, z_2 = (w_2)/2, z_3 = w_2 + (w_3)/2, \dots,$$

$$z_{N+2} = z_{N+1} + w_{N+1}$$

where in general

$$z_i = z_{i-1} + (w_{i-1})/2 + (w_i)/2$$

for $i=2, \dots, N+2$ with $w_1 = w_2$ and $w_{N+2} = w_{N+1}$

In the program, DELZ(I) denotes the layer thickness. The profile is defined in program lines 9-21 (symbol glossary, Appendix A). The distance used to calculate the hydraulic gradient is based on the distance between layer mid-points (program lines 20-21, Appendix A). Other distances, however, could be assumed in the definition of the gradient.

4.5.3 Fluxes

Fluxes into and out of layers are given by explicit finite difference approximations as:

$$Q_i = \bar{K}_i \left(\frac{h_{i+1} - h_i}{z_{i+1} - z_i} + 1 \right) \quad (i=1, \dots, N+1) \quad (4.2)$$

where $\bar{K}_i$ is an average conductivity between K_i and K_{i+1} :

$$\bar{K}_i = (w_i K_i + w_{i+1} K_{i+1}) / (w_i + w_{i+1}) \quad (4.3)$$

where $K_i = K(\theta_i)$ and $h_i = h(\theta_i)$ are evaluated at z_i . The total hydraulic potential at each node is:

$$\psi_i = h_i + z_i \quad (4.4)$$

Head (matric suction potential) and hydraulic conductivity are calculated from given functions of θ for three soil types (i.e., clay, loam, and sand).

4.5.4 Finite Difference Equation

During a time step Δt the change in water content $\Delta\theta_i$ within each compartment is described by the following finite difference approximation for Equation (4.1):

$$\Delta\theta_i = - \frac{\Delta Q_i}{\Delta z_i} \Delta t - S_i \Delta t \quad (4.5)$$

where

$$\Delta Q_i = Q_i - Q_{i-1} \quad (i=2, \dots, N+1)$$

and

$$\Delta z_i = z_i + (W_i)/2 - (z_i - (W_i)/2) = W_i$$

ΔQ_i is the net flow rate through the i^{th} layer. Equation (4.5) represents the actual explicit difference scheme. Most difference solutions of Equation (4.1) however, whether explicit or implicit, utilize an explicit definition of flux, like Equation (4.2). Notice that Δz_i defines the gradient of flux across a compartment. In an implicit scheme, the fluxes acting across compartments for time step Δt change the water content by ΔQ_i , which then determines the water contents and potentials at the next time $t+\Delta t$.

In the program, calculations of hydraulic properties and fluxes are found on lines 54-65 (Appendix A). To calculate the flux, an average of the logarithm of conductivity is used. Such a layer-weighted average, Equation (4.3), is used to correct for different compartment sizes. Compartments of greater size then have more influence on the flux between two adjacent compartments. An array, ISOIL, is used to indicate which soil type constitutes each layer.

4.5.5 Mass Balance

The soil-water mass balance is expressed as follows:

$$\begin{aligned}\sum_{i=2}^{N+1} \Delta \theta_i W_i &= - \sum_{i=2}^{N+1} \Delta Q_i \Delta t - \sum_{i=2}^{N+1} S_i W_i \Delta t \\ &= - (Q_{N+1} - Q_1) \Delta t - \sum_{i=2}^{N+1} S_i W_i \Delta t\end{aligned}\quad (4.6)$$

Equation (4.6) indicates that a change in soil-water storage plus plant transpiration equals the difference in surface flux (rainfall or evaporation) and drainage. Thus, the explicit finite difference formulation of the flow, Equation (4.5), will conserve mass at all times.

4.5.6 Boundary Conditions

Let θ_s and θ_m denote the saturated and minimum water contents, respectively. Rainfall is:

$$Q_1 > 0$$

where Q_1 is the surface flux. RAIN denotes rainfall rate (cm/day) in the program.

Infiltrability of the soil surface is given by Q_1 with $\theta_1 = \theta_s$ or $h_1 = 0$. The surface flux during rainfall is not allowed to exceed this infiltrability (program lines 67-68, Appendix A). Rainfall that exceeds infiltrability is considered as runoff lost from the system (program line 133, Appendix A).

4.5.7 Actual Evaporation

When sufficient soil-water is near the surface, evaporation takes place at the potential rate determined by atmospheric conditions, PE. However, when the soil surface is dry, actual evaporation is determined by the upward flux controlled within the soil. The surface evaporativity is given by Q_1 with $\theta_1 = \theta_m$, and the suction head takes its maximum value for air dry

conditions at the surface. Here, PE denotes potential evaporation (program lines 50-51 and 67, Appendix A). Notice that during evaporation the surface flux satisfies

$$Q_1 < 0$$

4.5.8 Lower Boundary Conditions

At the bottom of the simulated soil profile three distinct conditions could apply: a water table is present, the profile drains continually into a deeper region, or an impervious layer is present that does not allow any drainage. The key word LOWER is used to indicate which lower boundary condition prevails:

- LOWER = 1, a water table
- = 2, a unit hydraulic gradient
- = 3, a zero flux condition

If a water table is present (LOWER = 1), then drainage flux is given by Q_{N+1} for $\theta_{N+2} = \theta_s$. The drainage flux may be either up or down. A deep drainage condition with a unit hydraulic gradient (LOWER = 2) is specified by $\theta_{N+2} = \theta_{N+1}$ at all times. The profile without any drainage (LOWER = 3) is described by the condition $Q_{N+1} = 0$ (program lines 47-49 and 66, Appendix A).

4.5.9 Plant Sink

The plant sink $S(\theta, z)$ depends on both the soil water availability condition and the rooting distribution. Under optimal climate and soil water conditions, the sink will extract water at the potential transpiration rate PT. The PT is determined by partitioning PET into PE and PT based on the leaf cover of the soil and the growth conditions for the specific plant. The specific model used for the plant will be discussed later. The transpiration during each time step equals (program lines 136-137, Appendix A):

$$\sum_{i=2}^{N+1} S(\theta_i, z_i) W_i \Delta t \quad (4.7)$$

4.5.10 Time Step Control

The most complicated aspect of the water flow model is the time step control. Because the water content within each soil layer should remain within the physical limits of its air dry and saturation value, the fluxes between layers, Equation (4.2), must be continually adjusted to keep the system within those limits. Hillel (1977) simply used a constant, sufficiently small step to control accuracy in his compartmental soil-water flow model. For long-term simulations, however, such an approach would not be an efficient use of computer time. During evaporation and redistribution periods, it may be possible to apply a large time step, whereas during infiltration a small step may be necessary. A small time step is usually required to accurately describe the wetting fronts advance during infiltration. The maximum time step was taken as one day in this model, and two time steps were defined for evaporation and infiltration conditions. In addition, the applied time step Δt was adjusted so that the fluxes evaluated at t do not drive the water content at $t + \Delta t$ beyond physical limits (program lines 39-44, Appendix A).

4.5.11 Infiltration Adjustment

Next, consider a saturated wetting front that has advanced to z_k , so that

$$\theta_i = \theta_{si} \quad (i=1, \dots, k) \text{ and } \theta_{k+1} < \theta_{s, k+1} \quad (4.8)$$

It is assumed that Q_k controls the wetting front advance, and the saturated conductivity of the least conductive layer determines the possible infiltration. The plant sink is assumed to equal zero in a saturated zone during rainfall. Now if $(\theta_i + \Delta\theta_i) < \theta_{si}$ for $i \leq k$, then the change in water content is allowable. Otherwise, we take $Q_{i-1} = Q_i$ so that $\Delta\theta_i = 0$, and the water content does not exceed saturation (program lines 70-75, Appendix A).

4.5.12 Dry Limit Adjustment

The soil layers are kept from over desiccation by not allowing fluxes that remove soil water from air dry layers. Thus, if $\theta_i = \theta_{mi}$, then set $Q_{i-1} = 0$ if $Q_{i-1} < 0$ initially, and set $Q_i = 0$ if $Q_i > 0$ initially (program lines 76-79, Appendix A).

4.5.13 Time Step Adjustment

For water contents θ_i within the proper limits, the time step Δt is adjusted so that the next value $\theta_i + \Delta\theta_i$ stays within the dry and saturation limits. If $(\theta_i + \Delta\theta_i) > \theta_{si}$ or $(\theta_i + \Delta\theta_i) < \theta_{mi}$, then a new time step $\Delta t'$ is calculated:

$$\Delta t' = \frac{(\theta_{si} - \theta_i)}{\Delta\theta_i} \Delta t \quad \text{or} \quad \Delta t' = \frac{(\theta_{mi} - \theta_i)}{\Delta\theta_i} \Delta t \quad (4.9)$$

for

$$\Delta\theta_i \neq 0.$$

The minimum $\Delta t'$ of all adjustments is used for Δt . Thus, only one layer during a time step will attain either an air dry or saturated water content. This gives a controlled exchange of water between layers and mass balance is maintained (program lines 87-99, Appendix A). Note that the dry limit is assumed to be below the plant's root wilting point, so that the sink is zero in an air dry layer.

4.5.14 Soil Hydraulic Properties

The soil hydraulic properties can be defined in the program according to a user's own selection. The curves of Hillel (1977) provide some reasonable example data for clay, loam, and sand soils. Hydraulic properties are calculated in the program as the function HYPINT. HYPINT interpolates values directly from a representative set of data. Of course, the simple functions $h = a \theta^b$ and $K = c \theta^d$ could be applied directly in place of HYPINT. The advantage of this simple explicit finite difference program is that a smooth capacity function ($d\theta/dh$) is not required as in more complex unsaturated flow models (Feddes et al. 1978).

4.5.15 Improved Estimation Method

If the time step Δt is not small enough, it is likely that Q_i between compartments will not accurately represent an average flux that should act to change θ_i into its next value. An improved estimation method based on averaging $\Delta\theta_i$ over a time step can be constructed as follows. Let Q_i denote the flux calculated as before for the present θ_i and let Q'_i be that calculated for $\theta_i + \Delta\theta_i$. After time Δt , Q_i yields a change $\Delta\theta_i$ and Q'_i gives $\Delta\theta'_i$ after time $\Delta t'$. An improved estimate is obtained by taking

$$\theta_i + 1/2 (\Delta\theta_i + \Delta\theta'_i)$$

as the water content after a time $1/2 (\Delta t + \Delta t')$. This change in water content is produced by an average flux $\bar{Q}_i$ given by:

$$\bar{Q}_i = \left(\frac{\Delta t}{\Delta t + \Delta t'} \right) Q_i + \left(\frac{\Delta t'}{\Delta t + \Delta t'} \right) Q'_i \quad (4.10)$$

The method amounts to taking the average of θ_i and $\theta_i + \Delta\theta_i + \Delta\theta'_i$ for the change in water content after an average time $1/2(\Delta t + \Delta t')$. This method determines an iterative procedure that has been included in our version of the WTRFLX model. Its effect is to smooth oscillations in the solution of the flow equation. A disadvantage of this scheme, however, is that the number of calculations for each node doubles with each iteration (program lines 99-127, Appendix A).

4.5.16 Transpiration and Sink Model

It seems self evident that advantages of using a more complex soil-water flow model are realized only if a plant transpiration model of compatible complexity is applied. Feddes et al. (1978) has discussed in detail a plant sink model that is typical of many others. In fact, a general review of such models has been given by Molz (1981). We shall review here our interpretation of the current BIOTRAN plant-water uptake model and how it should be constructed for use in our version of WTRFLX.

Potential evapotranspiration PET is driven by a stochastically varying air temperature $R\Delta T$, superimposed on a sine wave of yearly variation:

$$T_0 = \frac{(T_{\max} - T_{\min})}{2} \left(\sin \left(2\pi \frac{(t - t_1)}{365} \right) + 1 \right) + T_{\min} \quad (4.11)$$

where temperature is

$$T = T_0 + R\Delta T \quad (^\circ\text{C}) \quad (4.12)$$

and

$$\text{PET} = 0.6 + 0.18T \quad (\text{mm/day}) \quad (4.13)$$

The formula applies to the top 250 mm of soil. Here, R refers to a random number. Roots are not present in a top 20 mm thick layer.

It appears that the plant-water uptake model used in the LANL version WATFLX is based on extending the fraction of PET based on field capacity to each soil layer. Letting θ_w and θ_{fc} denote wilting point and field capacity water content, respectively, the sink model is:

$$S(\theta, z) = \text{PT } r(z) \left(\frac{\theta - \theta_w}{\theta_{fc} - \theta_w} \right) \quad (\text{day}^{-1}) \quad (4.14)$$

where

PT = potential transpiration (mm/day)

$r(z)$ = root density distribution function (mm⁻¹)

and $r(z)$ satisfies

$$\int_0^{z_m} r(z) dz = 1 \quad (4.15)$$

z_m = maximum rooting (root penetration depth) depth (mm).

z_m depends on growth time, and is given by

$$z_m = [- \exp (-0.0001t)] * 9144$$

The root density function appears to be based on an exponential function:

$$\exp(-0.004z)$$

Actual transpiration TRANSP is obtained by integrating the sink over the root depth:

$$\text{TRANSP} = \int_0^{z_m} s(\theta, z) \, dz \leq \text{PT} \quad (4.16)$$

This plant sink model is similar to that proposed by Feddes (1978), and also coded into the UNSAT model. No attempt was made to include the sink model in our version of WTRFLX, and the particular model must be selected. The plant model described by Hillel (1977) is another approach.

The final step in defining a plant uptake model is to partition the PET with some method: $\text{PET} = \text{PE} + \text{PT}$. BIOTRAN does not seem to distinguish PT and PET at present. A method needs to be selected, and one based on leaf area index seems most appropriate since that variable is linked to biomass production (leaf growth).

4.5.17 Program Structure for WTRFLX

This subsection provides a summary of the operational steps included in the WTRFLX program. A complete FORTRAN listing of the WTRFLX code is provided in Appendix A.

Dimensions of arrays

I Data statements

- layer thickness (soil type index set)
- initial water contents

- lower boundary condition flag
- hydraulic property coefficients
- plant sink coefficients
- calculate layer depths

II Day calculation loop

- find rainfall
- find PET (partition into PE and PT)
- find depth of plant roots and distribution

III Each day loop

- set time step for rain or evaporation
- calculate suction head and conductivity
- calculate sink
- average conductivity between layers
- calculate fluxes
- adjust fluxes for wetting front and air dry conditions
- reduce time step and adjust changes
- calculate change in water contents of each layer and obtain new values
- increase time by applied step

IV Return to start of day loop until complete daily simulation is done, III.

V Calculate cumulatives of infiltration, evaporation, transpiration, drainage, storage.

VI Return to start of next day of year

END program

4.6 SUMMARY

4.6.1 Conclusions and Recommendations

The UNSAT code should not be included directly as a subprogram of BIOTRAN. These models are conceptually and operationally different and should not be combined within the same code. UNSAT is a model based on a detailed dynamical description of moisture flow and plant-water uptake, whereas BIOTRAN is based on an averaged, compartmental view. UNSAT is best suited for applications

involving a detailed description of water movement. On the opposite side, BIOTRAN describes the averaging of soil-water flow over large spatial and temporal steps. The parameter needs of these models are considerably different since they represent physical processes on entirely different scales of space and time.

The following alternative recommendations are made:

1. Develop an improved compartmental model for moisture movement compatible with other sub-models now in BIOTRAN. An explicit finite difference approach (WTRFLX) which only provides a more inaccurate representation of theory now included in UNSAT is not recommended. A continuous model based on certain analytical solutions for basic moisture movement phenomena would seem to be a better approach. The research of Eagleson (1978) provides an example of such a model. In that kind of model, the basic processes of infiltration, drainage, and evaporation are described by approximate analytical equations and finite difference techniques, which require numerical control, are not employed. The soil profile model can also be represented by a few major layers, as currently conceptualized in BIOTRAN. An exact water balance, including a groundwater reservoir to receive drainage and leaching losses, can be maintained. Moreover, the approach of Eagleson was designed to accommodate stochastic inputs for the system parameters. That aspect is consistent with the modeling view point already taken in BIOTRAN.
2. Apply the UNSAT code in a quasi-uncoupled mode that does not attempt to include the code as a permanent part. Recommendation is based on scientific reasons and should not be interpreted to mean that UNSAT, or its major components, could not be coded into BIOTRAN. The models would be operated in a quasi-uncoupled mode by relegating all moisture flow, plant-water uptake, and plant growth aspects to UNSAT. All biomass accumulation and TRU transport aspects would remain in BIOTRAN, however. Certain aspects of plant growth would be duplicated in both codes, as well as the external climatic forces that drive both water movement and plant growth. In an uncoupled

mode, UNSAT would be run first to establish soil-plant moisture flow over a selected period. Moisture flow variables (water content, fluxes, and plant root-sink transpiration) would then be read into BIOTRAN to control plant growth and TRU transport. An intermediate averaging or integration of flow variables might be necessary to make moisture flow details conform to the particular soil levels utilized in BIOTRAN.

4.6.2 Coupling of BIOTRAN and UNSAT

Some reasons why UNSAT should not be simply substituted into BIOTRAN are summarized as follows.

1. BIOTRAN is constructed for fixed soil levels (layers) and soil type is not accounted for. In UNSAT, each soil layer is usually represented by many nodes which are used to control computational accuracy. Flow variables would require averaging over the layers used by BIOTRAN.
2. BIOTRAN uses relatively large time steps (daily changes) that are consistent with the lumped daily input of rainfall and evapotranspiration. UNSAT uses small, variable time steps to estimate infiltration during rainfall. Small steps are required because UNSAT is a mechanistic and dynamic simulator of soil-water flow. Moreover, it is known that the detailed daily pattern of rainfall influences the yearly water balance. Daily rainfall patterns and correlation between rainfall events would need to be accounted for in order to properly apply the UNSAT model. There is no provision to take such detail into account in BIOTRAN. That is, the models of plant growth and TRU uptake in BIOTRAN are much less dynamic and could not make effective use of the additional moisture flow detail.
3. The modeling of evapotranspiration by BIOTRAN is not of sufficient dynamical detail to be compatible with the surface boundary condition control usually required by UNSAT. An accurate division of PET into soil surface evaporation and plant transpiration must be performed in UNSAT in order to control water balance. At present, this level

of modeling detail is not required in BIOTRAN. This aspect of the difference between the BIOTRAN and UNSAT codes is a major reason for recommending that the codes be used in a quasi-uncoupled mode.

An essential part of calculating actual plant transpiration is a root sink model. A plant-water uptake model like those reviewed by Moly (1981) is recommended. UNSAT is usually applied to a single species of plant so that the root sink model is simplified. However, BIOTRAN describes a plant community on an averaged basis. This aspect would need further research and consideration before coupling the codes.

4. A main objective of BIOTRAN is to describe transport of TRU through a plant ecosystem. However, the common accepted theory of representing solute transport in soil does not appear to be employed. That is, the movement of TRU does not appear to be coupled to water flow by convective or dispersive transport. Movement of soil-water and TRU appear to occur as concurrent, but separate processes within BIOTRAN.

The modeling of TRU movement by BIOTRAN is perhaps adequate under its present conceptual design; but if coupled with UNSAT, the detailed moisture fluxes in a soil profile will not be useful unless BIOTRAN is modified to account for at least convective movement of solute. The selective absorption of TRU by plant roots should be accounted for also by a mechanistic model, which depends on a dissolved TRU concentration.

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5.0 SIMPLIFIED MULTIMEDIA CONTAMINANT ENVIRONMENTAL EXPOSURE ASSESSMENT METHODOLOGY AND ITS APPLICATION TO MORTANDAD CANYON IN LOS ALAMOS, NM

This chapter discusses the preliminary application of the proposed Multimedia Contaminant Environmental Exposure Assessment (MCEA) methodology as it relates to the Mortandad-South Mortandad Canyon site in New Mexico.

5.1 INTRODUCTION

To evaluate the ability of a radionuclide disposal site to contain radioactive substances, a site-evaluation methodology must be capable of predicting the long-term integrity of environment in curtailing radionuclide migration in the biosphere. Radioactive substances released from the disposal site undergo complex interactions in the biosphere. Since mathematical models can integrate these complex interactive mechanisms into a single system, they must be an integral part of a site-evaluation methodology.

Currently, Los Alamos National Laboratory (LANL) and Pacific Northwest Laboratory (PNL) are jointly developing a site-evaluation methodology. The goal is to develop an assessment methodology that permits: 1) the consideration of site-specific conditions and characteristics, 2) the simulation of realistic environmental transport mechanisms, and 3) comparative evaluation of radionuclide disposal consequences over many hundreds of years. To arrive at a suitable system for simulating the dynamics of radionuclide transport in the ecosystem, several models were assembled at appropriate interfaces (Figure 5.1).

Models representing terrestrial plants, land, surface water, and aquatic sediment (hatched portions in Figure 5.1) were selected as a scaled-down version of the MCEA methodology. Efforts to include air transport and saturated and unsaturated groundwater transport (shaded portions in Figure 5.1) into the overall methodology are also currently underway, as discussed in Chapters 3 and 4.

Prior to the full development of the proposed assessment methodology described in Figure 5.1, the scaled-down version of the MCEA methodology

FIGURE 5.1. Schematic Diagram Illustrating the Interactions Between the Various Transporting Media and How They Affect Man through His Environment

was applied to simulate the migration of ^{239}Pu from Area C, a shallow-land disposal site located near the head of South Mortandad Canyon on the LANL site in New Mexico. The scenario studied herein assumed that through natural processes of plant growth and radionuclide uptake, dryfall, and litter decomposition, ^{239}Pu would be deposited on the land surface. Runoff events would then transport ^{239}Pu to and in the canyon. Hence, the terrestrial-plant, overland, surface-water, and aquatic-sediment compartments of the methodology were used for this study. Detailed description of this study was reported in Onishi, Whelan, and Skaggs (1982).

5.2 CONCLUSIONS AND RECOMMENDATIONS

Because the migration and fate of radionuclides in a given environment are controlled by a complex set of mechanisms, the models must be capable of simulating dynamic processes of transport, decay, intermedia transfer, and biological uptake to predict radionuclide exposure levels in the environment. Under this task, models representing terrestrial plants, land and surface water, and sediment (Figure 5.1) were selected as integral parts of the MCEA methodology. The models are BIOTRAN, a terrestrial ecology model (Wheeler 1977 and Gallegos et al. 1980); ARM, an overland transport model, (Donigian and Crawford 1976); DKWAV, an in-stream hydrodynamic model (Whelan 1980); and TODAM, an instream sediment-contaminant transport model, which was developed by modifying the two dimensional model, SERATRA (Onishi et al. (1979), into a one-dimensional model.

A scaled-down version of the methodology consisting of the BIOTRAN, ARM, DKWAV, and TODAM models simulated the migration of ^{239}Pu (with the assumed source strength of 800 pCi/g) from Area C. The terrestrial plant modeling with BIOTRAN was performed by LANL, while overland and instream modeling with ARM, DKWAV, and TODAM were conducted by PNL. After 100 yr of simulation with BIOTRAN, radionuclide concentrations on the land surface of the waste-disposal site were predicted to be 5×10^{-6} pCi/g or 6×10^{-9} times the original ^{239}Pu concentration disposed of in the ground under a natural condition (recreational land use). Over the 2-yr simulation period following the 100-yr BIOTRAN simulation, 1% of ^{239}Pu on the land surface had been removed by soil erosion events and transported to the canyon. The simulation also revealed

that, once in the canyon, up to 99% of the ^{239}Pu was carried by sediments during occasional runoff events. Simulation results revealed that all of the ^{239}Pu eroded from Area C remained in the canyon. Hence, the study reveals that the environment around Area C has integrity high enough to curtail radionuclide migration under recreational land use. Although radioactivity levels are extremely low, deposition of contaminated sediment in the channel may become a long-term source of contamination, because radioactive contaminants concentrate in the bed sediment.

The following conclusions and recommendations were derived from this study:

1. The MCEA methodology discussed herein has demonstrated that it is capable of evaluating how specific sites curtail radionuclide migration.
2. The methodology could be used as:
 - a scientific decision-making tool for regulating the management of radioactive wastes
 - a research tool for evaluating the relative effectiveness of natural and man-made features at the site in curtailing radionuclide migration to the biosphere
 - a research tool for estimating the relative significance of environmental pathways and radionuclide transport and fate mechanisms
 - a means of providing a rational base for analyzing field sampling data.
3. Since the methodology is physics-based and simulates dominant dynamic processes in the environment, its data requirements are rather extensive but still judged reasonable to simulate the complex processes of radionuclide transport and fate. The methodology application requires a moderate effort.
4. Although their sophistication, time frames and land-surface areas of the models BIOTRAN, ARM, DKWAV, and TODAM under consideration

differ, these models are reasonably coupled in the MCEA methodology. Since the methodology is currently being expanded to include atmospheric and groundwater compartments, the framework for coupling the models must be further improved. We also recommend that TODAM be combined with an appropriate hydrodynamic model to include feed back of sediment-contaminant transport results to flow conditions, thus enabling longer morphological changes of a stream system in an analysis.

5. Limited data were used to partially test the methodology's validity. Additional tests are strongly recommended.

5.3 MODEL SELECTIONS

As a first step for developing the MCEA methodology, terrestrial plant, overland, and in-stream models were selected in this task.

Model selection was guided by the following four principal considerations:

1. the models must be capable of simulating dynamic environmental processes with a moderate degree of resolution in space and time
2. the models must be generic but, at the same time, capable of being calibrated on a site-by-site basis. They should not require excessive data or require data that are difficult, expensive, or time consuming to acquire
3. the models must be capable of being coupled to each other so that the simulation includes radionuclide migration in multimedia and the ensuing aspects of exposing humans to the radionuclide
4. all of the models must be based on conceptually sound algorithms and all of the models must currently be in use.

After reviewing various models, the following models were selected.

5.3.1 Overland Radionuclide Transport Modeling

The Agricultural Runoff Management (ARM) model was selected for this purpose. ARM predicts runoff, sediment, and contaminant loadings at the edge of a stream. Model input includes meteorological data, physical and chemical properties of a chemical, chemical application rates and practices, and

watershed characteristics. ARM provides continuous simulation of runoff, and sediment and contaminant loadings by modeling:

- hydrologic response of watersheds
- soil erosion
- contaminant adsorption and removal
- contaminant decay or degradation.

5.3.2 Surface Water - Radionuclide Transport Modeling

The sediment-contaminant transport model, TODAM, used here is a finite element model which predicts time-varying longitudinal distributions of sediments and toxic contaminants (radionuclides) in rivers and estuaries. The model consists of the following three submodels coupled to describe sediment-contaminant interaction and migration:

- sediment transport
- dissolved contaminant transport
- particulate contaminant (i.e., contaminants adsorbed by sediment) transport.

The sediment transport submodel simulates transport, deposition, and scouring for three size fractions (or sediment types) of cohesive and noncohesive sediments. The transport of particulate contaminants is also simulated for those associated with each sediment size fraction. The contaminant submodels include the mechanisms of: 1) advection and dispersion of dissolved and particulate contaminants; 2) chemical and biological degradation resulting from hydrolysis, oxidation, photolysis, biological activities, and radionuclide decay where applicable; 3) volatilization; 4) adsorption/desorption; and 5) deposition and scouring of particulate contaminants. TODAM also computes changes in river (both tidal and nontidal) bed conditions for sediment and contaminants.

Since TODAM requires depth and velocity distributions as input data, DWOPER (Fread 1973), a dynamic wave model for rivers, was selected to supply these inputs to TODAM. However, since DWOPER cannot handle conditions of low intermittent flows with small depths and steep slopes as occurring at the LANL site, a kinematic wave model, DKWAV, was selected for the LANL site

application. The model is an unsteady, one-dimensional, second-order, explicit, finite difference model which simulates the hydrodynamics in dendritic river systems to obtain time-varying distributions of depth and velocity in a channel.

5.3.3 Terrestrial Plant Growth and Radionuclide Uptake Modeling

The BIOTRAN model was selected for this purpose by LANL.

5.4 MORTANDAD CANYON APPLICATION

Prior to the full development of the proposed MCEA methodology, LANL and PNL decided first to apply a scaled-down version of the methodology (involving terrestrial plants, overland, and surface water compartments) to an actual waste disposal site. The purpose of this effort was to evaluate and, at the same time, demonstrate the attributes of the methodology. We evaluated 1) the capability of each component of the methodology to simulate radionuclide transport within its media--inclusive of the major mechanisms of radionuclide migration and fate, 2) the soundness of coupling several components of the methodology and the ability of the integrated methodology to simulate radionuclide migration in several media, and 3) the applicability and limitations of the integrated methodology and its required input data.

The Los Alamos National Laboratory is located on the eastern slope of the Jemez Mountains, a portion of the Pajarito Plateau in north-central New Mexico (Figure 5.2). The plateau is dissected by numerous canyons, all of which eventually drain into the Rio Grande River. Waste burial sites are located on the tops of finger-like mesas with a relief of 25 to 60 m above the floors of adjacent canyons. The area has a semi-arid, continental mountain climate. Annual precipitation averages about 46 cm at the higher elevations (2200 m), and about 18 cm at the lower elevations (1650 m). Summer rainfall accounts for about 75% of the annual precipitation (Hakonson et al. 1976). During major storms and snow melts, large surface water flows traverse along canyons and most of the time, flows disappear into the alluvium (Hakonson et al. 1976). Area C, a small shallow land disposal site, is located in a side-canyon (South

FIGURE 5.2. Topography of the Los Alamos Area in New Mexico

or South Fork Mortandad Canyon) within the Mortandad Canyon drainage. Figure 5.3 presents Mortandad and South Mortandad Canyons. Figure 5.3 also presents the 13 segments into which the canyons were divided for the modeling scenario.

FIGURE 5.3. Mortandad and South Mortandad Canyons Upstream of the "Garden" Location

A waste management scenario was developed for the Area C disposal site affecting South Mortandad and Mortandad Canyons to provide a basis for demonstrating the methodology's applicability. It was assumed that management of Area C had ceased, and that natural vegetation had become reestablished over a period of 100 yr. Ponderosa pine, deciduous shrubs (e.g., oak), and cool season grasses, in succession, were the three plant types simulated by BIOTRAN.

The disposal site conditions were assumed to be as follows:

- Soil properties are approximately 28% field capacity, 35% holding capacity, and have a wilting point of 10%.
- Plants grow over the radioactive disposal trenches, which are characterized as having a 1.5 m cap containing no radioactivity and a layer of fill 6.5 m deep that is uniformly contaminated with ^{239}Pu to a concentration of 800 pCi/g.
- All plants are assumed to have essentially the same depth and distribution of roots; all roots are present in the first 2 cm, 75% of the roots appear in the next 25 cm, 18% appear in the following 25 cm, 4% in the following, and so on until only a small fraction ($1.5 \times 10^{-2}\%$) of the roots actually makes contact with the first layer (25 cm) of waste. We assume that none of the trench cover is lost to wind or water erosion.

Through the natural process of plant uptake, litter dryfall, and litter decomposition, ^{239}Pu is deposited on the land surface. Runoff events produced by successive rainfall and snowmelt transport ^{239}Pu , in both dissolved and particulate forms, to South Mortandad Canyon (which joins Mortandad Canyon). Transport, deposition, and resuspension of sediments in the channel within the canyon spread the contaminants downstream in the canyons.

The modeling approach for the above scenario involves simulating 100 yr of plant growth at Area C with BIOTRAN. Then, using the plutonium deposition that BIOTRAN has predicted, the other models - ARM, DKWAV, and TODAM simulate the overland and in-stream transport of ^{239}Pu for the next 2 yr. Figure 5.4

MODEL INTERACTIONS

FIGURE 5.4. Model Coupling and Information Transfer

presents the model coupling and information transport scenario. As shown in Figure 5.4, BIOTRAN provides ^{239}Pu levels on the land surface as an initial condition for ARM. The runoff events produced by ARM are provided to DKWAV for the hydrodynamic simulation. Outputs of runoff, overland soil erosion, and the plutonium flux predicted by ARM and DKWAV represent initial and boundary conditions for TODAM. TODAM then simulates sediment-radionuclide transport and accumulation in the canyon channels. This report briefly discusses the results of using ARM, DKWAV, and TODAM. A more detailed discussion of this study can be found in Onishi, Whelan, and Skaggs (1982).

Before ARM was applied to each of the 13 subcatchments ranging in size from 7 to 246 acres, ARM was calibrated by applying it to the 246-acre subcatchment located at the head of the Mortandad Canyon (Figure 5.3). As an example of the ARM calibration, a comparison of the simulated and measured runoff for the July 21, 1976 storm event is shown in Figure 5.5, revealing reasonable agreement. After ARM was calibrated, the hydrodynamic model,

FIGURE 5.5. Comparison of Simulated and Measured Runoff for the Storm of 7/21/76

DKWAV, was calibrated to select appropriate channel roughness coefficients and seepage velocities. After many calibration runs, the Manning roughness coefficient and the seepage velocity for Mortandad Canyon were selected to be 0.045 and 2.35×10^{-5} m/s, respectively. For South Mortandad Canyon, the seepage velocity was also selected to be the same as that in Mortandad Canyon. However, the Manning coefficients used on South Mortandad Canyon were 0.065 and 0.055 for the upper and lower half of the canyon, respectively. Using the

ARM output as input at the stream gaging station at GS-1 (Figure 5.3), DKWAV then calculated the flow rate at the gaging station GS-2. Comparisons of these results with measured data for the September 15, 1974 and July 16, 1976 storm events indicated reasonable agreement (Figures 5.5, 5.6, and 5.7).

The in-stream sediment-contaminant transport model, TODAM, was then calibrated. Because sediment information existed at location GS-2 for the September 15, 1974 flood event and because peak discharge, water depth, and flow velocity for the September 15, 1974 flood event ($0.30 \text{ m}^3/\text{s}$, 0.31 m , 1.5 m/s , respectively) were comparable to the computer results provided by DKWAV ($0.35 \text{ m}^3/\text{s}$, 0.31 m , and 1.1 m/s , respectively) for the July 16, 1976 flood event, TODAM was calibrated based on the sediment information of September 15, 1974 at location GS-2. Predicted sediment discharge agreed well with measured data (Figure 5.8). Predicted flow rates and sediment discharges (for sand, silt and clay) at GS-1 and at the confluence of Mortandad and South Mortandad Canyons are shown in Figures 5.9 through 5.12, respectively, for the July 16, 1976 storm event. The predicted net sediment deposition and erosion along the canyon are shown in Figure 5.13.

After the calibration, ARM, DKWAV, and TODAM were then applied to these two canyons (Figure 5.3). The simulation period for the application of ARM to Mortandad and South Mortandad Canyons above the Garden was from June 1, 1975 to May 30, 1977. The overland flow, and sediment and radionuclide transport simulation results for Area C are shown in Figures 5.14, 5.15 and 5.16. One of the significant events was the storm occurring on July 16, 1976. This event produced a peak discharge of $0.02 \text{ m}^3/\text{s}$ from Area C, maximum sediment concentration of about 17 kg/m^3 , and radionuclide concentration of $1.7 \times 10^{-4} \text{ pCi/m}^3$. Over the simulation period of approximately two years, only 1% of the initial 502 pCi of ^{239}Pu deposited on the land surface at Area C was transported from Area C into South Mortandad Canyon.

The models, DKWAV and TODAM, were then applied to Mortandad and South Mortandad Canyons to simulate the movements of flow, sediment and ^{239}Pu for the same 2-yr period as ARM was applied to. TODAM simulated the migration of sand, silt, clay, particulate ^{239}Pu adsorbed by sand, particulate ^{239}Pu adsorbed by silt, particulate ^{239}Pu adsorbed by clay, and dissolved ^{239}Pu . Over the 2-yr period, only several storms produced runoff, as shown in the

FIGURE 5.6. Simulated Flow Rate by ARM with Measured Data at GS-1 for the September 1974 and July 1976 Storm Events

FIGURE 5.7. Simulated Flow Rate by DKWAV with Measured Data at GS-2 for the September 1974 and July 1976 Storm Events

predicted temporal discharge distribution in South Mortandad Canyon at its confluence with Mortandad Canyon (Figure 5.17). The predicted total sediment discharge at the confluence reflected the flow variation (Figure 5.18). TODAM predicted a large increase in the total sediment flux, especially sand, from the head of the canyon to its confluence with Mortandad Canyon due to erosion of the channel bed (98% of which is composed of sand).

As discussed earlier, less than 1% of the available ^{239}Pu on the land surface in Area C reached the stream's edge during the simulation period. Furthermore, of the ^{239}Pu transported from Area C to the canyon, 99% was carried by the eroded sediment. Predicted particulate ^{239}Pu flux in South

FIGURE 5.8. Simulated Total Sediment Flow Rates by TODAM with Measured Data at GS-2 on Mortandad Canyon for the 15 September 1974 and 16 July 1976 Storms

Mortandad Canyon at its confluence with Mortandad Canyon is shown in Figure 5.19. Despite the fact that sand consists of ~85% of the suspended sediment, TODAM predicted that clay carries ~83% due to high adsorptive capacity of clay and that sand carries only 3%. The rest (14%) was associated with silt. Predicted dissolved ^{239}Pu flux (Figure 5.20) was <1% of the total ^{239}Pu flux. Predicted particulate, dissolved, and total ^{239}Pu concentrations are presented in Figures 5.21, 5.22 and 5.23. Note that the particulate ^{239}Pu concentrations are in pCi/kg. Comparison of Figures 5.22 and 5.23 indicates that the major transporting agent of ^{239}Pu is sediment, and that the dissolved concentrations are two to three orders of magnitude less than the particulate concentrations. This clearly indicates that deposition and resuspension of contaminated sediment are important mechanisms in the migration and fate of ^{239}Pu in the aquatic environment. Since the half-life of ^{239}Pu is very long, bed contamination may become an important concern as a source of long-term contamination. Figure 5.24 presents the simulated longitudinal distribution of bed contamination by the sediment size fraction in South Mortandad

FIGURE 5.9. Simulated Discharges Distributed in Time at GS-1 on Mortandad Canyon for the 16 July 1976 Storm

FIGURE 5.10. Simulated Sediment Flow Rates Distributed in Time at GS-1 on Mortandad Canyon for the 16 July 1976 Storm

FIGURE 5.11. Simulated Discharges Distributed in Time at the Confluence on Mortandad Canyon for the 16 July 1976 Storm

FIGURE 5.12. Simulated Sediment Flow Rates Distributed in Time at the Confluence on Mortandad Canyon for the 16 July 1976 Storm

FIGURE 5.13. Simulated Longitudinal Variation of the Net Change in the the Bed Elevation on Mortandad Canyon for the 16 July 1976 Storm

Canyon. As expected, the degree and location of contamination followed the same pattern of the bed elevation change which occurred during the simulation period due to sediment deposition and resuspension. Contamination was predicted to be greatest where the deposition of sediments was predicted to be highest and the resuspension of sediments was lowest. Because silt and clay are generally being carried through the system and because sand is the major sediment type being deposited and resuspended, most of the contaminant inventory is associated with the sand in the bed.

As described above, the current simulation predicted that over a 100-yr simulation period, only an extremely small quantity (6×10^{-9} times the original concentration) of buried ^{239}Pu was taken up by plants and deposited on the land surface. Only a small fraction (~1%) of that contamination was further removed by soil erosion from the site and carried to the canyon, where it remained. Hence, the study reveals that the environment around Area C has integrity high enough to curtail LLW migration under natural, recreational land use.

FIGURE 5.14. Simulated Discharge, Area C

FIGURE 5.15. Simulated Total Sediment Concentrations, Area C

FIGURE 5.16. Simulated Total Radionuclide Concentrations, Area C

FIGURE 5.17. Simulated Discharges Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.18. Simulated Total Sediment Flow Rates Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.19. Simulated Total Particulate Flow Rates Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.20. Simulated Dissolved ^{239}Pu Flow Rates Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.21. Simulated Total Particulate Concentrations in PC/kg Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.22. Simulated Dissolved ^{239}Pu Concentrations Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.23. Simulated Total ^{239}Pu Concentrations Distributed in Time at the Confluence on South Mortandad Canyon

FIGURE 5.24. Simulated ^{239}Pu Bed Contamination on South Mortandad Canyon

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6.0 PROGRESS REPORT: MULTIMEDIA RADIONUCLIDE EXPOSURE ASSESSMENT

MODELING OF LOS ALAMOS - PUEBLO CANYONS, NEW MEXICO

This chapter presents the progress of the radionuclide multimedia exposure assessment modeling of Los Alamos-Pueblo Canyon in New Mexico for FY-1981. It presents background information on the site and possible pathway and modeling methodologies.

6.1 INTRODUCTION

Potential environmental impacts from radioactive substances released into the aquatic environ must be assessed to ascertain potential levels at downstream locations. Researchers at the Pacific Northwest Laboratory (PNL) have been active for a number of years developing, modifying, and updating contaminant transport codes pertaining to various environments (i.e., rivers, lakes, estuaries, reservoirs, oceans, bays, etc.). This chapter describes the progress made in FY-1981 in assessing the potential migration and fate of transuranics in Los Alamos and Pueblo Canyons, New Mexico. Specifically, the transport of radionuclides in Los Alamos and Pueblo Canyons will be simulated to determine under what conditions a significant amount of radionuclides will migrate towards the Rio Grande. PNL is performing this work in cooperation with Los Alamos National Laboratory (LANL).

The first section of this chapter contains a summary which includes a description on the state of the catchment, potential problems, and a brief pertaining to the modeling scenario. The second section contains background information pertaining to the history of the Los Alamos area as presented in the Formerly Utilized MED/AEC^(a) Sites Remedial Action Program (FUSRAP) report (LANL 1981). The third section discusses the characteristics of Los Alamos and Pueblo Canyons, while the fourth section explains the proposed pathway and modeling methodology. The final section then proceeds to discuss the modeling scenarios and calibration methodology.

(a) MED and AEC are the acronyms of Manhattan Engineering District and Atomic Energy Commission, respectively.

6.2 SUMMARY

Radioactive effluent was discharged into Acid and DP Canyons (Figure 6.1) since 1943 as a result of the MED atomic bomb project. From data gathered in the Los Alamos Area, ^{239}Pu appears to be of a major concern, while other radioactive material appear less significant.^(a) Plutonium-239 migrates in two forms: dissolved and particulate (adsorbed onto sediment) phases. The transport of ^{239}Pu in solution is relatively insignificant during runoff events as ~99% is transported with the sediment in a particulate phase. The radionuclides generally do not desorb at a high rate with the bulk of ^{239}Pu being carried by suspended or bed sediments. The bulk of the radionuclide activity is associated with the larger-sized particles, even though the finer particles have a greater affinity for contaminants. This is because the larger-sized particles are much more abundant than the finer ones. In general, the ^{239}Pu concentrations are above background levels in all of the canyons: Acid Canyon, middle and lower Pueblo Canyon, and lower Los Alamos Canyon. The highest concentrations of ^{239}Pu are located at the outfall (waste disposal location) in Acid Canyon with the concentrations in the channels decreasing as the distance from the outfall increases.

Sediment-contaminant migration over the last 30 to 35 years, due to runoff events from precipitation and snowmelt, resulted in a major portion of the contaminants in Acid Canyon to move into lower Pueblo Canyon and, to a much smaller degree, lower Los Alamos Canyon. Sixty-seven percent of the plutonium in Pueblo Canyon is located in Lower Pueblo Canyon. This is expected because at this location the channel widens and flattens reducing the flow velocity and depositing contaminated suspended sediment.

The banks or inactive channel areas tend to have higher concentrations than the active channel. This is expected since the runoff events tend to resuspend active channel sediments and transport them downstream. In addition, the ephemeral stream flows tend to inundate bank areas less often

(a) Plutonium-239 signifies the sum of ^{239}Pu and ^{240}Pu (LANL 1981)

FIGURE 6.1. Acid-Pueblo and DP-Los Alamos Canyons

and tend to deposit finer sediment, so the concentrations of ^{239}Pu remain high. The activity level is generally confined to the top 30 cm of the bed. In general, no consistent vertical distribution of ^{239}Pu exists in the canyons. The inventory in the lower Los Alamos area appears to be of a steady-state nature with annual contaminant inflow equaling contaminant outflow. It has been estimated, though, that relatively little ^{239}Pu has reached the Rio Grande, even though 75% of contaminant released into DP Canyon have been transported into lower Los Alamos Canyon.

Major precipitation events could possibly result in flows resuspending a major portion of the contaminated sediments in lower Pueblo Canyon (area with a significant ^{239}Pu inventory) and transporting them to lower Los Alamos Canyon and possibly to the Rio Grande. There is a considerable amount of uncertainty in predicting the eventual spacial and temporal distribution of contaminants in the Los Alamos area. Complex phenomena and uncertainty in predicting meteorological events are largely responsible. Essentially, no data is available on flow rates for estimating flood frequency curves and maximum discharges for summer storms in the canyons (LANL 1981).

Three numerical codes have been selected to simulate overland runoff of a major precipitation event(s) and the resulting migration and fate of sediment and radionuclides in Acid-Pueblo and DP-Los Alamos Canyons. ARM will simulate the movement of flow and sediment (and radionuclides, if any) overland to the stream's edge; MODSEEP will simulate the in-stream hydrodynamics; and TODAM will simulate the in-stream migration and fate of sediment and radionuclides. The codes will be calibrated on DP and upper Los Alamos Canyons with partial records of data which exist for this area. A major precipitation producing flood event or sequence of events will be simulated in the Los Alamos area in order to analyze the migration of radionuclides downstream towards the Rio Grande. It should be remembered that if the storm or storms in the modeling scenario are too small then the banks and inactive channel regions may not be inundated. This becomes significantly important when one considers the fact that a significant inventory of plutonium exists in these regions. In addition, the flows should be large enough so that the contaminated sediments are entrained. The bed material is sufficiently large (coarse to very coarse

sand) and, if the flow events are too small, a significant amount of contaminants may not be transported downstream. On the other hand, if the events are too large, the in-stream contaminant concentrations, due to dilution, could drop below significant levels, or the contaminants could be carried completely through the Los Alamos site to the Rio Grande where the effects due to contamination may be insignificant. It must be remembered that it is possible for areas downstream of Los Alamos and Pueblo Canyons, regardless of the precipitation event, not to be significantly impacted.

6.3 FUSRAP BACKGROUND

Background information describing the Los Alamos area and its history is presented below. This information was originally presented by LANL (1981) in the form of a report for the Formerly Utilized Sites Remedial Action Program (FUSRAP) sponsored by the U.S. Department of Energy (DOE). Figure 6.1 presents a schematic representation of the Los Alamos area, while Figure 6.2 presents the land ownership or management in the study area.

"Liquid radioactive wastes were generated by research with nuclear materials at Los Alamos, New Mexico, for the World War II MED atomic bomb project starting in 1943, and subsequently by work conducted for the AEC. Untreated effluents were discharged into Acid Canyon (Figure 6.1) from 1944 until 1951. A treatment plant was constructed on the rim of Acid Canyon and discharged treated effluents from 1951 until 1964. Following decommissioning of the plant and decontamination of the site and part of Acid Canyon, ownership of the property was transferred to Los Alamos County by the federal government in 1967" (LANL 1981).

"Acid Canyon is a small branch of Pueblo Canyon, which in turn, joins lower Los Alamos Canyon. Acid Canyon and part of Pueblo Canyon are currently controlled by the County of Los Alamos. The federal government has an easement across the county land generally following the course of the normally dry channel from the discharge point at the head of Acid Canyon for collecting samples and maintaining test wells. The remainder of Pueblo Canyon and a small part of lower Los Alamos Canyon are currently controlled by the DOE. Most of lower Los Alamos Canyon, down to the point where it joins the Rio

FIGURE 6.2. Land Ownership or Management in Study Area (LANL 1981)

Grande, is controlled by the San Ildefonso Indian Pueblo (Figure 6.2). Some residual radioactivity attributable to the effluents is found on soils and sediments in the channels of each of these canyons. Intermittent runoff events transport and redistribute sediments periodically (LANL 1981). Current land use includes occasional recreational use of Acid and Pueblo Canyons, commuter traffic on State Road 4 in lower Los Alamos Canyon, several households, a commercial sand and gravel operation, and some cattle grazing in lower Los Alamos Canyon" (LANL 1981).

"Some highlights of the occurrence and distribution of radioactivity on the sediments and soils affected by the liquid effluents may be useful in evaluating future management alternatives and describing possible future changes from natural hydrologic processes. Transuranium elements... are present in all affected areas at levels with statistical significance above those normally observed as background in northern New Mexico from world wide fallout. The highest concentrations occur in areas of limited extent at the county-owned site of the former waste treatment plant (in Acid Canyon)... and along the natural drainage course which carried the untreated effluent. Within the canyons, most contaminated material is near-surface (<0.5 m). The largest average concentrations and about 16% of the total inventory occur in the county-owned Acid Canyon. Intermediate average concentrations and about 12% of the inventory occur in the county-owned middle Pueblo Canyon... Similar concentrations, but about 67% of the inventory, occur in DOE-controlled lower Pueblo Canyon. The lowest average concentrations, and about 6% of the inventory, occur in lower Los Alamos Canyon (on San Ildefonso Indian Pueblo land)... Other radioactive contaminants including fission products are present at low but statistically significant levels above background in some, but not all, areas. Their major contribution to estimated risks is from external penetrating radiation that would be experienced only in the immediate vicinity of the contamination, e.g., the channels and banks" (LANL 1981).

"Major future runoff events in Pueblo Canyon could result in movement of the large proportion of the transuranic inventory, now accumulated in the broad

channel of lower Pueblo Canyon, further downstream and into lower Los Alamos Canyon... During the year of a major event, it is possible that the average concentration of plutonium on suspended sediments in the Rio Grande in White Rock Canyon down to Cochiti Dam (about 20 km downstream from the junction with Los Alamos Canyon) would be higher than that typically observed in the river due to worldwide fallout. The maximum levels would be about the same as the concentration considered by the EPA to be average for soils throughout the U.S." (LANL 1981).

6.4 LOS ALAMOS AND PUEBLO CANYONS

The area under study, as presented in Figure 6.3, is located in north-central New Mexico about 100 km (62 mi) north-northeast of Albuquerque and 40 km (25 mi) northwest of Santa Fe (LANL 1981). Two major drainage basins comprise the overall catchment: DP - Los Alamos (DP-LA) Canyon and Acid-Pueblo (A-P) Canyon. The drainage basins are east-west oriented with DP and Pueblo Canyons as tributaries of Los Alamos Canyon (see Figure 6.1). The area has a semi-arid, continental mountain climate (Onishi, Whelan, and Skaggs 1982). The vegetation and climatic changes are commensurate with the elevational gradation westward from the Rio Grande (LANL 1981). The transition zones of over-story vegetation range from juniper and grasslands at lower elevations along the Rio Grande to fir, spruce, and subalpine grasslands at the higher elevations (LANL 1981). In general, the catchment has grasses and shrubs growing along the banks with some boulders and blocks dislodged from the canyon walls. For the most part, canyon walls are steep with a narrow canyon floor. The watershed characteristics of the individual catchments are presented in Table 6.1.

Moisture that infiltrates the ground from precipitation or snowmelt penetrates about 4 to 5 m at a maximum and is re-evaporated into the air (LANL 1981). Streams are intermittent by nature with surface runoff occurring in association with summer thunderstorms, with a highly variable intensity and distribution. The remaining precipitation occurs as snow during the winter months (LANL 1981). In addition, the average annual precipitation increases from about 23 cm along the Rio Grande to as much as 76 cm along the crest of the mountains to the west (LANL 1981).

FIGURE 6.3. Regional Location of Study Area (LANL 1981)

TABLE 6.1. Watershed Characteristics(a)

Canyon	Drainage Area	Average Channel Gradient	Channel Length	Elevation Drop in Catchment
DP	1.6 km ² (0.6 mi ²)	0.061	1.8 km (1.1 mi)	213 m (700 ft)(c)
Los Alamos	25.9 km ² (10.0 mi ²)(b)	0.026	14.5 km (9.0 mi)(b,c,d)	1280 m (4200 ft)(c)
Acid	1.1 km ² (0.4 mi ²)(c)	—	—	140 m (460 ft)(c)
Pueblo	21.2 km ² (8.2 mi ²)(c)	0.017	9.8 km (6.1 mi)	1158 m (3800 ft)(c)
DP-LA	27.5 km ² (10.6 mi ²)(b)	—	—	—
A-P	22.3 km ² (8.6 mi ²)	—	—	—

(a) Information gathered from LANL (1981), Purtymun (1974) and topographic and watershed characteristic maps.

(b) Upstream of Pueblo-Los Alamos Canyon confluence

(c) Estimate

(d) Downstream of the reservoir on Los Alamos Canyon (see Figure 6.1).

(e) Downstream of Acid-Pueblo Canyon Confluence

The average July temperature at the lower elevations is about 23°C (73°F), and on the plateau about 19°C (66°F), while average January temperatures are -6°C (21°F) and -7°C (19°F), respectively (LANL 1981). The temperature drops even lower as the elevation increases and snow stays on the peaks until late May or early June. Pan evaporation for the laboratory area is estimated at about 150 cm/yr. Considerable variability can be expected due to differences in elevation and aspect, but no data exists (Wheeler 1979).

Some data does exist regarding the distribution of sediments and radio-nuclides in DP-LA and A-P Canyons. The sediments in A-P Canyon result from chemical and mechanical weathering of acid volcanic rock (LANL 1981). The granules are composed mainly of tuff, pumice, latite, and rhyolite rock fragments with minor amounts of quartz and sanidine crystals (LANL 1981). The

fractions of fine to coarse sand consist mainly of quartz and sanidine crystals and crystal fragments with minor amounts of rock fragments. The silt and clay fractions are composed mainly of clay minerals, montmorillonite, and illite (LANL 1981). Tables 6.2 and 6.3 present sediment distributions (as percent by weight) at various locations (as indicated by Figure 6.4) on Acid and Pueblo Canyons.

In Los Alamos Canyon, sediments are derived from weathering of the Tschiconia Formation and Bandelier Tuff. The channel in Los Alamos Canyon is composed of gravel and sands with cobbles and boulders. In DP Canyon, the larger material is composed of tuff which breaks down rapidly with transport during storm runoff. Tables 6.4 through 6.6 present sediment distributions (as percent by weight) at various locations (as indicated by Figure 6.4) in DP and Los Alamos Canyons. As these tables indicated (Tables 6.2 through 6.6) the bulk of the sediment is fairly large (coarse sand). The median-sized sediment diameters for Tables 6.2 through 6.6 ranged from 0.43 mm to >2.00 mm.

The bulk of the radionuclide activity is associated more with these larger-sized sediment particles than with the finer sediment particles. This is because the larger-sized particles are much more abundant than the finer particles, even though the finer ones have a greater affinity for contaminants. The ^{239}Pu concentrations are above background levels in Acid, middle and lower Pueblo, and lower Los Alamos Canyons with the highest levels at the outfall (waste disposal location) in Acid Canyon. In general, the concentrations decrease with an increased distance from the outfall. These results are presented in Figure 6.5. Figure 6.5 indicates that banks and inactive channel areas tend to have higher concentrations than the active channel. This is expected since intermittent runoff events inundate these areas less frequently, thereby resuspending less of the contaminated sediment. The activity level of the radionuclides is generally confined to the top 30 cm of the bed. It should be noted that the extremely large concentration ($21,000 \pm 49,000$ pCi/g) depicted at the treatment plant site in Figure 6.5 is not associated with the

TABLE 6.2. Particle-Size Distribution of Channel Sediments from Acid-Pueblo Canyon (LANL 1981)

Classification	Size Range (mm)	Distribution (% by Weight)							
		Acid Canyon		Pueblo Canyon					
		AC-4	Acid Weir	PC-1	PC-5	PC-7	PC-9	APSC	
Granules	2.36 to 3.96	4.5	6.5	3.0	10.5	5.0	2.0	1.0	
Very coarse sand	1.17 to 2.36	47.0	42.5	36.5	34.5	28.0	10.0	17.0	
Coarse sand	0.589 to 1.17	44.0	39.5	50.5	37.0	31.0	40.0	50.5	
Medium sand	0.295 to 0.589	2.0	6.0	7.0	11.0	19.0	21.0	19.0	
Fine sand	0.147 to 0.295	1.0	1.5	1.0	3.0	11.5	9.5	7.0	
Very fine sand	0.074 to 0.147	1.0	1.0	0.5	1.5	2.5	6.5	2.0	
Silt and clay	<0.074	0.5	3.0	1.5	3.0	3.0	11.0	3.5	

TABLE 6.3. Particle-Size Distribution of Channel Sediments from Acid-Pueblo Canyon^(a)

Size Range (mm)	Distribution (% by Weight)		
	Acid-Pueblo Canyon		
	AP-I	AP-II	AP-III
>2.0	23.82	8.14	7.44
1.168 to 2.00	15.83	16.95	20.55
0.500 to 1.168	32.04	39.70	49.10
0.105 to 0.500	22.50	21.91	19.38
0.053 to 0.105	1.48	6.42	1.43
<0.053	4.33	6.88	2.10

(a) Samples taken 17.8 to 25.4 cm from top by staff at the Los Alamos National Laboratory

FIGURE 6.4. Monitoring Net in Acid-Pueblo and DP-Los Alamos Canyons, 1949-1975 (LANL 1981)

TABLE 6.4. Particle-Size Distribution of Channel Sediments from DP-Los Alamos Canyon (LANL 1981)

Classification	Size Range (mm)	Distribution (% by Weight)								
		DP Canyon		Upper Los Alamos Canyon				Lower Los Alamos Canyon		
		DPS-1	DPS-4	LAO-C	LAO-1	LAO-3	LASC	CAS-3	CAS-4	CAS-7
Granules	2.36 to 3.96	8.0	4.0	16.5	<0.5	0.5	4.5	0.5	1.0	10.5
Very coarse sand	1.17 to 2.36	48.5	42.5	38.0	23.0	13.0	26.0	7.0	17.0	29.5
Coarse sand	0.589 to 1.17	29.0	36.0	32.0	53.0	40.0	33.0	25.0	47.0	38.5
Medium sand	0.295 to 0.589	8.0	10.5	10.5	18.5	23.5	19.0	37.0	19.5	11.5
Fine sand	0.147 to 0.295	3.0	4.5	2.0	4.0	11.0	10.5	21.0	9.5	4.0
Very fine sand	0.074 to 0.147	1.5	1.0	0.5	0.5	4.5	4.0	6.0	2.0	2.0
Silt and clay	<0.074	2.0	1.5	0.5	0.5	7.5	3.0	3.5	4.0	4.0

TABLE 6.5. Particle-Size Distribution of Channel Sediments from DP-Los Alamos Canyon(a)

Size Range (mm)	Distribution (% by Weight)						
	DP Canyon DPS-3	Upper Los Alamos Canyon			Lower Los Alamos Canyon		
		LA-I	LA-VI	LA-V	LA-II	LA-III	LAS-IV
>2.0	6.81	65.36	62.72	4.26	45.83	31.03	29.90
1.168 to 2.00	13.76	7.12	9.68	28.94	14.75	15.50	16.82
0.500 to 1.168	35.88	12.77	19.59	49.85	22.17	29.73	36.57
0.105 to 0.500	38.48	11.95	6.40	15.60	12.89	20.83	19.59
0.053 to 0.105	3.29	1.23	0.50	0.92	2.37	1.64	2.74
<0.053	1.76	1.59	1.12	0.52	1.99	1.27	4.37

(a) Samples taken 17.8 to 25.4 cm from top by staff at the Los Alamos National Laboratory

TABLE 6.6. Average Particle-Size Distribution of Weathered Tuff, Channel and Suspended Sediments in DP Canyon (Purtymun 1974b)(a)

Classification	Size Range (mm)	Distribution (% by Weight)		
		Weathered Tuff	Channel Sediment	Suspended Sediment
Very fine gravel	2.00 to 4.00	1	5	0
Very coarse sand	1.00 to 2.00	10	37	6
Coarse sand	0.500 to 1.00	16	39	14
Medium sand	0.250 to 0.500	12	12	13
Fine sand	0.125 to 0.250	10	5	15
Very fine sand	0.062 to 0.125	9	0.5	17
Silt and clay	<0.062	42	1.5	35

(a) Average of five analyses

channel but with sediment within the Bandelier Tuff nearby. Tables 6.7 and 6.8 also present the longitudinal variation of plutonium and cesium concentrations from the outfall location in A-P and DP-LA Canyons, respectively. These results were gathered from a special study performed in 1972. The results of a special study in 1973 which present estimated ^{239}Pu inventory in the channels are given in Tables 6.9 and 6.10.

These tables present the longitudinal and vertical distribution of ^{239}Pu in A-P and DP-LA Canyons, respectively. The vertical variation of ^{239}Pu generally does not follow any specific trends. The highest concentrations of plutonium reported were in Pueblo Canyon at Station 2560 m (see Table 6.9). The concentrations ranged from 369 to 2250 pCi/g with depth. These values were not consistent with other data collected in the canyon. It may have represented an analytical error or a point of accumulation of plutonium (LASL 1981) which has now dispersed.

The majority of the ^{239}Pu inventory is located in lower Pueblo Canyon. The estimated inventories of ^{239}Pu in Acid-Pueblo and Los Alamos Canyons are

FIGURE 6.5. Concentration of ^{239}Pu on Soils and Sediments by Location (LANL 1981)

TABLE 6.7. Plutonium and Cesium on Sediments from Acid-Pueblo Canyon Special Study, 1972 (Cushing 1975; LANL 1981) (analyses in pCi/g)

<u>Location^(a)</u>	<u>^{238}Pu</u>	<u>^{239}Pu</u>	<u>^{137}Cs</u>
Control	0.009	0.20	0.36
Outfall	0.02	2.3	0.02
20	0.09	2.2	1.5
40	0.03	6.9	0.74
80	1.0	54	14
160	0.08	8.5	1.1
320	0.08	12	1.5
640	0.08	11	1.1
2,560	0.02	1.5	0.31
5,120	0.01	0.35	0.20
10,240	0.02	0.74	0.33

(a) m below outfall

TABLE 6.8. Plutonium and Cesium on Sediments from DP-Los Alamos Canyon Special Study, 1972 (Cushing 1975; LANL 1981) (analyses in pCi/g)

<u>Location^(a)</u>	<u>^{238}Pu</u>	<u>^{239}Pu</u>	<u>^{137}Cs</u>
Control	0.02	0.03	0.3
Outfall	2.1	28	1700
20	1.5	7.9	190
40	0.06	0.58	5.9
80	0.20	2.5	49
160	0.15	0.61	24
320	0.17	0.50	15
640	0.23	0.70	51
2,560	0.03	0.17	13
5,120	0.03	0.36	3.6
10,240	0.05	0.13	1.6

(a) m below outfall

TABLE 6.9. Plutonium in Sediments from Acid-Pueblo Canyon Special Study, 1973 (LANL 1981) (analyses in pCi/g)

Location ^(a)	Depth of Sediment in cm			
	0 to 2.5	2.5 to 7.5	7.5 to 12.5	>12.5 ^(b)
Control	0.122	0.137	---	---
Outfall	16.6	8.52	---	---
20	16.8	---	---	---
40	5.78	8.72	11.4	28.7
80	6.21	6.60	21.1	505
160	8.61	10.1	---	20.4
320	8.28	7.92	10.8	12.3
640	7.86	12.4	10.4	19.1
2,560	36.6	369	2250	---
5,120	1.39	---	0.617	1.65
10,240	0.40	0.518	0.435	---

(a) m below outfall

(b) remainder varied from 12.5 to 30 cm

TABLE 6.10. Plutonium in Sediments from DP-Los Alamos Canyon Special Study, 1973 (LANL 1981) (analyses in pCi/g)

Location ^(a)	Depth of Sediment in cm			
	0 to 2.5	2.5 to 7.5	7.5 to 12.5	>12.5 ^(b)
Control	0.036	0.036	0.044	0.051
Outfall	957	1640	---	---
20	24.8	16.4	2.63	---
40	18.2	---	11.4	0.488
80	---	10.4	1.87	0.831
160	0.332	2.25	0.369	0.328
320	0.196	0.252	0.225	2.34
640	0.344	0.481	0.445	---
1,280	0.864	0.878	0.644	1.78
2,560	0.183	0.090	0.114	---
5,120	0.599	0.186	---	---

(a) m below outfall

(b) remainder varied from 12.5 to 30 cm

presented in Figure 6.6. The ^{239}Pu inventories were estimated as a product of the average concentrations in the channel and banks of each segment and the estimated mass of affected sediments and soils derived from averaged measured dimensions and density (LANL 1981). This figure also indicates the degree in which the sediments in the inactive channel and banks are contaminated relative to the sediments in the active channel.

Sixty-seven percent of the ^{239}Pu is located in lower Pueblo Canyon. This is expected because at this location the channel widens and the gradient decreases reducing the flow velocity and depositing contaminated suspended sediment (LANL 1981).

6.5 PATHWAY AND MODELING METHODOLOGY

A preliminary analysis of natural phenomena, which could result in an increase of radionuclides downstream of the Pueblo-Los Alamos Canyon confluence, showed that the key pathways requiring detailed evaluation were the overland and in-stream pathways. Precipitation and snowmelt events transport water and sediment overland to the in-stream channel system. Once in the channel, water, sediment, and radionuclides can migrate downgradient through a continuous process of in-stream sediment transport, deposition, and resuspension. Because most of the contamination exists in the bed of the stream channels, the dynamic processes describing the history of the bed, distribution of sediments and radionuclides in the bed, aggradation, and degradation should be included in any modeling scenario. The types of models included for the modeling scenario are 1) an overland runoff-soil erosion-contaminant transport model, 2) an in-stream hydrodynamic model, and 3) an in-stream sediment-radionuclide transport model. The first and third models should include algorithms for computing the migration of radionuclides in their particulate (adsorbed to sediment) and dissolved states.

6.5.1 Model Selection

The primary criteria for initial selection of models were the availability of state-of-the-art modeling capabilities in each of the areas mentioned above and the adequacy of the models in describing the unique characteristics of the sites. Acid-Pueblo and DP-Los Alamos Canyons represent a unique region, which

FIGURE 6.6. Estimated Inventory of ^{239}Pu on Soils and Sediments by Location (LANL 1981)

calls for models with certain unique features. This region's channels are generally dry between storms. The channels may be described as ditch-like, with high representative roughness values as opposed to the more conventional river bed. Low-flow discharges and depths are typical in the region. Channel slopes are also quite high ($>1\%$).

PNL has been active for a number of years on the subject of overland and in-stream contaminant transport. They have developed and are now refining models to predict radionuclide migration in rivers, lakes, estuaries, and oceans. Three codes which PNL has used in the past have been selected for the modeling scenario: ARM (Agricultural Runoff Management Model), MODSEEP, and TODAM (Transient One-Dimensional Degradation and Migration Model). As discussed in Chapter 5, ARM and TODAM are two components of the MCEA Methodology.

Processes controlling overland runoff, soil erosion, and contaminant transport on land surfaces are continuous in nature even though the bulk of contaminant migration may take place only through runoff producing storm events. A continuous simulation model must be selected not only to simulate contaminant transport during a storm event, but also to simulate the processes that change a soil's moisture content and the events that influence soil and contaminant conditions between storms. Furthermore, a model must handle the migration of both dissolved and particulate (those adsorbed to the soil) phases of a contaminant. One overland contaminant-transport model which meets these criteria is the Agricultural Runoff Management (ARM) model (Donigian et al. 1977, and Donigian and Davis 1978). ARM has been extensively tested and used throughout the United States (Donigian et al. 1977, Donigian and Davis 1978, Donigian and Crawford 1976a, 1976b, 1979, and Crawford and Donigan 1973). The documentation for the understanding and implementation of the model is excellent. The code is not so large that it cannot be handled in an efficient manner, yet it considers many of the important mechanisms related to contaminant migration such as snowmelt, adsorption/desorption, degradation, sediment transport, mineralization, nitrification/denitrification, immobilization, nitrite leaching, etc.

Two new codes recently introduced to the contaminant-transport modeling community are the CREAMS (Chemical, Runoff, and Erosion from Agricultural Management Systems; Knisel 1980) and HSPF (Hydrological Simulation Program-Fortran, Johanson et al. 1980) models. HSPF is a systems model based on ARM, NPS (Nonpoint Source model, Donigian and Crawford 1976b, 1979), and HSP (Hydrological Simulation Program, Hydrocomp 1976, 1977). The HSPF software is not merely a translation of the above models, but a new system with a framework designed to accommodate a variety of simulation modules. HSPF has been written in a top-down format with approximately 500 modules included. This format is designed to allow the user to update any mechanism or physical phenomena not considered state-of-the-art.

CREAMS was developed by over 60 scientists, researchers, and technicians contributing ideas, direction, and data. Knisel (1980) reports that "CREAMS is a physically-based, daily simulation model that estimates runoff, erosion/sediment transport, plant nutrient, and pesticide yield from field-sized areas." CREAMS also includes many of the important mechanisms related to contaminant migration such as foliar interception, degradation, washoff, adsorption, desorption, degradation in the soil, etc.

One of the criteria for model selection is the extensive past application. Since ARM includes all major mechanisms for contaminant transport with extensive documentation and usage, ARM was chosen as the model for simulating the movement of water and sediments (and possibly contaminants) overland. For further information regarding various contaminant-transport models refer to Overcash and Davidson (1980), Brandstetter (1977), Brown et al. (1977), EPA (1976), and USFS (1977).

MODSEEP is a one-dimensional flood routing model which accounts for seepage through the channel bed. The model is based on a formulation, developed by Cunge (1969) and advanced by Ponce and Yevjevich (1978), in which wave attenuation is incorporated into a flood propagation model. A seepage function, which is proportional to the wetted perimeter, has been added to the flood routing code to increase the capability of MODSEEP.

Data required for model execution are elevation-width cross-sectional information, Manning's roughness coefficient, seepage velocity, initial flow conditions, lateral inflow, and upstream flow boundary conditions. Model results include discharges, depths, and velocities at each cross-section and time interval.

As a flood routing code, the model has been well-tested in actual streams. The channel bed seepage routine has been successfully applied to hypothetical streams where both initially wet and dry beds were used.

MODSEEP is an economical and user-oriented model. It is, however, limited to streams where downstream control and significant storage effects are not present.

TODAM is a one-dimensional, unsteady, sediment-contaminant transport code. It represents a one-dimensional version of the two-dimensional, sediment-contaminant code SERATRA (Onishi 1977 and Onishi et al. 1976, 1981). TODAM is composed of the following three submodels joined to describe sediment-contaminant interaction and migration: sediment transport, dissolved-contaminant transport, and sorbed-contaminant (contaminants adsorbed by sediment) transport. These submodels solve an advection-diffusion equation with decay and sink/source terms with appropriate initial and boundary conditions. These submodels use the finite element computation method with the Galerkin weighted residual technique. Since the movement and adsorption capacities of sediments vary significantly with grain size, the sediment transport submodel solves the migration (transport, deposition, and scouring) for three size fractions or types. TODAM also computes changes in river bed conditions, including bed elevation, sediment size distribution, and sorbed contaminant distribution within the bed. For further information regarding the capabilities of TODAM, refer to Parkhurst et al. (1981) and Onishi, Whelan, and Skaggs (1981).

6.5.2 Model Coupling

To adequately simulate the migration of radionuclides through the water-sediment transport pathways, the selected models had to be coupled at appropriate interfaces. Figure 6.7 presents the coupling methodology for the models and the information transferred at each interface. ARM is the first model in

FIGURE 6.7. Model Coupling and Information Transfer

the system. Meteorological information (precipitation, solar radiation, dew point temperatures, max-min temperatures, wind speed, etc.) is supplied to ARM so ARM parameters controlling evapotranspiration, interception, snowmelt, and soil erosion (as it is affected by forest density) can be estimated. ARM generates two types of information, which provide boundary conditions to the models MODSEEP and TODAM. ARM produces information on overland runoff and edge-of-stream sediment and radionuclide loadings. The second model in the system, MODSEEP performs the hydrodynamic simulation in the channel and provides the in-stream flow discharge, cross-sectional area, flow depth, shear stress, net inflow, and wetted perimeter for use by TODAM. TODAM, the third model in the system, simulates the in-stream migration and fate of sediments and radionuclides. For this particular modeling scenario the storms should be significantly large so as to encompass all active and inactive bank radionuclide storage areas. These storage areas would then be inundated with channel flows, requiring an in-stream modeling simulation as opposed to an overland modeling simulation. If smaller storms are employed in the modeling scenario the banks and inactive channel regions may not be inundated by the storm. This becomes particularly important when one considers the fact that a significant inventory of plutonium exists in these regions. Therefore, within this modeling scenario, ARM probably will not be used to simulate the migration and fate of radionuclides overland. ARM will be used, though, to simulate the movement of water and sediment overland.

6.6 MODELING SCENARIOS AND CALIBRATION METHODOLOGY

For approximately 30 years, radionuclide effluent has been discharged into A-P and DP-LA Canyons. Over this time, radionuclides (mainly ^{239}Pu) have adsorbed to sediment, and the banks and bed of the canyons have been contaminated at various depths with various activity levels. As mentioned earlier, Figures 6.5 and 6.6 and Tables 6.7 through 6.10 present levels and locations of the radioactive contamination. Under certain conditions (i.e., extreme flood events), the contaminated sediment may be resuspended and transported downstream towards the Rio Grande. The objective herein is to investigate the conditions under which a significant amount of radionuclides will be resuspended and transported downstream.

6.6.1 Flood Frequency

Because the size of the flood event determines the amount of contaminants transported downstream, return periods for A-P and DP-LA Canyons have been estimated. In addition, these estimates could be used to correlate the recurrence intervals of precipitation events and corresponding return periods of simulated flood events. It should be noted, though, that the return periods for precipitation and corresponding flood events do not have to be the same. The corresponding flood event is a function of the areal distribution, duration, intensity, etc., of the precipitation event and watershed characteristics at the time of occurrence of the event. The FUSRAP report (LANL 1981) presents various return periods (i.e., 2-yr, 5-yr, 10-yr, 25-yr, and 50-yr) for A-P and DP-LA Canyons. These are presented in Table 6.11.

TABLE 6.11. Flood Frequency and Maximum Discharge for Acid-Pueblo and DP-Los Alamos Canyons (LANL 1981)

<u>Frequency</u>	<u>Maximum Discharge</u> <u>(m³/s)</u>	
	<u>Acid-Pueblo</u>	<u>Upper Los Alamos</u>
2 year	3.1	3.0
5 year	7.1	6.8
10 year	10	11
25 year	17	16
50 year	21	20

These return periods were based on research by Scott (1971).^(a) Larger return periods may be estimated using more information provided by Scott (1971). He presents Log-Pearson Type III relationships for many of the canyons surrounding the Los Alamos area. Because of limited Los Alamos data, flood events representing larger return periods may be estimated by comparing recurrence interval curves from the Los Alamos area with those of surrounding canyons with similar characteristics. The correlations could be checked through numerical simulation, if it is assumed that the return period for a given precipitation event is similar to the return period of the corresponding flood event. In other words, a 25-year precipitation is not expected to produce a 200-year flood event (barring snow-melt conditions).

6.6.2 Calibration Procedure

In order for numerical codes (ARM, MODSEEP, and TODAM) to respond to changes within the watersheds, each code will have to be calibrated with data pertinent to the catchments. The calibration procedure of the models may proceed as follows:

- (a) ARM can simulate runoff from a precipitation event on DP Canyon. Parameters will be adjusted until the simulated and observed runoff events are similar.
- (b) ARM can then simulate runoff on Los Alamos Canyon upstream of LAGS-1 for the same precipitation event as that used in Step (a). If the output appears reasonable, the edge-of-stream flow will be routed by the hydrodynamic code from the reservoir to LAGS-1. These results will then be compared with measured data.
- (c) Steps (a) and (b) may have to be repeated until a satisfactory match between simulate and observed flood hydrographs are achieved.
- (d) TODAM will then be calibrated (depending on the availability of data) on the channel upstream of LAGS-1.

(a) Scott (1974) and Scott and Kunkler (1976) present further information pertaining to floods from small drainage areas in New Mexico.

- (e) A precipitation event will then be simulated on the watershed. If the return period for the precipitation event is not similar to the return period of the flood event, then the entire methodology will be re-examined (including the flood frequency analysis).

6.6.3 Data

Various groups of data should be collated so as much information pertaining to the A-P and DP-LA Canyons can be used in the modeling scenario:

- (a) A significant amount of relevant data exists from several Mortandad Canyon studies (Onishi, Whelan, and Skaggs 1982, Purtymun 1974, Hakonson, Johnson, and Purtymun 1973, Hakonson, Nyhan, and Purtymun 1976). Mortandad Canyon is located just south of Los Alamos Canyon (see Figure 6.2). Much of the meteorological data gathered for that study would probably be useful for calibrating ARM, MODSEEP, and TODAM. In addition, values obtained in the calibration procedure on Mortandad Canyon for various parameters in the numerical codes could be used as a starting point of the calibration procedure of the codes on the Los Alamos site.
- (b) A great deal of information on the Los Alamos area also exists in the FUSRAP report (LANL 1981). This report describes watershed conditions and characteristics. In addition, levels, types, and locations of contamination are described.
- (c) Reports and various supplemental information supplied by LANL and other agencies have been obtained (Hakonson et al. 1973, Purtymun et al. 1966, Abrahams et al. 1961, Hakonson et al. 1975, Nyhan et al. 1978). This information includes meteorological, hydrogeological, topographical, hydraulic, and hydrologic information.

6.6.4 Modeling Scenarios

In order to analyze the migration and fate of significant quantities of radionuclides, three models have been selected for use in the simulation: ARM,

MODSEEP, and TODAM (see Section 6.5). ARM and MODSEEP will be used in computing the precipitation-generated flood events overland and in-stream, respectively, while TODAM will simulate the migration and fate of in-stream sediments and radionuclides.

Care must be insured when simulating the precipitation-generated flood events so that the modeling objective is met. If the flood events are too large, the in-stream contaminant concentrations could drop below significant levels due to dilution. In addition, a large flood event could carry the contaminated effluent completely through the Los Alamos site to the Rio Grande where its effects may be insignificant.

If the flood events are too small, banks and inactive areas, where a significant amount of radionuclides exist, may not be inundated, thereby not being transported downstream. Because the modeling scenario considers seepage of flows in the channel, a small storm event may be significantly decreasing the discharge and depositing contaminated suspended sediments before they are transported from Pueblo Canyon. Lower Pueblo Canyon may be very susceptible to this, due to its shallow gradient and broader cross section. In addition, the flows should be large enough so that the contaminated sediments are entrained. It must be remembered that the bed material is fairly large (coarse to very coarse sand) and some flood events will not move significant amounts of contaminated sediment.

Finally, it is possible for areas downstream of Los Alamos and Pueblo Canyons, regardless of the precipitation event, not to be significantly impacted.

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APPENDIX A

WTRFLX COMPUTER CODE

```

C      PROGRAM *** ATRFLX ***
C      DEVELOPED AS A SIMPLIFIED WATER FLOW MODEL FOR RIOTRAN
C
C      AUTHOR: C.S. SIMMONS          OCT. 1981
C      BATTELLE PACIFIC NORTHWEST LAB. RICHLAND WASH.
C
C      SYMBOL GLOSSARY:
C      SOIL PROFILE:
C      LAYERS  = NUMBER OF SOIL LAYERS OR COMPARTMENTS
C      NPTS   = NUMBER OF NODES USED TO DEFINE SOIL PROFILE
C              = LAYERS+2
C      DELZ(I) = THICKNESS OR WIDTH OF EACH LAYER (MM)
C      Z(I)    = DEPTH (MM) OF LAYER MIDPOINTS (I=2,NPTS-1)
C              Z(1) AND Z(NPTS) LOCATE BOUNDARY VALUES
C      THETA   = VOLUMETRIC WATER CONTENT OF EACH LAYER
C      H       = SUCTION HEAD (MM) AT MIDPOINT OF EACH LAYER
C      COND    = HYDRAULIC CONDUCTIVITY (MM/DAY) AT LAYER MIDPOINT
C      AVCOND  = LAYER-WEIGHTED CONDUCTIVITY THAT DEFINES DARCY
C              FLUX BETWEEN LAYERS
C      FLUX(I) = SOIL WATER FLUX (MM/DAY) BETWEEN LAYERS I AND I+1
C              (I=1,NPTS-1). FLUX(1) IS AT THE SURFACE AND
C              FLUX(NPTS-1) IS THE DRAINAGE.
C      THDATA  = WATER CONTENT FOR THE SOIL WATER CHARACTERISTIC CURVE
C              WITH SOIL TYPE INDEX GIVEN BY ISOIL(I). DATA INPUT
C              IN INCREASING ORDER.
C      HOATA   = SUCTION HEAD VALUES CORRESPONDING TO THDATA (MM).
C      CDATA   = HYDRAULIC CONDUCTIVITY (MM/DAY) CORRESPONDING TO THDATA
C      NDATA   = NUMBER OF DATA POINTS FOR SOIL TYPE INDEX ISOIL(I)
C              DATA POINTS ARE FOR J=1,NDATA.
C      ISOIL   = SOIL TYPE INDEX FOR LAYER I
C              = 1 FOR CLAY (HILLEL, 1977)
C              = 2 FOR LOAM
C              = 3 FOR SAND
C      LOWER   = LOWER BOUNDARY CONDITION INDEX
C              = 1 FOR A WATER TABLE AT PROFILE BASE
C              = 2 FOR UNIT HYDRAULIC GRADIENT DRAINAGE
C              = 3 FOR A PROFILE WITHOUT DRAINAGE
C
C      CUMULATIVE WATER BALANCE TERMS:
C      STORGE  = SOIL WATER STORAGE (MM) WITHIN ENTIRE PROFILE
C      EVAPO   = EVAPORATION (MM) FROM SOIL SURFACE
C      RINFIL  = RAINFALL INFILTRATION (MM) INTO PROFILE
C      DRAIN   = DRAINAGE (MM) FROM BOTTOM OF PROFILE
C      RUNOFF  = EXCESS RAINFALL NOT INFILTRATED (MM)
C      TRANSP  = PLANT TRANSPIRATION AS (MM) OF WATER
C
C      CLIMATE PARAMETERS:
C      PET     = POTENTIAL TOTAL EVAPORATION AND TRANSPIRATION
C              FOR EACH DAY (MM)
C      PE      = POTENTIAL EVAPORATION (MM)
C      PT      = POTENTIAL PLANT TRANSPIRATION (MM)
C      RAIN    = RAINFALL RATE (MM/DAY) FOR EACH DAY
C      TEMP    = AIR TEMPERATURE AVERAGE FOR EACH DAY (DEG C)
C
C      PLANT SINK PARAMETERS:
C      SINK(I) = PLANT ROOT SINK TERM FOR WATER EXTRACTION
  
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C          UNITS ARE MM WATER PER MM LAYER THICKNESS PER DAY
C      THFC      = FIELD CAPACITY WATER CONTENT
C      THHYD     = HYDROPHOBIC WATER CONTENT LIMIT NEAR SATURATED
C                  CONDITIONS (FEDDES, 1977)
C      THWLT     = WILTING POINT WATER CONTENT ABOVE AIR DRY CONDITION
C
C      CONTROL PARAMETERS:
C      NDAYS     = NUMBER OF SIMULATION DAYS
C      DELTE     = TIME STEP (FRACTION OF DAY) USED DURING EVAPORATION
C      DELTR     = TIME STEP USED DURING RAINFALL
C                  MAXIMUM TIME STEP IS ONE DAY
C      DELTM     = MINIMUM TIME STEP ALLOWED WITHIN EACH DAY
C      PERCNT    = FRACTIONAL CHANGE IN WATER CONTENT ALLOWED
C                  FOR EACH TIME STEP, I.E. DELTH/THETA LESS THAN PERCNT,
C                  BUT SO THAT STEP REMAINS GREATER THAN DELTM.
C      ITERAT    = NUMBER OF ITERATIONS TO CALCULATE FLUX WITHIN EACH
C                  TIME STEP. FLUX IS AVERAGED OVER ITS PRESENT AND
C                  PREDICTED VALUES FOR EACH ITERATION
C
0001      DIMENSION DELZ(22),Z(22),OZ(22),THETA(22),H(22),COND(22),
          1DELTH(22),SINK(22),SSINK(22),ISOIL(22),THSAT(3),THMIN(3)
          2,FLUX(22),FLUXS(22),THETAS(22),DELTHS(22)
0002      DIMENSION THDATA(11,3),HDATA(11,3),CDATA(11,3),NDATA(3)
0003      COMMON X(11,3)
C      SOIL DATA:
0004      DATA NDATA/3*11/
0005      DATA THDATA/,.049,.069,.097,.129,.188,.286,.384,.448,.495,.52
          1,.521,.023,.064,.108,.147,.203,.280,.353,.413,.461
          2,.48,.481,.02,.041,.072,.118,.162,.206,.308,.390,.427
          3,.44,.441/
0006      DATA HDATA/2.E5,8.91E4,3.24E4,1.18E4,3.51E3,1.04E3,311,.113.
          1,.33,6,10,.0,.2.E5,5.26E3,1.04E3,465,.254,.138,.92.4
          2,.61,7,27.5,10,.0,.2.E5,1.04E3,380,.169,.113,.75.5,41.2
          3,.27.5,18.3,10,.0./
0007      DATA CDATA/2.61E-14,3.94E-11,3.94E-9,9.80E-8,4.94E-6,2.44E-4
          1,4.73E-3,.032,.183,.72,.72,2.18E-18,7.82E-8,1.57E-5
          2,2.14E-4,3.57E-3,4.2E-2,.226,.692,1.61,2.52,2.52
          3,3.06E-24,5.94E-7,4.40E-5,1.63E-3,.0133,.0611,.907
          4,4.0,7.23,9.0,9.0/
C      NOTE: UNITS ARE IN (CM) AND (CM/HR).
C      NOTE: A CAPILLARY FRINGE IS NOT ALLOWED FOR THETA VS H.
C-----
0008      OPEN(UNIT=1,NAME='WTRFLX.IN',TYPE='OLD',READONLY)
C      READS THE INPUT CONTROL FILE
C-----
0009      READ(1,*) LAYERS,NDAYS,LOWER,DELTE,DELTR,DELTN,PERCNT,ITERAT
0010      IF(PERCNT.LE.0.) PERCNT=0.5
0011      NPTS=LAYERS+2
0012      NPT=NPTS-1
0013      READ(1,*) (DELZ(I),I=2,NPT),(ISOIL(I),I=2,NPT)
C      READS INITIAL WATER CONTENTS OVER THE PROFILE
0014      READ(1,*) (THETA(I),I=2,NPT)
C      THETA(1) AND THETA(NPTS) ARE THE SURFACE AND BOTTOM VALUES
C      SET BY BOUNDARY CONDITIONS,RESP.
C
C      FINDS LAYER MIDPOINT DEPTHS. Z(1) AND Z(NPTS) ARE THE

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      C      3BOUNDARY POINT LOCATIONS.
0015      DELZ(1)=DELZ(2)
0016      DELZ(NPTS)=DELZ(NPT)
0017      Z(1)=DELZ(1)*0.5
0018      DO 100 I=2,NPTS
0019      100  Z(I)=Z(I-1)+0.5*(DELZ(I)+DELZ(I-1))
      C
      C      FINDS GRADIENT DISTANCE BETWEEN LAYERS I AND I+1.
0020      DO 105 I=1,NPT
0021      105  DZ(I)=Z(I+1)-Z(I)
      C
      C      SETS SOIL TYPE INDEX FOR SURFACE AND BOTTOM
0022      ISOIL(1)=ISOIL(2)
0023      ISOIL(NPTS)=ISOIL(NPT)
      C
      C      SETS THE AIR DRY AND SATURATED WATER CONTENT LIMITS
0024      DO 110 K=1,3
0025      THMIN(K)=THDATA(1,K)
0026      110  THSAT(K)=THDATA(NDATA(K),K)
      C
      C      LOG TRANSFORMS SUCTION HEAD AND CONDUCTIVITY DATA FOR
      C      INTERPOLATION, CHANGES TIME UNITS FROM HRS TO DAYS.
0027      DO 115 K=1,3
0028      DO 115 J=1,NDATA(K)
0029      X(J,K)=THDATA(J,K)
0030      HDATA(J,K)=ALOG(1.+HDATA(J,K))
0031      115  CDATA(J,K)=ALOG(24.*CDATA(J,K))
      C
      C      FINDS INITIAL SOIL WATER STORAGE IN PROFILE
0032      DO 116 I=2,NPT
0033      116  STORGE=STORGE+THETA(I)*DELZ(I)
      C-----
      C      BEGINS DAILY CALCULATION LOOP FOR NOAYS
      C-----
0034      DO 199 IDAY=1,NOAYS
0035      DAY=IDAY
      C
      C      READS OR FINDS CLIMATE VARIABLES FOR EACH DAY
0036      IF(IDAY.EQ.1) READ(1,*) PET,RAIN,TEMP
0037      PE=PET
0038      PT=0
      C
      C      READS OR FINDS PLANT ROOTING PARAMETERS FOR EACH DAY
      C      (TO BE INCLUDED FROM BIOTRAN)
      C      FINDS ROOT DISTRIBUTION FOR THE DAY
      C      (TO BE INCLUDED)
      C-----
      C      BEGINS CALCULATION LOOP WITHIN EACH DAY
      C-----
      C
      C      SETS TIME TO ZERO AND INITIALIZES TIME STEP CONTROL
0039      TIME=0
0040      200  DELT=DELTE
0041      IF(RAIN.GT.0.) DELT=DELTR
      C
      C      CHECKS THE ONE DAY LIMIT AND ADJUSTS LAST TIME STEP

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0042      IF(1.=TIME,LT,DELT) DELT=1.=TIME
0043      IF(TIME,GE,1.) GO TO 299
0044      TTIME=DAY=1+TIME

      C
      C      SETS ITERATION COUNTER AT START
0045      ICOUNT=0
0046      201 CONTINUE

      C
      C      SETS THE LOWER BOUNDARY CONDITION
0047      THETA(NPTS)=THSAT(ISOIL(NPTS))
0048      IF(LOWER,EQ,2) THETA(NPTS)=THETA(NPT)
0049      IF(LOWER,GE,3) THETA(NPTS)=THMIN(ISOIL(NPTS))

      C
      C      SETS THE SURFACE BOUNDARY CONDITION
      C      EVAPORATION CONDITIONS
0050      THETA(1)=THMIN(ISOIL(1))
0051      FSURF=PE

      C      RAINFALL CONDITIONS
0052      IF(RAIN,GT,0.) THETA(1)=THSAT(ISOIL(1))
0053      IF(RAIN,GT,0.) FSURF=RAIN

      C
      C      FINDS HYDRAULIC PROPERTIES BY INTERPOLATION AND CALLS
      C      THE PLANT SINK MODEL
0054      DO 120 I=1,NPTS
0055      J=ISOIL(I)
0056      H(I)=EXP(HYPINT(THETA(I),HDATA,NDATA(J),J))-1.
      C      HERE "COND" IS THE LOG OF CONDUCTIVITY
0057      120 COND(I)=HYPINT(THETA(I),CDATA,NDATA(J),J)
0058      CALL PLANT(SINK,THETA,Z,NPT,PT,DAY)

      C
      C      FINDS THE FLUX BETWEEN LAYERS USING A LAYER=WEIGHTED
      C      CONDUCTIVITY
0059      DO 125 I=1,NPT
0060      AVLOG=(DELZ(I)*COND(I)+DELZ(I+1)*COND(I+1))/(DELZ(I)+DELZ(I+1))
      C      SETS THE EVAPORATION CONDUCTIVITY
0061      IF(FSURF,LT,0.AND,I,EQ,1) AVLOG=COND(2)
0062      AVCOND=EXP(AVLOG)
      C      SAVES THE AVERAGE CONDUCTIVITY
0063      COND(I)=AVCOND
0064      125 FLUX(I)=AVCOND*(H(I+1)-H(I))/DZ(I)+AVCOND
0065      COND(NPTS)=EXP(COND(NPTS))

      C
      C      SETS NO FLOW LOWER BOUNDARY CONDITION
0066      IF(LOWER,EQ,3) FLUX(NPT)=0.

      C
      C      LIMITS SURFACE FLUX TO INFILTRABILITY OR EVAPORABILITY
      C      ALLOWED BY SOIL CONDITIONS
0067      IF(RAIN,EQ,0.AND,FSURF,LT,FLUX(1)) FSURF=FLUX(1)
0068      IF(RAIN,GT,0.AND,FSURF,GT,FLUX(1)) FSURF=FLUX(1)

      C
      C      SETS SURFACE FLUX DETERMINED BY RAINFALL OR
      C      EVAPORATION CONDITIONS
0069      FLUX(1)=FSURF

      C
      C      ADJUSTS FLUXES FOR A SATURATED WETTING FRONT ADVANCE
0070      DO 130 I=1,NPTS=2

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0071      K=NPTS=I
0072      THLOW=1.0001*THMIN(ISOIL(K))
0073      THMAX=0.9999*THSAT(ISOIL(K))
0074      IF(THETA(K).LT.THMAX) GO TO 205
0075      IF(FLUX(K-1).GT.FLUX(K)) FLUX(K-1)=FLUX(K)

      C
      C      ADJUSTS FLUXES SO WATER CONTENT REMAINS GREATER THAN
      C      THE MINIMUM. FLOW OUT OF A DRY LAYER IS NOT ALLOWED.
0076      205      IF(THETA(K).GT.THLOW) GO TO 130
0077      IF(FLUX(K-1).GE.FLUX(K)) GO TO 130
0078      IF(FLUX(K).GT.0.) FLUX(K)=0.
0079      IF(FLUX(K-1).LT.0.) FLUX(K-1)=0.
0080      130      CONTINUE

      C
      C      SETS THE ACTUAL SURFACE FLUX NOW DETERMINED BY PROFILE CONDITIONS
0081      FSURF=FLUX(1)

      C
      C      FINDS CHANGE IN WATER CONTENT AND ADJUSTS TIME STEP TO REMAIN
      C      WITHIN AIR DRY AND SATURATED LIMITS
0082      DELTO=DELT
0083      DO 135 I=2,NPT
0084      DELTH(I)=-((FLUX(I)-FLUX(I-1))/DELZ(I)+SINK(I))*DELT
0085      IF(DELTH(I).EQ.0.) GO TO 135
0086      THETAN=THETA(I)+DELTH(I)

      C
      C      TESTS IF WATER CONTENT CHANGE EXCEEDS CONTROL LIMIT
0087      TEST=DELTH(I)/THETA(I)
0088      IF(TEST.LE.PERCNT) GO TO 206
0089      DELTN=PERCNT*DELT/TEST
0090      IF(DELTN.LT.DELTM) DELTN=DELTM
0091      IF(DELTN.LT.DELTO) DELTO=DELTN
0092      206      IF(THETAN.LE.THSAT(ISOIL(I))) GO TO 210
0093      DELTN=(THSAT(ISOIL(I))-THETA(I))*DELT/DELTH(I)
0094      GO TO 215
0095      210      IF(THETAN.GE.THMIN(ISOIL(I))) GO TO 135
0096      DELTN=(THMIN(ISOIL(I))-THETA(I))*DELT/DELTH(I)

      C
      C      FINDS THE MINIMUM TIME STEP
0097      215      IF(DELTN.LT.DELTO) DELTO=DELTN
0098      135      CONTINUE

      C
      C      WATER CONTENT CHANGE IS NOW CORRECTED FOR NEW TIME STEP
      C      AND WATER CONTENT IS UPDATED.
0099      TRATIO=DELT/DELT
0100      IF(ICOUNT.EQ.0) DELTS=DELT
0101      *TS=DELTS/(DELTS+DELT)
0102      *T=1.-*TS
0103      DELTS=0.5*(DELTS+DELT)
0104      DO 140 I=1,NPT

      C
      C      ADJUSTS THE CHANGE IN WATER CONTENT
0105      DELTH(I)=DELTH(I)*TRATIO

      C
      C      SAVES THE FIRST VALUES BEFORE PERFORMING ITERATIONS
0106      IF(ICOUNT.GT.0) GO TO 220
0107      THETAS(I)=THETA(I)
0108      DELTHS(I)=DELTH(I)
0109      FLUXS(I)=FLUX(I)
0110      GO TO 225
  
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      C      AVERAGES VALUES OVER ITERATIONS
0111      220      DELTHS(I)=0.5*(DELTHS(I)+DELTH(I))
0112              FLUXS(I)=WTS*FLUX3(I)+WT*FLUX(I)
0113              FLUX(I)=FLUXS(I)
0114      225      THETA(I)=THETAS(I)+DELTHS(I)
0115      140      CONTINUE
      C
      C      TEST PRINT
0116      IF(TTIME.LT.TCHECK) GO TO 250
0117      *WRITE(S,*) 'TIME=',TIME,' DELT=',DELTS,' COUNT=',ICOUNT
0118      *WRITE(S,320) (ISOIL(I),Z(I),THETA(I),H(I),COND(I),FLUX(I),
      I=1,NPTS)
0119      320      FORMAT(X,I1,X,F8.1,X,F5.4,X,F8.1,X,E10.4,X,E10.4)
0120      *WRITE(S,*) ' '
0121      *WRITE(S,*) 'CONTINUE ITERATIONS?'
0122      READ(S,*) BLANK
      C
      C      UPDATE THE ITERATION COUNTER AND REPEAT FLUX CALCULATION
0123      250      ICOUNT=ICOUNT+1
0124      IF(ICOUNT.GT.ITERAT) GO TO 230
0125      GO TO 201
      C
      C      TIME IS UPDATED
0126      230      DELT=DELTS
0127      TIME=TIME+DELT
      C
0128      *WRITE(S,*) 'NEW DELT=',DELT,' TIME=',TTIME
0129      *WRITE(S,*) 'ENTER NEXT TIME CHECK'
0130      IF(TTIME.GE.TCHECK) READ(S,*) TCHECK
      C
      C      CUMULATIVES ARE UPDATED
0131      IF(FSURF.GT.0.) RINFIL=RINFIL+FSURF*DELT
0132      IF(FSURF.LE.0.) EVAPO=EVAPO-FSURF*DELT
0133      IF(RAIN.GT.0.) RUNOFF=RUNOFF+(RAIN-FSURF)*DELT
0134      DRAIN=DRAIN+FLUX(NPT)*DELT
0135      DO 145 I=2,NPT
0136      SSINK(I)=SSINK(I)+SINK(I)*DELZ(I)*DELT
0137      145      TRANSP=TRANSP+SSINK(I)
      C
      C      RETURN TO TOP OF DAY LOOP
0138      GO TO 200
0139      299      CONTINUE
      C-----
      C
      C      FINOS FINAL SOIL WATER STORAGE FOR THE DAY AND CALCULATES
      C      THE WATER MASS BALANCE FOR PROFILE
0140      CUMWTR=0.
0141      DO 150 I=2,NPT
0142      150      CUMWTR=CUMWTR+THETA(I)*DELZ(I)
0143      BALANS=STORGE+RINFIL-CUMWTR-EVAPO-TRANSP-DRAIN
      C
      C      PRINTS DAILY SIMULATION RESULTS
0144      PRINT*, 'DAY:', IDAY
0145      PRINT*, 'WATER CONTENTS OF PROFILE'
0146      PRINT 300, (Z(I),THETA(I),I=2,NPT)
0147      300      FORMAT(X,F8.1,2X,F5.4)

```

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WTRFLX.FTN /TR:BLUCKS/WR

14:21:22

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```
0148      PRINT 310, STORGE,CUMWTR,RINFIL,RUNOFF,EVAPO,DRAIN,TRANSP,  
          1BALANS  
0149      310  FORMAT(/X,'INITIAL STORAGE',5X,F8.2/X,'FINAL STORAGE',7X,F8.2/  
          1X,'INFILTRATION',8X,F8.2/X,'RUNOFF',14X,F8.2/X,'EVAPORATION'  
          2,9X,F8.2/X,'DRAINAGE',12X,F8.2/X,'TRANSPIRATION',7X,F8.2/X  
          3,'MASS BALANCE ERROR',2X,F8.2)  
          C-----  
0150      199  CONTINUE  
0151      STOP  
0152      END
```

PROGRAM SECTIONS

NAME	SIZE	ATTRIBUTES
SCODE1	005556 1463	R*,I,CON,LCL
SPDATA	000206 67	R*,D,CON,LCL
SIDATA	000400 128	R*,D,CON,LCL
SVARS	003364 890	R*,D,CON,LCL
STEMPS	000016 7	R*,D,CON,LCL
.3333.	000204 66	R*,D,OVR,GBL

TOTAL SPACE ALLOCATED = 012172 2621

```

      C
      C      HYDRAULIC PROPERTY INTERPOLATION FUNCTION
0001      FUNCTION HYPINT(XPT,Y,N,J)
0002      DIMENSION Y(11,3)
0003      COMMON X(11,3)
      C      ASSUMES THAT X IS AN INCREASING SEQUENCE
0004      DO 1 I=1,N
0005      IF(XPT.LT.X(I,J)) GO TO 2
0006      1      CONTINUE
0007      I=N
0008      2      IO=I-1
0009      IF(IO.GT.0) GO TO 3
0010      IO=1
0011      I=IO+1
0012      3      SLOPE=(Y(I,J)-Y(IO,J))/(X(I,J)-X(IO,J))
0013      HYPINT=SLOPE*(XPT-X(IO,J))+Y(IO,J)
0014      RETURN
0015      END
  
```

PROGRAM SECTIONS

NAME	SIZE	ATTRIBUTES
3CODE1	000332 109	RW,I,CON,LCL
\$IDATA	000016 7	RW,D,CON,LCL
\$VARS	000010 4	RW,D,CON,LCL
\$STEMPS	000002 1	RW,D,CON,LCL
,\$SS\$,	000204 66	RW,D,UVR,G8L

TOTAL SPACE ALLOCATED = 000566 187

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```
      C
      C      PLANT SUBPROGRAM DEFINED HERE
0001      SUBROUTINE PLANT(SINK,THETA,Z,NPT,PT,T)
0002      DIMENSION SINK(NPT),THETA(NPT),Z(NPT)
0003      RETURN
0004      END
```

PROGRAM SECTIONS

NAME	SIZE	ATTRIBUTES
SCODE1	000104 34	RW,I,CON,LCL
SIDATA	000060 24	RW,O,CON,LCL

TOTAL SPACE ALLOCATED = 000164 58

NO FPP INSTRUCTIONS GENERATED

,LP:=NTRFLX

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