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Title: INTEGRATION OF COMPUTATIONAL MODELING FOR THE LOS ALAMOS NATIONAL LABORATORY LOW LEVEL RADIOACTIVE WASTE DISPOSAL PERFORMANCE ASSESSMENT

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INTEGRATION OF COMPUTATIONAL MODELING FOR THE LOS ALAMOS NATIONAL LABORATORY LOW LEVEL RADIOACTIVE WASTE DISPOSAL PERFORMANCE ASSESSMENT

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ABSTRACT

The preliminary Performance Assessment for the Los Alamos National Laboratory Low Level Radioactive Waste Disposal Facility at Area G is drawing to completion. The disposal site is located on the top of a finger mesa in the complex terrain of a semi-arid region which leads to considerable complications in the atmospheric and subsurface transport and in the requisite modeling. Infiltration and run-off are evaluated for the proposed disposal unit closure configuration. A new analytic source release model characterizes the disposal unit performance utilizing detailed source term characterization from the inventory data base. This analysis provides input to the subsurface modeling done by the sophisticated finite element transport code, FEHM, using realistic 2-D cross-sections of the geologic units stratigraphies and the disposal units. Subsurface transport via lateral flow to intermittant alluvial waters in adjacent canyons is evaluated in addition to the usual deep aquifer. Vapor phase flow has been treated separately and calibrated to field data for tritium migration. Atmospheric transport is based on Gaussian dispersion with a correction for complex canyon terrain evaluated from on-going 3-D atmospheric transport studies. Indications to date are that the Performance Assessment objectives are met for all migration pathways.

INTRODUCTION

The preliminary draft of the Performance Assessment (PA) for the Los Alamos National Laboratory (LANL) Low Level Radioactive Waste (LLRW) disposal facility at TA54, Area G, was presented to the US Department of Energy (USDOE) Peer Review Panel in August, 1995. Panel comments were received and are being incorporated into the complete draft for submittal to the USDOE during 1996. The on-going effort has involved a team of LANL technical staff and contractors including nine principle authors and more than a dozen additional contributors. This report summarizes the integration of the assessment teams, the technical data analyses, and the flow of the actual modeling effort.

The LANL disposal site at Area G is located on the top a narrow finger mesa averaging 300m wide, north to south, and about 30m above the adjacent canyons. The mesa is several kilometers long with the active disposal site occupying about 1 km west to east, and a proposed expansion area for future

projected waste occupying another half km to the west of the present site. The mesa is composed of Bandelier tuff, a porous volcanic residue in multiple stratigraphy layers of different volcanic ashes and flows[#].

The region is semi-arid, with about 14 in/year precipitation on average. The mesa top elevation is about 300m above the saturated aquifer. The adjacent canyons have perched alluvial systems, while vertical moisture profiles observed on most core samples beneath the mesa show a very low moisture content (1-2%). Hydraulic conductivities on core samples are consistent with negligible liquid phase flow through much of the vertical profile[#]. Vapor phase movement is expected to be significant for gas or vapor phase contaminants. The mesa top location, complex stratigraphy, and liquid and vapor phase movement make analyses of the subsurface transport a challenging modeling effort.

The release mechanisms expected from the site are summarized in a conceptual model in Fig.1. The liquid phase migration is indicated by the Darcy flux, q. Effort to date has focused on the downward movement to the aquifer, but movement may be laterally towards the mesa edge or even upward from the disposal unit if evaporation conditions prevail. These paths are currently under study. Biota translocation is projected to bring a small but steady transfer of contamination to the surface which is then available to the atmospheric path by resuspension and to canyon contamination and off-site exposure via the surface run-off path. Cliff retreat and surface erosion are predicted to uncover the remaining waste on the time scale of about 50,000 years and surface erosion contributes to increasing the biota translocation during erosion. These issues have been analyzed in the prelimnary draft PA. In this report, the discussion will focus on the groundwater and the atmospheric pathway assessments.

GROUNDWATER PATHWAY

A flow chart for the ground water pathway assessment is shown in Fig.2. Detailed numerical simulations followed the historical inventory and were used to generate scaling laws to apply to the future projected inventory. The inventory in the historical disposal units (pits and shafts which were active after the USDOE PA compliance order issuance in 1988) was screened to eliminate nuclides with half-lives less than five years. A second screen eliminated nuclides whose concentration in the waste was below the level that would be safe if conservatively ingested. i.e., the waste concentration leads to a concentration in leachate through the waste that would meet the PA dose objectives if ingested at the standard annual rate.

This screened inventory included 30 nuclides, with 15 being parents of decay chains. These 30 nuclides were sorted into four release categories defined by the release model parameters and the nuclide data base sorted on physical and chemical information in the 'waste code' information. This screened and categorized spreadsheet data base then contained concentrations (Ci/m3) and total historical inventory (Ci) information each sorted over 30 nuclides and over the four release form categories, rapid release, soil absorbed, concrete or sludge absorbed, and corrosion. This information is provided to the facility source release model.

Source Release Model

The source release model includes a compartment description of the waste packages and disposal unit, accounting for site parameters including waste type, waste form chemistry in Kds and elemental solubility limits by waste category, and infiltration and percolation characteristics. The average percolation rate through the facility of 4mm/yr was determined by detailed surface water balence simulations utilizing statistical precipitation data from the site#. Equilibration coefficients, Kd, and solubility limits, for waste forms in soil and in sludge, were derived from relevant literature values#. With this data base, the compartment release model provides an analytic solution for the time dependent release from the waste package provided it is not solubility limited. The elemental solubility limit must be applied to the sum of each nuclide contributing to the elemental concentration. Integration of this elemental concentration over the historical inventory of nuclides and multiple waste forms required the development of a numerical code. The output of this code is the time dependent efflux from the waste packages per nuclide (summed over release category), and this is distributed as a source term over each of the grid nodes within the disposal units in the 2-D unsaturated zone transport model.

Unsaturated Zone Transport

The unsaturated zone was modeled in detail using the FEHM code#, extensively applied and quality assured in Yucca mountain studies. A 2-D mesa top to ground water and canyon to canyon cross-section is modeled with full stratigraphy# and associated hydrologic transport propetries summarized as van Genutchen-Maulem fits#. Infiltration was varied to find the best overall fit to field data on vertical moisture profiles. The result is 1 mm/yr net infiltration

(Darcy flux), although some units fit better to a much lower and negligible vertical flux. On top of this, the 4mm/yr percolation derived for the disposal unit source term was added to the disturbed mesa surface areas represented by including five disposal units in a typical mesa cross-section. The resulting steady state moisture profiles for the mesa perturbed by disposal operations are shown in Fig.#, and the increased moisture content of the disturbed disposal units is clear. The horizontal bands near the elevation of the canyon floors is due to the different hydrologic transport properties in the stratigraphy layers.

Nuclide transport is imposed on this flow field, under the assumption that the long term behaviour is adequately described by the steady state flow solution. A source release term for Kd=0 in the waste (rapid release) was input to the unsaturated flow model for varying values of Kd in the Bandelier tuff. This showed that values of Kd > 0.3, did not traverse the unsaturated zone within the 10,000 years compliance period. Analysis of these results showed that only 17 of the 30 inventory nuclides needed to be modeled further based on a comparison of nuclide half lifes to the time for unsaturated zone transit.

The remaining 17 nuclides were modeled in detail through the unsaturated and saturated zones. An example is shown at successive times in Fig.# for uranium. The very slow progress for a small Kd = 1.8 is evident in the time scales. Only nuclides with Kd values approximately equal to zero in tuff, neptunium (with its non-secular equilibrium decay chain daughters, uranium and thorium) and carbon 14, reach the aquifer within the 10,000 year compliance period.

Transport to the saturated zone is conservatively approximated as transport to the top of the basalt layer, only about one third of the total 300m to the aquifer (this can be seen in Fig.# where the uranium contours 'flatten' or disappear at the basalt layer). Thus, no credit is taken for dilution or travel time throught the basalt (and deeper Puye) layers, because there is little or no site-specific data available for these layers. This likely incorporates a very large conservatism which may need to be revisited if this leads to PA objectives being exceeded considering the Legacy Waste (disposed of prior to 1988) to be estimated in the 1996 PA report.

Saturated Zone Transport

The 17 nuclides and decay chain products are then treated in the aquifer dilution model. Saturated zone transport occurs on a time scale very short compared to unsaturated movement at Area G and is treated analytically by

diluting the contaminant into the aquifer. Horizontal dispersion is negligible for the spatial scales of interest and the vertical dispersion is proportional to the dispersion length taken to be 0.1m. A simple boundary layer analysis leads to aquifer dilution factors of about 160 at the receptor well location 100m downstream. These concentrations drive the final dose assessment via the standard ground water dose pathways.

ATMOSPHERIC PATHWAY

The flow chart for the atmospheric transport assessment is shown in Fig. ?. The actual PA assessment was done completely on spreadsheets, with analyses and results from several supporting technical studies incorporated in two main areas. One, the gas phase source release models were analytic solutions to diffusive flux transport equations, which were compared to detailed numerical results of the diffusive transport profiles in time and in spacial distribution through the disposal unit. Mesa subsurface diffusion was calibrated to field data for tritium#. Two, the expected atmospheric dispersion was corrected for the complex terrain effects from a simple Gaussian estimate, based on site-specific data, on-going sophisticated modeling efforts and an assessment procedure to incorporate the complex terrain channeling effects into a predictive procedure for atmospheric dispersion.

Source Release Models

Atmospheric release source models were developed for the resuspension of surface contamination from the biota-erosion models, and for the diffusive release of gas or vapor phase contaminants, tritium, carbon 14, and radon. Site-specific resuspension values# based on standard EPA wind erosion estimates were used to convert surface contamination levels to an airborne source release term. Extensive field data on tritium surface effflux# and on core sample tritium concentrations# in the vicinity of the high level tritium disposal shafts was compared to 3-D simulations# to derive an effective diffusion coefficient, conservatively applied to all vapor or gas phase movement in the Bandelier tuff.

One-dimensional (vertical) and time dependent numerical simulations for gas phase release examined the concentration and flux profiles in space through the disposal unit. The transport equations differed primarily only in their source terms. Radon emanated from the radium in the disposal unit which included listed inventory and decay radium from the uranium series. Carbon 14 was

assumed released as a gas following the biodegradation of the estimated organic fraction of the total carbon inventory. The tritium release rate was determined empirically by comparison of the 3-D modeling to the field data.

Complex Terrain Dispersion

Data on wind flow and meteorologic conditions at Area G has been collected on six remote meteorological towers fielded in the Area G vicinity for over a year# to characterize the atmospheric transport in complex terrain at the site. Atmospheric dispersion is influenced by the complex terrain surrounding Area G, where the canyons can channel mesa top wind flow from several different directions leading to increased time averaged concentrations in the canyons upstream during the day or downstream during the night (estimated from Area G meteorological data to produce concentration increases by a factor of about 2.4 for the day or the night time cases). Reduced wind velocities in the canyons relative to the mesa top (observed to be about a factor of 1.7 for the canyons surrounding Area G) proportionately increases canyon contaminant concentrations. Recirculating flow in deep canyons (not apparently present near Area G) could additionally increase canyon concentrations.

These factors indicate that critical receptor locations (minimum atmospheric dispersion) will be in the adjacent canyons assuming that mesa top flow is entrained in those canyons. This assumption is supported by the site field data and by the simulations completed to date. An example of a 3-D simulation done for a normalized source at a nearby mesa top location is shown in Fig.#. The atmospheric dispersion and canyon channeling conditions are expected to be similar to that at Area G. The figure shows a morning time release which is carried to the north side canyon and then up canyon for a considerable distance before dispersing into the mesa top flow field. Once the airborne contaminant escapes the canyon flow and is entrained in the mesa top wind field, then the dispersion is greater than that in flat terrain due to the increased turbulence resulting from the 'rough surface' of the canyon systems.

Based on the site data, dispersion parameters were estimated for the up canyon and down canyon receptor locations, and combined with the release terms described above to generate the receptor location concentrations.

RESULTS

A set of standard dose pathways assumptions are used to convert the environmental concentrations, as described in the previous sections, to a dose rate. The dose results of the preliminary draft analyses (including the intruder scenarios not discussed in this paper) are summarized in Table I. The peak dose within the 10,000 year compliance time frame is shown for comparison to the PA dose objectives. In all cases, the PA dose objectives are met.

The peak dose for all time is also shown. These peak doses occur in the 80,000 to 600,000 year time frame depending upon the pathway and result from the ingrowth of daughter nuclides in decay chains especially the uranium series. The uncertainty associated with dose projections on these time scales is large.

Uncertainty associated with the 'mean dose estimates' summarized in Table I, is critical to interpreting the significance of the assessment and its implications for disposal operations and for supporting Waste Acceptance Criteria. The preliminary PA assessment included extensive discussion of the uncertainty associated with the various 'pieces' of the environmental transport and assessment and also a preliminary review of the overall sensitivity of final results to the models and their data input. The existing and on-going uncertainty and sensitivity analyses and their implications for the waste site operations are presently being pulled into a unified framework for presentation in the draft PA to the USDOE in 1996.

Table I A **Comparison of projected doses for the 10,000-year compliance period with DOE Performance Assessment (PA) Objectives**

Exposure Scenario	PA Objective (mrem)	Max. Dose (mrem) Total Inventory	Historic Pits	Historic Shafts	Future Pits	Future Shafts
Groundwater	4	0.08	n/a	n/a	n/a	n/a
Atmospheric	10	7.9	n/a	n/a	n/a	n/a
All Pathways Groundwater	25	6.8	n/a	n/a	n/a	n/a
All Pathways Surface Water	25	0.0001	n/a	n/a	n/a	n/a
Intruder Construction	500	n/a	1.6	0.8	3.8	1.0
Intruder Agriculture	100	n/a	22	8.2	53	11
Intruder Post-Drilling	100	na/	0.2	1.5	0.3	3.4

Table I B **Peak projected doses for time beyond 10,000 years**

Exposure Scenario	Peak Dose (mrem) Total Inventory	Historic Pits	Historic Shafts	Future Pits	Future Shafts
Groundwater	67	n/a	n/a	n/a	n/a
Atmospheric	500	n/a	n/a	n/a	n/a
All Pathways Groundwater	2.7	n/a	n/a	n/a	n/a
All Pathways Surface Water	35	n/a	n/a	n/a	n/a
Intruder Construction	n/a	24	5.5	55	13
Intruder Agriculture	n/a	310	69	690	160
Intruder Post-Drilling	na/	310	69	690	160

ACKNOWLEDGEMENTS

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REFERENCES

1.
2. NOT YET - no references are classified
3.

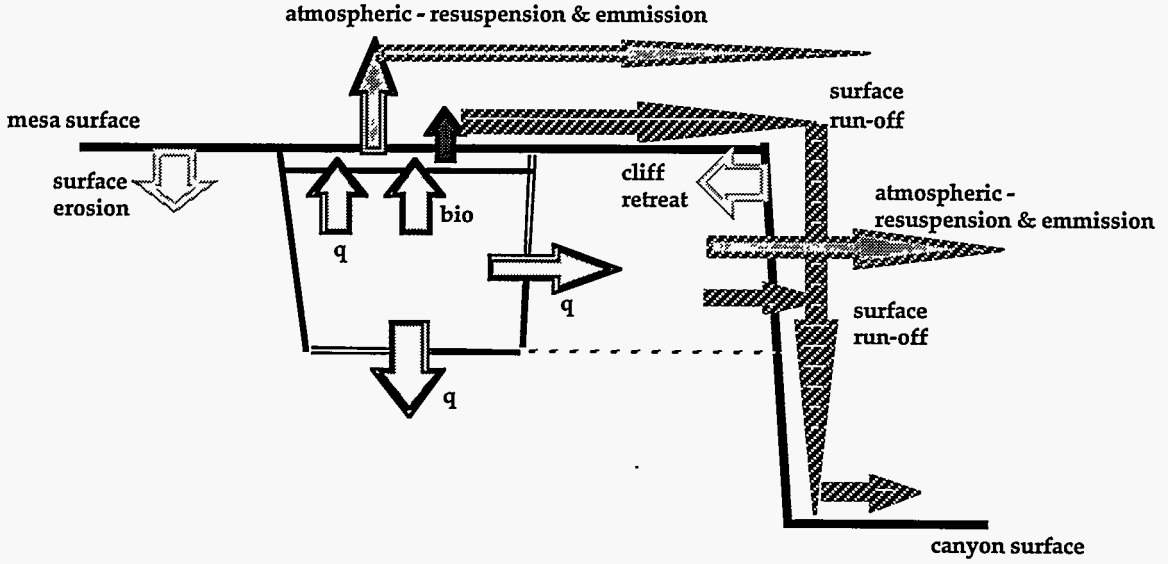


Fig.1 Conceptual model for source release mechanisms from the mesa top disposal site at Area G.

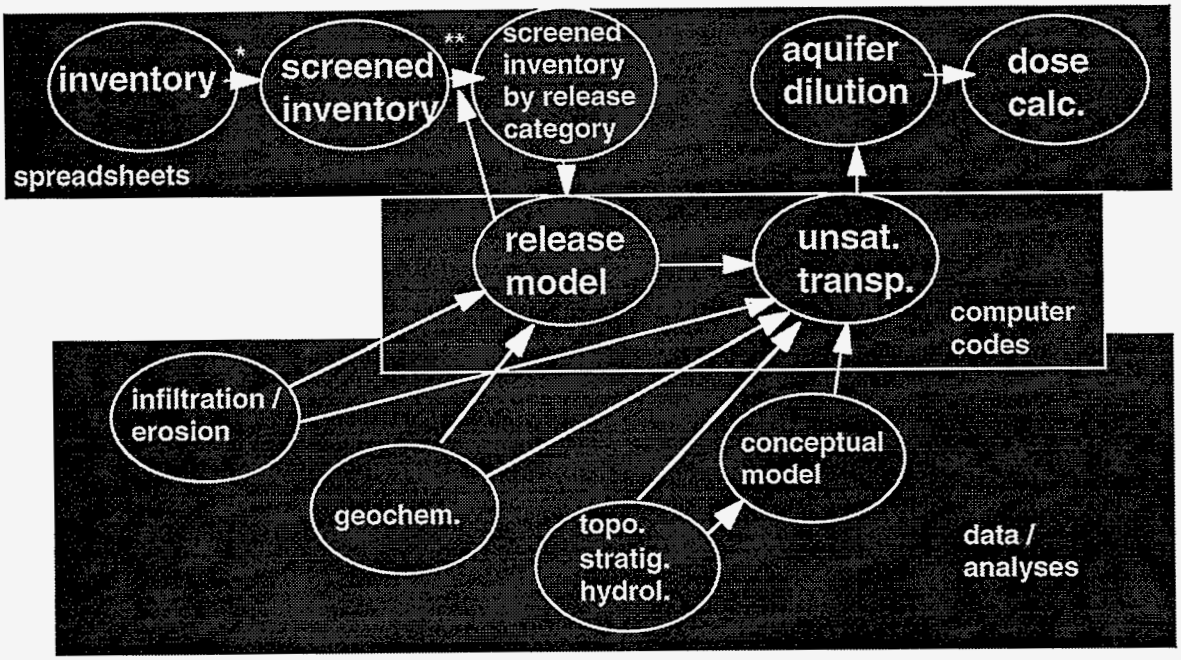


Fig. 2 Hydrogeologic transport calculations and data flow.

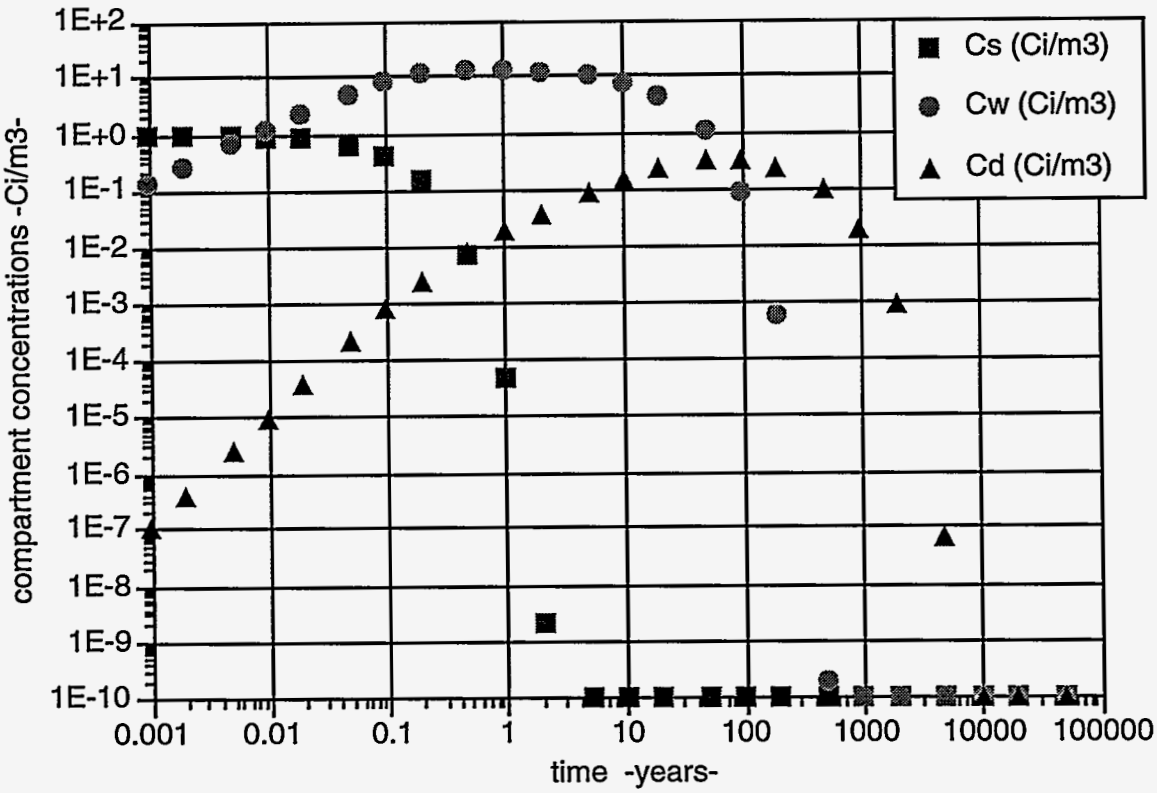


Fig.3 Compartment concentrations in the aqueous phase source release model for the base case conditions, with Kd = 0 in the waste form and in the disposal unit tuff, and with a rapid release characteristic time of 0.1 year. The model compartments, s, w, and d, are described in the text.

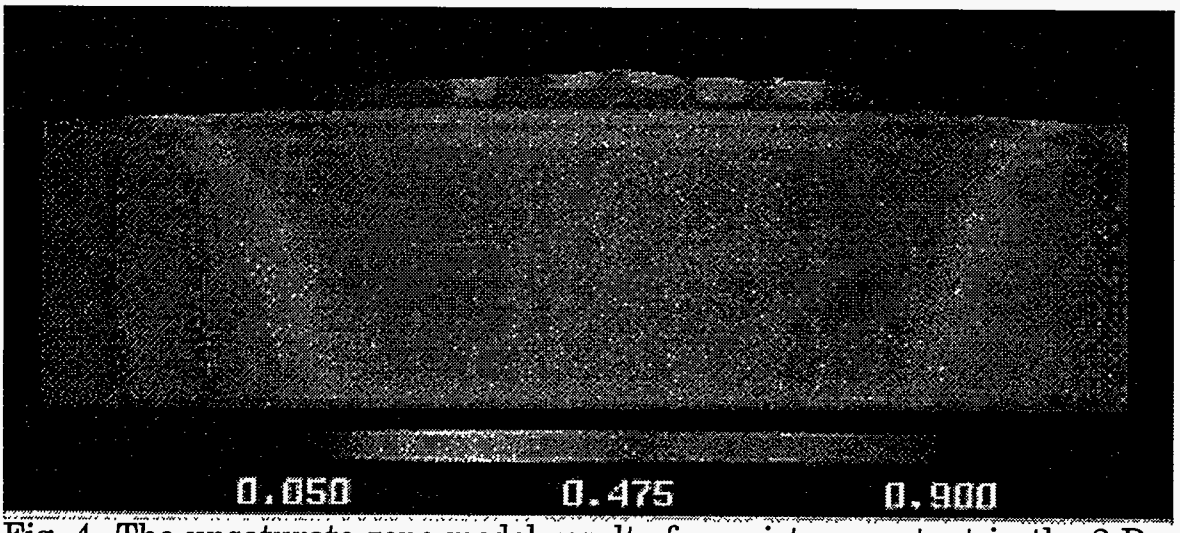
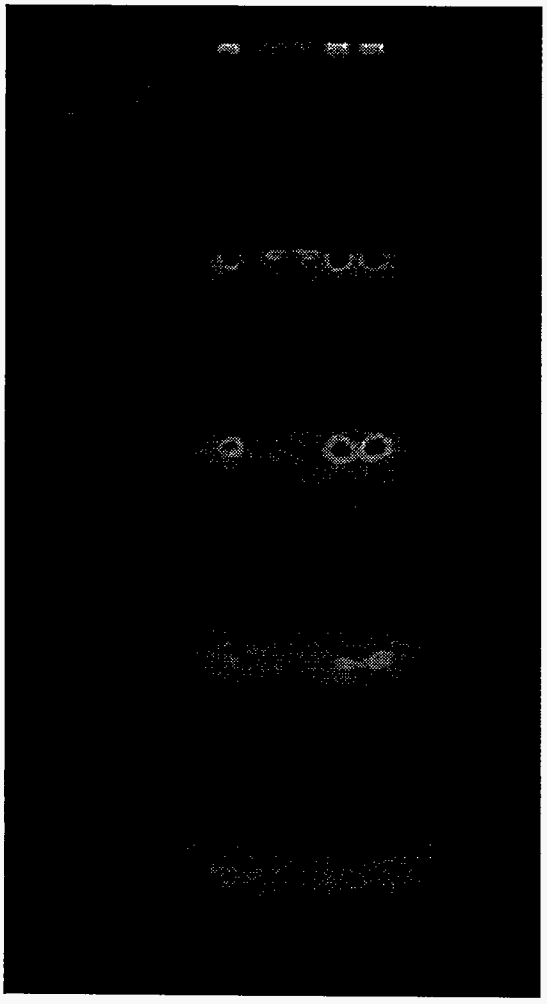


Fig. 4 The unsaturate zone model results for moisture content in the 2-D profile showing the mesa top and 5 representative disposal units. The moisture content is fixed at the canyon surfaces to the left and right of the mesa.



time = 5000 yrs

time = 20,000 yrs

time = 50,000 yrs

time = 80,000 yrs

time = 100,000 yrs

Fig. 5 Representative transport results for a species with Kd=1.8 in the Bandelier tuff (uranium) shown at several times.

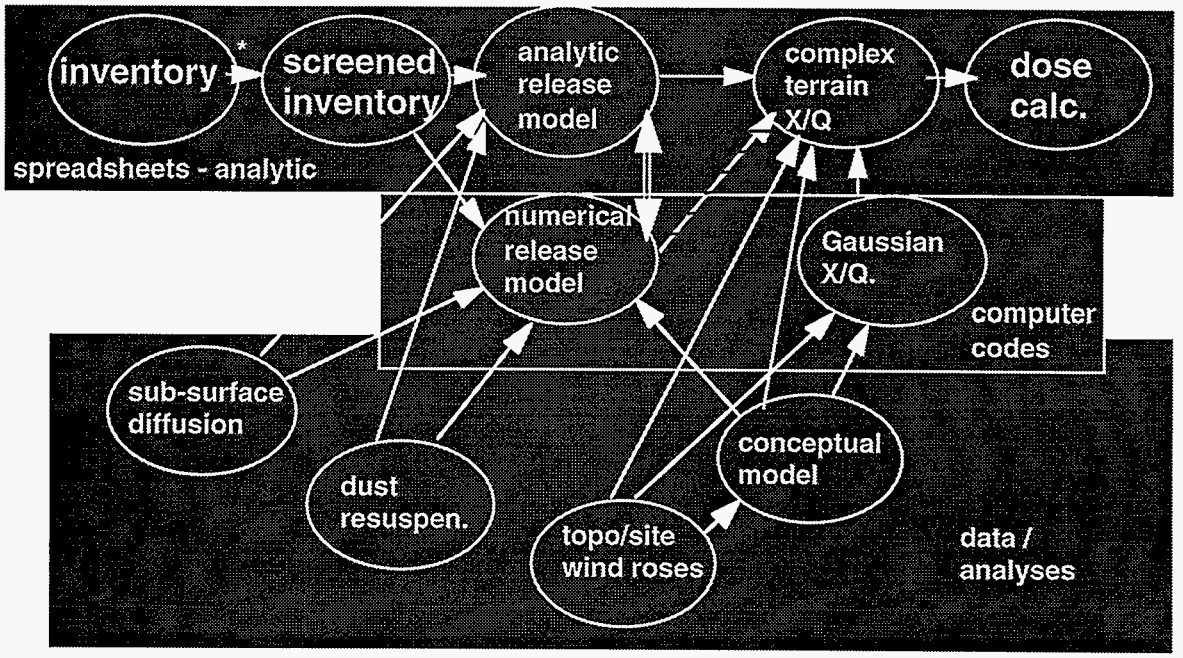


Fig. 6 Atmospheric transport and data flow for complex terrain dispersion.

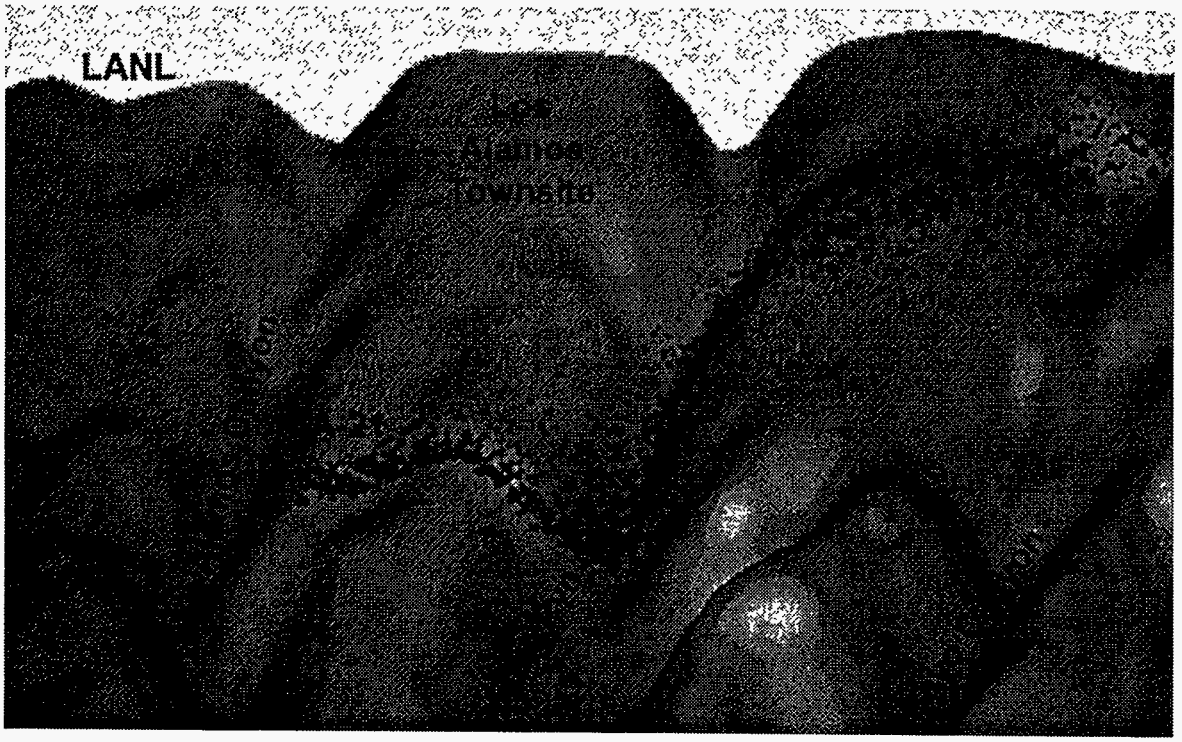


Fig. 7 Atmospheric disperson simulation in Los Alamos complex terrain (ref: J. Bossert #). A normalized source is located at TA-21. Similar results are expected from Area G, TA-54.