Evaluation of the Migration of Nitrogen Compounds from Septage/Sludge Land Disposal Facilities: Vadose Zone Predictive Computer Modeling

Summary Report

Prepared for:

New Mexico Environment Department Groundwater Quality Bureau

Prepared by:



A Duke Energy Company
1650 University Blvd. NE, Suite 300
Albuquerque, NM 87102
Telephone: (505) 246-1600

August 18, 2000

Evaluation of the Migration of Nitrogen Compounds from Septage/Sludge Land Disposal Facilities:

Vadose Zone Predictive Computer Modeling Summary Report

Table of Contents

Section	<u>on</u>	<u>Page</u>
LIST	OF FIGURES	4
	OF TABLES	6
1.0	INTRODUCTION AND OBJECTIVES	7
2.0	BACKGROUND	9
	2.1 Purpose of Study	
	2.2 Phase 1 Work	9
	2.2.1 Santa Fe Sludge Disposal Facility	10
	2.2.2 Taos Disposal Site	11
	2.3 Phase 2 Field Study Near Albuquerque	11
	2.4 Possible Transformation Processes for Nitrogen Compounds	
3.0	FIELD DATA SUMMARY	14
	3.1 Subsurface Soils	14
	3.1.1 Santa Fe Disposal Facility	14
	3.1.2 Taos Impoundment Basins	14
	3.1.3 Albuquerque Soil Amendment Facility	14
	3.2 Soil Physical Properties	14
	3.3 Model Calibration Data	17
4.0	CONCEPTUAL MODELS	
	4.1 General Conceptualization of Flow and Transport	
	4.2 Downward Seepage Rates	
	4.3 Loading Rates	
	4.4 Simplifying Assumptions and Their Potential Impacts	23
5.0	MATHEMATICAL FORMULATION OF CONCEPTUAL MODELS	
	5.1 Unsaturated Flow	
	5.1.1 Governing Equation	
	5.1.2 Functional Relationships Between Hydraulic Parameters	
	5.1.3 Nonlinearity of Richard's Equation	
	5.1.4 Calculation of Infiltration Rate Across an Impoundment Basin	Surface
	Layer26	
	5.2 Unsaturated Transport	
6.0	TECHNICAL APPROACH	
	6.1 Modeling Code	
	6.1.1 General Code Description	
	6.1.2 Data Requirements	
	6.1.3 Output Options	
	6.2 Vadose Zone Model Setup	29

	6.3 Input and Output Data	30
	6.4 Methods of Interpretation	31
7.0	MODEL CALIBRATION	32
	7.1 Data Assimilation	
	7.2 Santa Fe Clusters	
	7.3 Taos Clusters	33
	7.4 Albuquerque Clusters	
8.0	PREDICTIVE SIMULATIONS	
	8.1 Predictive Model Development	
•	8.2 Land Application of Sludge or Septage	
	8.4 Septage Impoundments	43
	8.5 Using Predictive Results for Site Evaluation	
	8.6 Predicting Downward Transport at Other Sites	43
9.0	SENSITIVITY ANALYSES	
	9.1 Perturbation Simulations	60
	9.1.1 Calibrated Models	60
	9.1.2 Predictive Model Sensitivity Runs	61
10.0	CONCLUSIONS	67
11.0	RECOMMENDATIONS	69
12.0	REFERENCES	70
APPI	ENDIX A	72

LIST OF FIGURES

<u>Figure</u>	<u>ge</u>
Figure 1. Observed and Computed Nitrate Concentrations in the Calibrated Model 1	for
Santa Fe Cluster 1.	35
Figure 2. Observed and Computed Nitrate Concentrations in the Calibrated Model 1 Santa Fe Cluster 2.	tor 36
Figure 3. Observed and Computed Nitrate Concentrations in the Calibrated Model for Ta	105
Cluster 1.	37
Figure 4. Observed and Computed Nitrate Concentrations in the Calibrated Model for Ta	ios
Cluster 2.	38
Figure 5. Observed and Computed Nitrate Concentrations in the Calibrated Model	for
Albuquerque Cluster 1.	39
Albuquerque Cluster 1. Figure 6. Observed and Computed Nitrate Concentrations in the Calibrated Model	for
Albuquerque Cluster 2.	40
Figure 7. Predicted Normalized Concentration of Nitrate, for Land Application on a Fir	1e-
Grained Surface Layer Overlying Coarse Sand Sediments.	45
Figure 8. Predicted Normalized Concentration of Nitrate, for Land Application on a Fir	1e-
Grained Surface Layer Overlying Medium Sand Sediments.	46
Figure 9. Predicted Normalized Concentration of Nitrate, for Land Application on a Fir	1e-
Grained Surface Layer Overlying Loamy Sand Sediments.	4/
Figure 10. Predicted Normalized Concentration of Nitrate, for Land Application on a Fir	1e-
Grained Surface Layer Overlying Sandy Loam Sediments.	48
Figure 11. Predicted Normalized Concentration of Nitrate, for Land Application on a Fir	1e-
Grained Surface Layer Overlying Silt Loam Sediments	49
Figure 12. Predicted Normalized Concentration of Nitrate, for Land Application on Coar	rse
Sand Sediments.	
Figure 13. Predicted Normalized Concentration of Nitrate, for Land Application on Media	3111 51
Figure 14. Predicted Normalized Concentration of Nitrate, for Land Application on Loan	111y
Sand Sediments. Figure 15. Predicted Normalized Concentration of Nitrate, for Land Application on San	22 My
Loam Sediments	53
Loam Segiments.	Silt
Figure 16. Predicted Normalized Concentration of Nitrate, for Land Application on St. Loam Sediments.	54
Figure 17. Predicted Normalized Concentration of Nitrate, for Septage Impoundment of	n a
Fine-Grained Surface Layer Overlying Coarse Sand Sediments.	55
Figure 18. Predicted Normalized Concentration of Nitrate, for Septage Impoundment of	n a
Fine-Grained Surface Layer Overlying Medium Sand Sediments	56
Figure 19. Predicted Normalized Concentration of Nitrate, for Septage Impoundment of	n a
Fine-Grained Surface Layer Overlying Loamy Sand Sediments	57
Figure 20. Predicted Normalized Concentration of Nitrate, for Septage Impoundment of	n a
Fine-Grained Surface Layer Overlying Sandy Loam Sediments	58
Figure 21. Predicted Normalized Concentration of Nitrate, for Septage Impoundment of	n a
Fine-Grained Surface Layer Overlying Silt Loam Sediments.	59

Figure 22.	Predicted	Nitrate	Concentrations	at	Santa	Fe	Cluster	2	Using	a	Five-I	Fold
Increas	se in the Ma	ain Sedin	nent Saturated H	[ydr	aulic C	ondi	activity.				••••••	. 64
Figure 23.	Predicted	Nitrate	Concentrations	at	Santa	Fe	Cluste	r 2	2 Usin	g '	Twice	the
Calibra	ated Model	Infiltrati	on Rate			•••••	•••••		•••••	••••	••••••	. 65
Figure 24.	Predicted	Nitrate	Concentrations	at 7	aos C	luste	r 1 Usi	ng	Half t	he	Calibra	ated
Model	Septage De	epth (ψ _s :	= 1.5 feet)			•••••	• • • • • • • • • • • • •			••••		. 66

LIST OF TABLES

<u>Table</u>		<u>Page</u>
Table 1.	Transformation Processes for Nitrogen Compounds	13
Table 2.	Physical Properties of Soils at the Santa Fe Sludge Disposal Facility	15
Table 3.	Physical Properties of Soils at the Taos Facility	16
Table 4.	Measured Moisture Contents and Nitrate Concentrations	18
Table 5.	Parameters Used in the Calibrated Models	34
Table 6.	Soil Hydraulic Parameters Used in the Predictive Simulations	42
Table 7.	Sensitivity Results for Land Application Predictions	63
Table 8.	Sensitivity Results for Septage Impoundment Predictions	63

1.0 INTRODUCTION AND OBJECTIVES

Downward and lateral migration of nitrogen compounds in the vadose zone from two types of sludge/septage disposal practices in New Mexico (NM) was simulated using numerical models. The two types of disposal consisted of land application of sludge or septage and discharge of septage into surface impoundments. This work was performed by Duke Engineering and Services (DE&S) (the authors) on behalf of the Ground Water Quality Bureau (GWQB) of the New Mexico Environment Department (NMED). The simulations were intended to support NMED's regulation of sludge/septage disposal facilities in the state. In addition to calibrating separate models for each of three sites at which nitrogen species concentration data and other information had been collected, predictive models were developed. The predictive models accounted for different scenarios, each of which was generally representative of conditions that could be observed at a site where sludge/septage disposal is proposed. To a large extent, the predictive models were patterned after the three sites at which extensive soil sampling and analysis for nitrogen contaminants had been performed.

The subsurface flow models developed under the project simulate variably saturated (saturated-unsaturated) flow and concomitant transport of nitrogen compounds. All of the simulations were based on the transport of a single species, nitrate, and were performed with the computer code known as VS2DT (Healy, 1990; Hsieh et al., 2000).

Findings from this project were intended to support the assessment and regulation of sludge/septage disposal sites in New Mexico. Accordingly, one of the goals of this study was to provide relatively generic findings regarding vadose zone transport of nitrogen compounds, rather than focusing exclusively on site-specific results. In keeping with such an approach, two sets of the predictive simulations were based on domains that consisted of two separate materials: (1) a surface layer consisting of relatively fine-grained soils and (2) a deeper, more coarse-grained material. Each of these materials was assumed to be homogenous. In a third set of predictive model runs, a single uniform material was applied to the entire simulation domain.

The results of the variably saturated flow and transport modeling are presented in this final report. The following text provides (1) descriptions of the sites modeled for calibration purposes; (2) descriptions of the conditions adopted for each generic, predictive simulation; (3) a detailed discussion of the modeling approach and model input parameters; (4) calibration steps with the model(s) and calibration results; and (5) graphical and textual explanations of simulation results. This report also summarizes study results regarding combinations of septage/sludge loading rates and generic site conditions that are protective of groundwater quality.

The objectives of this project were threefold:

(1) Develop and calibrate vadose zone flow and transport models for nitrate transport at three separate sites in New Mexico;

- (2) Develop generic models for predicting the transport of nitrogen below sludge and septage facilities;
- (3) On the basis of modeling results, develop conclusions and recommendations that will assist the NMED in assessing and regulating sludge/septage disposal facilities in New Mexico.

2.0 BACKGROUND

2.1 Purpose of Study

During the summer of 1999, the NMED began a project focused on assessing the downward migration of nitrogen compounds in vadose zone soils resulting from both land application of sludge or septage and surface impoundment of septage. This project, funded by the U.S. Environmental Protection Agency (EPA), was inspired by NMED's need to better understand the types of site conditions within the state that would be conducive to surface disposal of sewage waste while still being protective of underlying groundwater. The soils below the waste are commonly unlined, leaving a potential for nitrogen species and other wastewater constituents to be transported downward within the underlying vadose zone. NMED has been concerned about this potential migration and its potential detrimental impact on public health, the environment, and groundwater quality, despite the fact that vadose zones in arid New Mexico can be quite thick, sometimes approaching depths of 400 feet or more.

During Phase 1 of this project, the GWQB and one of its contractors collected soil samples from a septage impoundment facility in Taos, NM, and the municipal sludge disposal facility in the City of Santa Fe, NM. In addition to analysis for nitrogen compounds, the soil samples, collected up to a depth of 30 feet below ground surface, were analyzed for a variety of chemical and physical parameters.

During Phase 2 of the project, additional field work was performed to characterize nitrogen migration at the City of Albuquerque Soil Amendment Facility, located approximately 10 miles west of Albuquerque. The variably saturated flow and transport modeling described in this work plan was also part of the Phase 2 activities.

2.2 Phase 1 Work

The Phase 1 study was funded by EPA, managed by the NMED Ground Water Quality Bureau (GWQB), and conducted by John Shomaker and Associates, Inc. (JSAI) (Finch, 1999). The Phase 1 activities consisted of the following:

- (1) Reviewing existing site-specific information and performing a literature search of septage disposal practices;
- (2) Collecting climatic data for the Taos and Santa Fe sites in preparation for predictive computer modeling; and
- (3) Performing borehole investigation studies at the Taos and Santa Fe disposal facilities.

At each of the disposal sites studied under Phase 1 of the project, a cluster of three borings was advanced at each of three locations to measure both soil properties and nitrogen species concentrations with depth. Two of the cluster locations at a disposal site were placed within cells or basins that were actively being used for waste disposal; these cluster sites were referred to as "impacted locations." The third borehole cluster was placed at a locale

representative of background conditions that were not impacted by waste disposal practices; this latter cluster site was referred to as the "background location."

2.2.1 Santa Fe Sludge Disposal Facility

Sludge disposal at the Santa Fe site is accomplished by injecting treated sludge approximately 1 foot below ground surface into one of four land application areas. The disposal facility has been in operation since 1984. Finch (1999) presents graphs showing monthly quantities of combined sludge application to all four areas from the mid-1980s to late 1990s. Average disposal rates and concentrations of various nitrogen species are also reported in tabular form.

Monitor wells near the Santa Fe disposal facility have shown elevated nitrate concentrations, sometimes reaching levels as high as 13 mg/L nitrate as nitrogen. However, some of these elevated nitrate concentrations are thought by some investigators to result from seepage of effluent discharged into the Santa Fe River from the nearby Santa Fe Waste Water Treatment Plant, rather than from downward seepage of dissolved nitrate below the sludge application areas.

Drilling at the three borehole clusters at the Santa Fe site was conducted in June of 1999. At each cluster, a sandy silt was encountered in the uppermost 5 feet of soils, below which the sediments generally consisted of sand and gravel. Soil samples were collected from each cluster at depths of 3, 5, 10, 15, 20, and 30 feet below ground surface. The samples were sent to laboratories both for analysis of their physical properties and for the measurement of concentrations of total Kjeldahl nitrogen (TKN), nitrate as nitrogen, ammonia as nitrogen, chloride, and total organic carbon. Physical properties measured included bulk density, particle size distribution, porosity, hydraulic conductivity, and moisture content. The nitrogen composition of sludge prior to disposal at the impacted sites was available from analyses performed by the City of Santa Fe.

Measured ammonia concentrations at the Santa Fe site indicated that most of it either had volatilized or was converted into nitrate within the uppermost 3 feet of sediment below the application areas. Nitrate concentrations at the impacted locations were observed to stay relatively high in the top 5 feet of sediment, but then gradually began decreasing with increasing depth. Down to a depth of 15 feet, nitrate below the impacted locations occurred at levels above the observed background concentration for this constituent in the background cluster. Soil moisture below the impacted areas was greater than background measures of this parameter down to a depth of 20 feet. This latter observation suggested that the sludge that was being disposed of at the site contained residual moisture.

Another observation from the Santa Fe site investigation was that TKN concentrations below the impacted areas were relatively elevated between the 0- and 10-foot depths, but then hovered near background levels for this constituent between the 10- and 30-foot depths. Organic carbon contents beneath the impacted areas were usually elevated above background values over the full 30 feet of borings. The fact that these latter measures of carbon content

do appear to remain elevated may have some bearing on possible nitrate transformation processes occurring beneath the application areas.

2.2.2 Taos Disposal Site

The Taos disposal site has been operating since 1987. The facility operator discharges septage to unlined, infiltration/evaporation disposal cells. The total area covered by the cells is about 4 acres. The facility operator rotates between cells for the purpose of managing evaporative and infiltration processes. Since the facility began operation, some cells have been covered, and new ones have been developed.

Detailed data regarding the volumes of septage disposed of in specific cells at the Taos site are not available. Finch (1999) provides estimates of the range of annual disposal volumes, and also estimates the average concentration of nitrogen species in the septage using information provided in EPA's Guide to Septage Treatment and Disposal (1994).

Drilling and sediment sampling at the background and impacted cluster locations at the Taos disposal also took place in June of 1999. The sampling depths and sampling analyses were identical to those used at the Santa Fe disposal facility. As at the Santa Fe site, a finergrained soil, described by Finch (1999) as a clay loam to sandy silt, was found in the uppermost 5 feet of materials below the septage basins. Below the upper 5 feet, the sediments were generally characterized as sand and gravels with some clay and silt stringers occurring between a depth of 20 to 30 feet.

Soil moisture content in the upper 5 feet of sediments beneath the impacted locations and at the background location were elevated in comparison to soil moisture content in samples collected at greater depth. This phenomenon, which was quite obviously correlated with finer-grained sediments at the shallower depth, was most likely attributed to the different soil moisture characteristic curves characterizing shallower and deeper materials. As at the Santa Fe site, nearly all of the ammonia was observed in the uppermost 5 feet of soils below the septage cells, again suggesting that, below this depth, most of the ammonia in the shallow soils has been either volatilized or converted into nitrate.

Nitrate concentrations below the septage disposal cells were of the same general magnitude observed at the Santa Fe site, although slightly lower. A relatively steep drop-off in nitrate concentration was observed at one of the Taos impacted locations between the 5-foot and 20-foot depths, whereas the decrease in nitrate concentration with depth beneath the other disposal location is relatively subtle.

2.3 Phase 2 Field Study Near Albuquerque

The Albuquerque Soil Amendment Facility (ASAF) is located about 10 miles west-northwest of downtown Albuquerque, north of Interstate 70 on the West Mesa. The site began operation in 1988. Sludge is trucked to the site from the Albuquerque Sewage Treatment Plant and spread evenly on the land surface in any of 14 different spreading fields, where it is

subsequently tilled into the soil. The rates at which sludge is applied to the land vary both spatially and with time.

The activities associated with investigation of the Albuquerque disposal facility were similar to those discussed previously for the Phase 1 field sites. However, the drilling and sampling investigation at the Albuquerque site was conducted to a depth of 70 feet (Finch, 2000) rather than the 30-foot investigation depth applied at the other sites. As with the Phase 1 studies, two impacted location clusters were investigated at the ASAF. These were located in Fields 2 and 4.

The ASAF was chosen for study because the site's hydrogeologic setting is typical of sludge and septage disposal sites around New Mexico and the southwest (Finch, 2000). The site is covered with soil consisting of silt loam (SCS, 1977). The uppermost 8 to 12 feet soils at both impacted locations are described as consisting of silty sand, with the basal portion of this uppermost layer showing some calcification. Below the upper layer to a depth of 70 feet, the sediments are described as gravelly sand and sand (Finch, 2000). Thus the vertical soil profile at the Albuquerque site is similar to those observed at the Santa Fe and Taos facilities in that a surface layer of relatively fine-grained material overlies more coarse sediments. The depth to groundwater at the ASAF is approximately 920 feet.

Observation of various nitrogen species concentrations in the sediment profile at ASAF shows that nitrogen processes occurring here are similar to those observed at the Phase 1 sites. That is, nearly all of the ammonia is observed in the uppermost 5 feet, indicating that most of it, after application of the sludge, is either lost to volatilization or converted into nitrate.

2.4 Possible Transformation Processes for Nitrogen Compounds

During the Phase 1 investigations, efforts were made to better understand the various nitrogen forms that could exist in unsaturated porous media. The NMED recognized that development of such an understanding would help to interpret field data collected at the Santa Fe and Taos sites, and to determine which nitrogen transformation processes, if any, would need to be included in the predictive simulations.

As discussed in Finch (1999), there are six possible transformation processes that nitrogen can undergo in natural environments. All six are listed in Table 1 and are summarized in the following text. The likelihood that each specific process could be significant at the three sites upon which model calibration was based is also discussed.

Table 1. Transformation Processes for Nitrogen Compounds

Process	Result
Fixation	Conversion of nitrous oxide to ammonia or nitrate (nitrogen source process)
Ammonification	Biological conversion of organic nitrogen to ammonia (nitrogen source process)
Volatilization	Release of ammonia to the atmosphere
Synthesis	Uptake of nitrogen by biological processes
Nitrification	Biological oxidation of ammonia to nitrate
Denitrification	Conversion of nitrate to nitrogen gas

Most organic compounds of interest at sludge and septage disposal sites are derivatives of ammonia. Ammonia is first created by the degradation of organic nitrogen, a process referred to as ammonification. In the unsaturated zone, ammonia may be lost from the aqueous phase by being (1) adsorbed onto soil particles, (2) retained by the soil via cation exchange, or (3) released to the atmosphere via volatilization. Though all three of these latter transformation process appear to be viable at sludge and septage disposal sites, Finch (1999) presents information that indicates volatilization is likely to be the most prevalent of the three. Another transformation process for ammonia is nitrification, in which ammonia is converted into nitrate. This process is likely very prevalent in the unsaturated zone beneath sludge and septage disposal facilities. Quoting others, Finch (1999) reports that first order nitrification rates range from 1.11 day⁻¹ to 0.05 day⁻¹. These rates are the equivalent of half-lives for ammonia of 0.623 and 13.86 days, respectively.

Denitrification refers to the biological or chemical reduction of nitrate to molecular nitrogen gas or nitrous oxide. Finch (1999) states that anaerobic conditions are conducive to denitrification and Hantzshce and Finnemore (1992) report an additional three soil conditions are most favorable to this transformation process: (1) an abundance of organic carbon substrate, (2) high soil moisture content, and (3) high soil pH. Though none of these conditions appear to be significantly present at the Santa Fe and Taos disposal sites, Finch (1999) states that the range for first order denitrification rates is 0.1 day⁻¹ for sandy soils to 1.5 day⁻¹ for organic soils. These latter rates correspond to respective half-lives of 6.93 and 0.462 days.

3.0 FIELD DATA SUMMARY

3.1 Subsurface Soils

The soil types located below each of the disposal facilities were described in boring logs, characterized with respect to grain-size distribution, and further characterized through the measurement of such properties as porosity and saturated hydraulic conductivity. The following paragraphs provide descriptions of soils encountered at the field sites and data regarding their physical characteristics. In addition, the field data used to calibrate the flow and transport models for each impacted location are presented.

3.1.1 Santa Fe Disposal Facility

The uppermost 3 to 5 feet of sediments at the Santa Fe facility consist primarily slightly moist sandy silt, with some traces of organic matter. Below these shallow soils to a total sampling depth of 30 feet, the sediments consist almost exclusively of gravelly sand and sandy gravel. On the basis of descriptions given in well logs for both impacted locations at the Santa Fe site, the saturated hydraulic conductivity of the materials located between 5 and 30 feet deep is expected to be relatively large.

3.1.2 Taos Impoundment Basins

The uppermost 7 to 8 feet of sediments at the Taos facility consist of silty sands. The predominant soil type below these shallow materials to a depth of 20 feet is gravelly sand. Between the 20- and 30-foot depths, the soils are typically described as gravelly sand with stringers of silty clay and silty sand. On the basis of descriptions given in well logs for both impacted locations at the Taos site, the saturated hydraulic conductivity of the materials located between 8 and 30 feet deep is expected to be relatively large.

3.1.3 Albuquerque Soil Amendment Facility

The uppermost 7 to 12 feet of sediments at the Albuquerque facility consist of silty sands, the basal portion of which appears to be calcified. Between the 12- and 70-foot depths, the sediments are described as gravelly sands and sands. On the basis of descriptions given in well logs for both impacted locations at the Albuquerque site, the saturated hydraulic conductivity of the materials located between 12 and 70 feet deep is expected to be relatively large.

3.2 Soil Physical Properties

Measured physical properties of soils (porosity, saturated hydraulic conductivity, and dry bulk density) at the impacted location clusters at the Santa Fe and Taos field study sites are presented in Tables 2 and 3, respectively. None of these physical properties were measured at the ASAF. Consequently, estimates had to made for them during calibration of the flow and transport models developed for the Albuquerque site.

Table 2. Physical Properties of Soils at the Santa Fe Sludge Disposal Facility

Sample Depth (feet)	Porosity (unitless)	Saturated Hydraulic Conductivity (ft/day)	Saturated Hydraulic Conductivity (cm/sec)	Dry Bulk Density (lb/ft³)	Dry Bulk Density (kg/L)
Impacted 1	Location 1				
3	0.43			88	1.41
5	0.51	1.56E-02	5.52E-06	87.9	1.41
10	0.31			100.4	1.61
15	0.26	5.07E-01	1.79E-04	105.5	1.69
20	0.26			113.6	1.82
· 30	0.32			108.3	1.73
	Location 2		·	04.1	1.61
3	0.41			94.1	1.51
5	0.43	1.43E-01	5.04E-05	93.1	1.49
10	0.35			111.9	1.79
15	0.25			112.3	1.80
20	0.28			122.2	1.96
30	0.31			117.9	1.89

Table 3. Physical Properties of Soils at the Taos Facility

Sample Depth (feet)	Porosity (unitless)	Saturated Hydraulic Conductivity (ft/day)	Saturated Hydraulic Conductivity (cm/sec)	Dry Bulk Density (lb/ft ³)	Dry Bulk Density (kg/L)
Impacted I	Location 1				
3	0.42			87.4	1.40
5	0.47	3.69E-01	1.30E-04	77.3	1.24
10	0.33			106.9	1.71
15	0.27			112.6	1.80
20	0.42			92.2	1.48
30	0.36	2.68E-01	9.47E-05	103	1.65
<u>.</u>	Location 2			70.0	1.26
3	0.41			78.8	1.26
5	0.43	2.76E-02	9.72E-06	74.6	1.19
10	0.35			107.4	1.72
15	0.25	3.74E-01	1.32E-04	119.2	1.91
20	0.28			117.9	1.89
30	0.31			109.2	1.75

3.3 Model Calibration Data

Upon reviewing the field investigation reports (Finch, 1999; Finch, 2000), DE&S determined that the data that would be most useful for model calibration work were measured nitrate concentrations. It was decided that moisture contents would be helpful in developing input properties for the flow portions of the site-specific simulations, but that they would not be useful as specific calibration targets.

Because the nitrate concentrations were reported as soil concentrations in units of $\mu g/g$, yet the VS2DT calculates aqueous-phase concentrations using units of mass per unit volume, it was necessary to calculate the equivalent aqueous-phase concentrations using the equation

$$C_{w} = C_{t} \left(\frac{\varrho_{b}}{\theta} \right) \times \frac{1000 \text{ cm}^{3}}{\text{Liter}}$$
 (1)

where $C_w = \text{water concentration } (\mu g/L)$,

 C_t = soil concentration ($\mu g/g$),

 ρ_b = soil dry bulk density (g/cm³), and

 θ = volumetric moisture content (unitless).

Equation (1) is based on the assumptions that nitrate does not sorb to soil material and that it does not volatilize to nitrogen gas via denitrification.

Measured moisture contents and soil nitrate concentrations (in units of $\mu g/g$) at selected sampling depths for the Santa Fe, Taos, and Albuquerque sites are presented in Table 4. First attempts at determining equivalent aqueous-phase concentrations at each depth for the Santa Fe and Taos facilities using Equation (1) and the corresponding bulk densities and moisture contents shown in Tables 2 and 3 indicated that the trends observed in soil concentration with depth were not always the same as those occurring in soil moisture. That is, a decline in soil concentration from one depth to another did not actually coincide with an increase in aqueous-phase concentration, and vice versa.

There are several possible explanations for these observations. For example, it may be that the aqueous-phase concentrations are relatively good indicators of relative nitrate levels in soil moisture, and that soil concentrations alone are not capable of catching what occurs in the aqueous phase. Alternatively, it is possible that the values for θ and ρ_b used in Equation (1), and taken from Tables 2 through 4, do not necessarily correspond with the measured soil concentrations. Nonetheless, because the flow and transport simulations are based on flow of and transport within soil moisture, the models must be developed using computed aqueous-phase concentrations.

Table 4. Measured Moisture Contents and Nitrate Concentrations

_			· · · · · ·	1	Г	T	_	Γ.	Г	Г	Г		_			_		_	Г			_	_	Γ.		_
_	itrate ation	(mg/L)		55250.0	46277.8	31402.8	75.6	151.1	75.6	<47.2	<47.2	<47.2	<47.2	<47.2		93500.0	12037.3	2149.9	142.5	53.4	28.9	<47.2	<47.2	<47.2	<47.2	<47.2
nendment Facility	Aqueous Nitrate Concentration	(ng/L)	ocation 1	5.53E+07	4.63E+07	3.14E+07	7.56E+04	1.51E+05	7.56E+04	4.72E+04	4.72E+04	4.72E+04	4.72E+04	4.72E+04	ocation 2	8.80E+07	7.87E+06	8.56E+06	2.84E+05	1.13E+05	1.09E+05	4.72E+04	4.72E+04	4.72E+04	4.72E+04	4.72E+04
Albuquerque Soil Amendment Facility	Soil Nitrate Concentration	(g/gn)	Impacted Location 1	1170	086	599	9.1	3.2	1.6	∀	V	⊽		[>	Impacted Location 2	385	649	305	6.4	2.4	1.3	i>	! >			₽
Al	Moisture Content	(unitless)		0.007	0.132	0.057	0.036	0.034	0.019	0.018	0.021	0.028	0.033	0.013		0.007	0.132	0.057	0.036	0.034	610.0	0.018	0.021	0.028	0.033	0.013
	rate ion	(mg/L)			104.9	102.0	381.9	498.3	24.4	32.6							1562.9	441.7	259.5	2404.7	8.65	351.8				
sal Site	Aqueous Nitrate Concentration	(ng/L)	cation 1		1.05E+05	1.02E+05	3.82E+05	4.98E+05	2.44E+04	3.26E+04					cation 2		1.56E+06	4.42E+05	2.60E+05	2.40E+06	5.98E+04	3.52E+05				
Taos Disposal Site	Soil Nitrate Concentration	(g/gn)	Impacted Location 1		15.3	16.9	23	13	2.1	1.6					Impacted Location 2		238	58.1	7.4	58	2.6	30				
	Moisture Content	(unitless)			0.204	0.205	0.103	0.047	0.127	0.081							0.192	0.157	0.049	0.046	0.082	0.149				
	trate tion	(mg/L)			3054.4	4098.9	4712.1	0.9991	1202.2	1120.4							5416.0	5277.4	2936.3	1463.6	642.1	163.9				
isposal Facility	Aqueous Nitrate Concentration	(ng/L)	ocation 1		3.05E+06	4.10E+06	4.71E+06	1.67E+06	1.20E+06	1.12E+06					ocation 2		5.42E+06	5.28E+06	2.94E+06	1.46E+06	6.42E+05	1.64E+05				
Santa Fe Sludge Disposal Facility	Soil Nitrate Concentration	(B/Bn)	Impacted Location		410	545	264	8.06	46.3	47.2					Impacted Location 2		259	248	123	44.8	31.2	5.3				
5	Moisture Content	(unitless)			0.189	0.187	60'0	0.092	0.07	0.073							0.072	0.07	0.075	0.055	0.095	0.061				
	Sample Depth	(feet)		0	3	5	10	15	70	30	40	95	09	70		0	3	5	10	15	20	30	40	20	09	70

To develop somewhat less erratic data for equivalent aqueous-phase concentrations at the Santa Fe and Taos sites, a scheme was formulated in which a representative set of soil properties was developed for each of two depth intervals. At each site, the average moisture content and average bulk density was determined using, in one case, the values for these properties at the 3- and 5-foot sampling depths, and in the second case, the 10- through 30-foot sampling depths. The resulting shallow soil averages were used to compute aqueous-phase concentrations at the 3- and 5-foot depths, and the deeper soil equivalents were used to compute all other aqueous-phase nitrate concentrations. The rationale for applying this scheme was that the porosities (see Tables 2 and 3) and moisture contents (see Table 4) at the two shallowest sampling depths appeared to be very similar to each other, and differed markedly from equivalent values for these parameters at the greater depths.

Unlike the Santa Fe and Taos sites, the measured moisture contents at the Albuquerque facility were more uniform in value, with no distinct differences appearing in θ values between shallower soils and deeper ones. Consequently, the equivalent aqueous-phase nitrate concentrations at the Albuquerque site were computed using the average of all measured moisture contents and a uniform estimated bulk density of 1.7 kg/L.

4.0 CONCEPTUAL MODELS

4.1 General Conceptualization of Flow and Transport

Subsurface flow at all three of the field sites is conceptualized as being dominated by downward unsaturated flow of soil moisture. Though air also exists in the unsaturated zone, it is assumed that it has little to no effect on the downward movement of moisture. This assumption is tantamount to saying that the air within the unsaturated pores exists everywhere and at all times at atmospheric pressure, and cannot be at pressures greater than atmospheric. Accordingly, flow is considered to obey Richard's equation (Rawls et al., 1992), in which it is assumed that water movement is controlled only by processes occurring in the water itself. This assumption of "single phase flow" is generally adequate for most analyses of field conditions.

Because downward movement of moisture appears to be predominant, significant lateral flow of moisture is expected to occur only along the edges of the waste disposal areas. At the Phase 1 field sites, the sample cluster sites were located essentially in the middle of disposal areas, thus making it likely that the nitrate concentrations and other properties of soils measured at specific depths were primarily reflective of one-dimensional, vertically downward flow and transport. Assuming that waste loading rates to the subsurface are distributed uniformly over a site, the deepest penetration of contaminants would, accordingly, be expected near the center of the site. That is, lateral spreading of contaminants at the site center would not be expected to slow the rate of penetration of a contaminant front as might be anticipated along the site edge.

The field studies at the Santa Fe and Taos sites (Finch, 1999) and the Albuquerque facility (Finch, 2000) indicated that a significant portion of the nitrogen loaded to the subsurface in the form of ammonia was typically lost to volatilization within the uppermost 3 to 5 feet of sediments. On the basis of these studies, volatilization losses on the order of 25% of the nitrogen mass applied appeared to be viable, and the transport of aqueous-phase ammonia was believed to be insignificant.

The field investigations (Finch, 1999; 2000) also indicated that the non-volatilized portion of nitrogen loaded to the subsurface was converted to nitrate via nitrification. Thus, it appeared that nitrate was the only nitrogen species that was undergoing significant downward transport. Though the data collected at the field sites could not be directly used to estimate long-term, steady loading rates for nitrate, these rates could be backed out through calibration steps with the site-specific models.

Though Finch (1999; 2000) presents some evidence that nitrate can potentially volatilize to nitrogen gas via denitrification, the field data from all three sites indicate that subsurface conditions are not conducive to such a process. Specifically, organic carbon levels appear to be too low and moisture contents too low to promote denitrification. Moreover, there is no evidence to indicate that the anaerobic conditions required for denitrification occur in the uppermost 30 to 70 feet of soils at the sites.

The foregoing discussion regarding field study findings leads to three conclusions about how the model simulations can be prepared. First, the site-specific models can be limited to simulations of one-dimensional, downward flow and transport. Second, nitrate is the only nitrogen species that needs to be simulated. Third, simulation of the loss of nitrate to nitrogen gas is not warranted; by assuming that denitrification is not occurring, the simulations will be conservative in that the penetration depths for nitrate predicted by the models will be greater than would actually occur if denitrification had a notable influence on transport.

4.2 Downward Seepage Rates

One of the most influential factors affecting downward transport of nitrate is the long-term, downward seepage rate of moisture below each facility. At the sludge disposal sites, this rate might be close in magnitude to the background recharge rate resulting from infiltration of precipitation, or it may be enhanced due to the increased moisture content of the sludge that is applied to the land surface. Because precipitation rates and sludge moisture contents at a site vary temporally, infiltration rates can also be expected to vary with time. However, infiltration pulses are typically dampened out within the top 2 to 3 feet of a soil column, resulting in a relatively constant downward seepage rate in the materials lying below this depth (Charbeneau and Daniel, 1993). Consequently, it is not unreasonable to assume that the long-term downward transport of dissolved constituent at depths below 2 to 3 feet can be effectively modeled using a steady, long-term infiltration rate.

A variety of methods can be considered to estimate long-term, background infiltration rates at land application facilities as a result of precipitation alone. For example, long-term records from nearby weather stations may be examined to ascertain how monthly precipitation compares to estimates of monthly quantities of evaporation. However, such an approach fails to account for the actual quantities of excess precipitation during individual storms or for periods of a few days or less. Moreover, examination of weather records alone does not account for the specific effects of a soil type on infiltration. As an alternative, much more reliable estimates of background infiltration rates can be developed by utilizing the results of field studies that have been aimed specifically at the measurement of long-term downward seepage rates in the unsaturated zone.

Fortunately, the findings from some field studies in New Mexico have been reported in which long-term downward seepage rates have either been directly measured or estimated. Stephens and Knowlton (1986), McCord and Stephens (1987), and Phillips et al. (1988) have used a variety of techniques, including isotope measurements and hydraulic calculations based on measured unsaturated zone properties, to calculate natural, long-term infiltration rates at the Sevilleta Wildlife Refuge located between Albuquerque and Socorro. The resulting estimates of the seepage rate tend to fall into a range of about 0.5% to 3% of annual precipitation. Alternatively, Sandia National Laboratories (SNL), also using actual field measurements at several inter-fluvial (i.e. between surface runoff channels) sites on its property, has estimated long-term recharge rates that vary between 0.002 and 0.02 feet per year (ft/yr) (0.06 – 0.61 cm/yr). (SNL, 1996). The surface soils at SNL in which and below

which testing has been performed are typically described as silty sands or sandy silts. Of all of these field-derived estimates of background infiltration rates due to natural events only, those developed for SNL sites are probably most similar to the infiltration rates that occur at the Santa Fe and Albuquerque facilities included in this study. However, it should be kept in mind that the actual downward seepage rate at these two facilities might be somewhat higher than was observed on Sandia land because of the additional moisture that can occur within the applied sludge.

Development of initial estimates of long-term seepage rates below septage impoundments involves more analysis than simply transferring data from a site where such rates have been measured. This observation occurs partly because the depth of liquid that is maintained in waste impoundments typically varies both with site and with time. In addition, the formation of a flow-impeding clogging layer at the base of an impoundment is possible. Such a clogging layer, whether formed by biological processes or the simple filtration of fine-grained particles in septage below an impoundment, can be expected to reduce the infiltration rate below that which would be expected if no clogging layer formed. Thus a more defensible method for arriving at a reasonable estimate of infiltration rates below septage disposal facilities is to determine a combination of clogging layer properties and average septage depths that are in accordance with the depths to which nitrate transport below a facility has been observed. This can be accomplished through some form of calibration of a flow and transport model to site-specific observations, such as is performed for the Taos site in this report.

4.3 Loading Rates

The conceptual models that apply to the sites reported on in this study can be clarified somewhat by providing an explanation as to what is referred to as a "loading rate." In this report, a loading rate comprises the product of an average, long-term downward seepage rate and the aqueous-phase concentration of the nitrogen species that is being investigated. This distinction is important because loading is sometimes defined in other ways, such as a finite number of pounds of sludge spread over a given number of acres. To effectively use the results of this modeling investigation, it is necessary to convert given mass loading information into expressions of concentration times seepage.

The reasons for using the report-specific definition of loading rate are found in the discussion presented above as to why one-dimensional, downward transport is expected to dominate the transport process. Specifically, simulation of one-dimensional, downward flow and transport means that the predicted depth of penetration for a given nitrogen species will be conservative in comparison to shallower penetration depths predicted by a multi-dimensional simulation that allows the species to diffuse laterally. The physical principles of flow and advective transport establish that, for a given soil profile with a distinct set of hydraulic and transport properties, the depth of penetration of a contaminant is governed only by the seepage rate. In other words, the aqueous-phase concentration in the source material does not influence the penetration depth. The one exception to this rule occurs if molecular diffusion of the contaminant in soil moisture is of the same general magnitude as the rate of the contaminant's migration in response to unsaturated flow. However, because aqueous-

phase diffusion rates in most soils are typically small in comparison to the transport rates brought about by advection and mechanical dispersion, the effects of the contaminant's concentration on its vertical penetration are not expected to be significant. This observation allows predictions of nitrate migration to be based on normalized, dimensionless concentrations, an approach that is applied in Chapter 8.

4.4 Simplifying Assumptions and Their Potential Impacts

The nature of this modeling study required that several simplifying assumptions regarding flow and transport be adopted. Specifically, because the ultimate study products were to comprise generic modeling predictions, DE&S and the GWQB decided that some site-specific features affecting flow and transport would not be directly taken into account. For example, during calibration of each of the site models, the number of soil materials used to represent the soil vertical profile was limited to two, with one representing the shallowest 5 to 12 feet of materials, and the other representing all remaining materials to the full investigation depth. No other forms of soil heterogeneity were explicitly taken into account

Model calibration was also performed assuming constant long-term infiltration rates and concomitant nitrate source loading rates. This simplified approach to handling source terms at the ground surface at each disposal area was taken because it was impossible to know how conditions at the ground surface actually varied in time at the disposal sites. In the cases of sludge applied to the land surface or just below the land surface, the constant infiltration rate was viewed as representing the long-term average, downward seepage due to net precipitation and/or moisture draining from the sludge. For surface impoundments, the constant infiltration rate represented net downward seepage over several years as a result of an average pond depth and liquid movement across a basal clogging layer.

MATHEMATICAL FORMULATION OF CONCEPTUAL MODELS 5.0

5.1 **Unsaturated Flow**

5.1.1 Governing Equation

Downward flow of water in the unsaturated zone at each of the three disposal sites is represented by the one-dimensional (1-D) form of Richard's equation

$$\frac{\partial}{\partial z} \left[k_r(h) K_s \frac{\partial h}{\partial z} \right] = C(h) \frac{\partial h}{\partial t} - Q$$
 (2)

where h = hydraulic head (L),

> = saturated hydraulic conductivity (L/T), K.

= relative hydraulic conductivity (unitless),

= specific moisture capacity (1/L),

= volumetric flow rate, via sources or sinks, per unit medium volume Q

of porous medium (1/T),

= elevation (L), and

= time (T). t

Hydraulic head is made up of two components, i.e.

$$h = \psi + z \tag{3a}$$

$$\psi = \frac{p}{\rho g} \tag{3b}$$

= pressure head (L), where ψ

= pressure in soil water (ML^2/TL^2) ,

= density of water (M/L^3) , and = acceleration due to gravity (L^2/T) .

Because the elevation z is constant at a given location in the subsurface, the 1-D form of Richard's equation can also be stated in terms of pressure head, i.e.

$$\frac{\partial}{\partial z} \left[k_r(\psi) K_s \frac{\partial \psi}{\partial z} \right] = C(\psi) \frac{\partial \psi}{\partial t}$$
(4)

Boundary conditions for the one-dimensional unsaturated flow problem can be expressed as prescribed heads or prescribed fluxes, i.e.

$$\psi = \psi_o \qquad \text{on } \Gamma_1 \tag{5}$$

$$u = u_n$$
 on Γ_2 (6)

where Γ_1 is the portion of the domain boundary where ψ is prescribed as ψ_o , and Γ_2 is the portion of the boundary where the moisture flux into the domain u is prescribed as u_n . Initial conditions in the flow model are given as prescribed pressure heads.

5.1.2 Functional Relationships Between Hydraulic Parameters

In unsaturated soils, pressure head ψ varies with changes in moisture content θ . The relationship between these two variables for a given soil is commonly referred to as the soil moisture characteristic. Sometimes it can be shown that, depending on whether a soil is wetting or drying, different values of pressure head occur in conjunction with a given value of moisture content, a phenomenon that is referred to as hysteresis. In the interest of problem simplification, however, we ignore hysteresis in this study, and assume that, for a given porous medium, there is a one-to-one correspondence between each value of ψ and θ . Under such an assumption, it follows that there is also a one-to-one correspondence between each θ - ψ pair and the soil's unsaturated hydraulic conductivity.

The nonlinear relationships between θ , ψ , and k_r can be expressed in the form of several sets of corresponding measurements of these parameters or, alternatively, described with mathematical relationships between them. The latter approach is taken in this study because it simplifies the steps involved in model development and simulation. The specific relationships used were developed by van Genuchten (1980), whose formulation begins with the following definition

$$S_{e} = \frac{\theta - \theta_{r}}{\varphi - \theta_{r}} \tag{7}$$

where S_e = effective saturation (unitless),

 θ = volumetric moisture content (unitless),

 θ_r = residual moisture content (unitless), and

 φ = porosity (unitless).

Under van Genuchten's scheme, effective saturation is related to pressure head by

$$S_{e} = \left[\frac{1}{1 + (\alpha \psi)^{s}}\right]^{m}$$
 (8)

where α (1/L) and β (unitless) are fitting parameters, and $m = 1-1/\beta$. The corresponding equation relating relative hydraulic conductivity to moisture content is

$$k_{r} = (S_{e})^{1/2} \left\langle 1 - \left[1 - \left[S_{e} \right]^{1/m} \right]^{m} \right\rangle^{2}$$
 (9)

An advantage of using the functional relationships like those of van Genuchten, rather than tabulated data describing the relationships between moisture content, pressure head, and hydraulic conductivity, is that estimates of corresponding values of these three parameters can be arrived at directly rather than having to estimate them by interpolation between tabulated values. In addition, van Genuchten's model is useful because it represents the full soil moisture characteristic curve, rather than only describing that portion of the curve at pressure heads less than the pressure at which air enters the soil (Rawls et al., 1993) There are a variety of sources that can be accessed to develop initial estimates of these parameters, including a list of recommended ranges for each parameter provided in Lappala et al. (1997) and the UNSODA database (Leij et al., 1996).

5.1.3 Nonlinearity of Richard's Equation

The product of k_r and K_s is defined as unsaturated hydraulic conductivity, and is always a fraction of saturated hydraulic conductivity under unsaturated conditions, or equal to saturated hydraulic conductivity when the porous medium is saturated. Accordingly, k_r takes on values that vary from 0 to 1.

Specific moisture capacity is defined by

$$C = \frac{d\theta}{dw}$$
 (10)

Because both relative hydraulic conductivity and specific moisture capacity are dependent on the state variable in Richard's equation (i.e., pressure head or hydraulic head), the governing equation is inherently nonlinear. This means that unsaturated hydraulic conductivity and specific moisture capacity for a given point in space and time cannot be determined until pressure head has been solved for, and vice versa. Thus an iterative scheme is required to solve Richard's equation.

5.1.4 Calculation of Infiltration Rate Across an Impoundment Basin Surface Layer

The long-term, steady-state infiltration rate used in simulations of flow and transport below land application sites comprises a model input. In contrast, the infiltration rate associated a column of septage liquid standing above the bed of an impoundment basin is a function of the liquid depth and the hydraulic properties of the soils underlying it. In some instances the properties of the shallowest soils may be impacted by the clogging of pores. Consequently, the steady-state infiltration rate below septage impoundments is calculated within the model. Assuming that the surface layer of soil just below an impoundment is somewhat fine-grained (as has been observed at the Phase 1 and Phase 2 field sites), and that it is entirely saturated

while septage enters the subsurface, the long-term infiltration rate can be approximated by the Darcy's Law expression (Peterson and Zhang, 2000)

$$q_{s} = \frac{K''}{B} (h_{s} - h_{b} - \psi_{b})$$
 (11)

where q_s = infiltration rate (L/T),

K'' = saturated hydraulic conductivity of the surface layer (L/T),

B = thickness of the surface layer (L),

h_s = hydraulic head at the base of the impoundment basin (L),

h_b = elevation at the base of the surface layer (L), and

 ψ_b = pressure head at the base of the surface layer (L).

5.2 Unsaturated Transport

The equation describing 1-D, downward advective-dispersive transport of a dissolved constituent in porous media that is not affected by sorption to soil materials is (Charbeneau and Daniel, 1993)

$$\frac{\partial}{\partial z} (q C_w - \theta D \frac{\partial C_w}{\partial z}) = \frac{\partial (\theta C_w)}{\partial t}$$
 (12)

where q = volumetric flow of water given by Darcy's Law (L/T),

= hydrodynamic dispersion coefficient (L^2/T), and

all other parameters are as previously defined.

The hydrodynamic dispersion coefficient D actually accounts for the two additive phenomena of molecular diffusion and mechanical dispersion, and for a 1-D problem is expressed as

$$D = \tau D_{m} + \omega_{\ell} v \tag{13}$$

where v = pore water velocity = q/θ (L/T),

 D_m = molecular diffusion coefficient (L^2/T),

 τ = a tortuosity factor that depends on moisture content (unitless), and

 ω_{ℓ} = longitudinal dispersivity (L).

Two types of boundary conditions can be employed in a 1-D transport analysis: (1) prescribed concentration on the boundary or (2) prescribed concentration of incoming water. Initial conditions are established as prescribed water concentrations.

6.0 TECHNICAL APPROACH

6.1 Modeling Code

All of the model runs conducted under this study were performed with the code known as VS2DT (Healy, 1990; Hsieh et al., 2000), a finite-difference simulator developed and distributed by the U.S. Geological Survey (USGS). VS2DT was used to solve Richard's equation for unsaturated flow and concomitant advective-dispersive transport of nitrate. The flow solution in the code is essentially the same as that developed by Lappala (1997) in the simulator known as VS2D, a precursor to VS2DT. The flow and transport simulations were mostly carried out within the Windows-based graphical user interface (GUI) known as VS2DI (Hsieh et al., 2000), developed for the VS2D family of codes by the USGS.

6.1.1 General Code Description

VS2DT is a computer program developed by the USGS for solving problems of water flow and solute transport in variably saturated porous media. VS2DT originated as a stand-alone program that reads simulation setup data from input files, and writes simulation results to output files. Prior to the release of the present software, version 3.0, VS2DT was released as version 2.5. In revising VS2DT from version 2.5 to 3.0, no new features were added. Rather, the code was modified so that it can be run in an interactive manner (Hsieh et al, 2000), and the definition of the van Genuchten parameter α was revised to be consistent with established usage. The present software integrates VS2DT 3.0 with a preprocessor and postprocessor so that simulations can be run in a visual-interactive environment.

Major features of VS2DT 3.0 include the following:

- Use of finite-difference approximations to solve the Richard's equation for flow, and the advection-dispersion equation for transport.
- Simulated regions can be one-dimensional columns, two-dimensional vertical cross sections, or three-dimensional axially symmetric cylinders.
- Boundary conditions for flow include: specified pressure head, specified flux, infiltration with ponding, plant transpiration, bare soil evaporation, and seepage faces.
- Unsaturated hydraulic characteristics may be represented by: van Genuchten, Brooks-Corey, and Haverkamp equations, as well as tabular data.
- Transport processes include advection, dispersion, first-order decay, equilibrium adsorption as described by Freundlich or Langmuir isotherms, and ion exchange.

6.1.2 Data Requirements

In using VS2DT, a conceptual model of the geometry and boundaries of the region to be simulated is of prime importance. Initial conditions in terms of pressure heads or moisture contents for flow simulations and concentrations for transport simulations are needed. Hydraulic and transport properties of the porous media are also required. These values can be different for different sediments. Flow simulations require values for saturated hydraulic

conductivity and for relative hydraulic conductivity and moisture content as functions of pressure head. Solute transport simulations require values for dispersivity and molecular diffusion. Other information may be needed, depending on the program options that are selected.

Model input files contain ASCII data that are read by the numerical model VS2DT 3.0. When a model user has entered all required data in the preprocessor, and the postprocessor has also been invoked within VS2DI, two model input files (vs2dh.fil and vs2dh.dat) are generated in the working directory. This is done automatically and requires no handling by the user.

6.1.3 Output Options

Simulation results from VS2DI can be displayed as contours of pressure head, moisture content, saturation, concentration, and velocity or flux for each time step, thus creating a simple animation. The graphical displays may be printed or saved as bitmap files. Text (or ASCII) output can be obtained for pressure head, total head, volumetric moisture content, saturations, velocities, and solute concentrations, each of which can be presented graphically using alternative plotting programs. Time histories and spatial profiles of the data can be obtained. In addition, the user may opt to view time histories of up to 72 mass balance parameters.

6.2 Vadose Zone Model Setup

The model runs performed under this study focused on one-dimensional flow and transport. All of the site-specific and predictive model runs were made with a domain that was 100 feet deep, with the base of the domain representing a hypothetical water table, and the top representing ground surface.

To calibrate the flow model to measured moisture contents at land application sites, a constant infiltration rate was prescribed at the ground surface. To calibrate the corresponding transport model, a prescribed concentration was assigned to the water that infiltrates the ground surface. The mass loading rate under this approach was equal to the product of the infiltration rate and prescribed concentration.

All of the site-specific models and most of the predictive simulations took into account the occurrence of a relatively fine-grained sediment in the shallowest depths of the simulation domain. A prescribed pressure head was used above this surface layer to represent the standing liquid that comprises septage. A uniform depth of 3 feet of liquid was used to represent the septage depth in all of the calibrated model runs and the predictive simulations based on septage impoundment.

To match observed nitrate concentrations at the field site, properties of both the surface layer and underlying sediments were manipulated. This resulted in the estimation of a reasonable long-term infiltration rate. In calibrating the transport model of the impacted locations at the

Taos site, prescribed concentrations were assigned to the finite-difference block representing the bottom of each septage basin.

Initial estimates of a subsurface soil's moisture characteristic and relative hydraulic conductivity information were developed by examining particle size analyses and borehole logs from the Phase 1 and Phase 2 field investigations. These types of information were taken compared with similar data provided in EPA's UNSODA (Leij et al., 1996) database. Initial estimates of soil hydraulic properties were developed by selecting porous media materials within the database that have similar textural and descriptive properties to those measured in the field investigations.

The 100-foot long simulation domain was divided into finite-difference blocks that were 0.5 feet long. This discretization scheme facilitated the matching of measured nitrate concentrations at the Phase 1 and Phase 2 field sites, while still allowing flow and transport models to be completed within a period of several minutes.

6.3 Input and Output Data

Two general types of data, hydraulic and transport, were used as input to the models. Hydraulic input parameters consisted not only of the varying pressure head and hydraulic conductivity properties of affected soils with varying moisture, as determined with van Genuchten relationships, but also included information that defines flow model boundary conditions. Transport data comprised the parameters that influence the movement of nitrogen species given a specific flow field.

Two required input parameters for the flow simulation portion of each model run were saturated hydraulic conductivity and residual moisture content. Additional flow simulation input comprised the parameters used to represent boundary conditions at the top and bottom of the simulation domain. In the case of surface or shallow subsurface applications of sludge, the boundary condition at the ground surface consisted of a prescribed infiltration rate. For septage impoundments, the upper boundary condition consisted of a prescribed pressure head to represent standing water on the ground surface. The boundary condition assigned to the base of the domain was a prescribed pressure head of zero, which is representative of a water table.

The advection component of transport was determined by flow velocities calculated within the flow portion of the code; consequently, dispersivity and aqueous-phase diffusion coefficient were the only transport properties required as input.

Output consisted of computed pressure heads, corresponding hydraulic heads and moisture contents, and nitrate concentrations. These state variables were viewed using graphical means with the VS2DI post-processor and, subsequently, in ASCII output files. For this report, graphical results were prepared primarily in the form of vertical profiles of computed nitrate concentrations. To help assure that model output was reasonable, mass balance components of both the flow and transport simulations were inspected.

6.4 Methods of Interpretation

Results from both the calibration model runs and the predictive simulations were examined in both graphical and numerical form. Because of the relatively limited number of data points for nitrate concentrations at each sample cluster, DE&S based model calibration on a visual best-fit between simulated and observed data, rather than using a specific algorithm that provides a measure of the differences between observed and simulated values. This approach removed the possibility of producing nitrate profiles that do well in minimizing the differences between observed and computed values (i.e., model residuals), but do not necessarily capture the most important features of the observed concentration profiles.

7.0 MODEL CALIBRATION

7.1 Data Assimilation

Data from the Phase 1 investigations that were considered in developing models for the Santa Fe, Taos, and Albuquerque sites included: (1) lab-derived saturated hydraulic conductivities, (2) porosities, (3) bulk densities, (4) moisture contents, and (5) nitrate concentrations. Additional information from the Phase 1 field investigations that was utilized in developing the vadose zone models included particle-size analyses of the soil samples collected and the borehole logs. Each of these latter pieces of information was useful for arriving at initial estimates of a representative soil moisture characteristic in modeled soils and associated relative hydraulic conductivity changes with moisture content and pressure head.

DE&S believed that the computed infiltration rates stemming from calibration efforts would provide the greatest insight into the general magnitude of potential infiltration rates. Initial estimates of the long-term infiltration rates to be used in the models of land application sites were developed using values within the range of inter-fluvial recharge rates measured at Sandia National Laboratories (SNL, 1996).

7.2 Santa Fe Clusters

Total simulation time in the models developed for Clusters 1 and 2 at the Santa Fe Sludge Disposal Facility was 16 years, the period between facility start-up in 1984 and the field investigation in 1999. Saturated hydraulic conductivity and long-term infiltration rate were the parameters adjusted most to achieve calibration of the models. Minor adjustments were also occasionally made to other parameters affecting unsaturated flow, such as van Genuchten's α and β , but none of these latter parameters appeared to have much influence on simulation results.

The flow and transport parameters ultimately used in the calibrated models for this site are listed in Table 5. A plot of nitrate concentrations with depth at Santa Fe Cluster 1, both those computed by the calibrated model and observed concentrations, is presented in Figure 1. The equivalent plot for Cluster 2 is presented in Figure 2.

Two of the parameters used in the calibrated Santa Fe models – saturated hydraulic conductivity and long-term infiltration rate- are worthy of further discussion. Obviously, the K_s value of 50 ft/day is at least two orders of magnitude larger than the measured values of this parameter shown in Table 2. Reasons for ultimately using such a large value for this parameter were two-fold. First, it falls within the range of K_s values typically reported in the literature for the sand and gravel sediments that predominate at depths greater than 5 feet below ground surface at the Santa Fe site. Alternatively, the measured K_s values are much lower than would be expected for soils of this kind. Secondly, calibration could have only been achieved with saturated K_s values similar to measured ones by using much larger than reasonable infiltration rates.

The long-term infiltration rate used in the calibrated models varies from 8.99E-05 ft/day (1.0 cm/yr) at Cluster 1 to 7.37E-05 ft/day (0.8 cm/yr) at Cluster 2. Both of these rates are somewhat higher than the range of inter-fluvial recharge rates of 0.002 to 0.02 ft/yr (0.06 to 0.61 cm/yr) measured at Sandia National Laboratories (SNL, 1996). Thus, assuming the rates based on calibration are of the same general magnitude as those that actually occur, it may be deduced that the downward migration of nitrate stemming from sludge application at this site is potentially enhanced by moisture within the emplaced sludge.

7.3 Taos Clusters

The models developed for Clusters 1 and 2 at the Taos facility assumed that 3 feet of septage liquid was always present above the floor of an impoundment. Total simulation time was 13 years, which corresponded to the period between facility start-up in 1987 and the time of field investigation in 1999. Calibration of the models was accomplished mostly by adjusting the saturated hydraulic conductivity of both the surface layer and the underlying soils. As in the case of the Santa Fe Clusters, some adjustments were also made to van Genuchten parameters, but little to no effect on simulation results was again observed.

The flow and transport parameters ultimately used in the calibrated models for this site are listed in Table 5. A plot of nitrate concentrations with depth at Taos Cluster 1, both those computed by the calibrated model and observed concentrations, is presented in Figure 3. The equivalent plot for Cluster 2 is presented in Figure 4.

The very low saturated hydraulic conductivities used for the surface layer at this site (2.5E-06 to 8.9E-05 ft/day) suggest that some clogging of this layer by biological means or filtration of fine particles may be occurring. However, it is also possible that the average depth of septage in the impoundments that were tested may be significantly less than 3 feet, in which case a larger hydraulic conductivity would have resulted in a calibrated model.

7.4 Albuquerque Clusters

Total simulation time at the Albuquerque impacted locations was 13 years, which corresponds to the period between facility startup in 1988 and the Phase 2 field investigation conducted in 2000. The flow and transport parameters ultimately used in the calibrated models for this site are listed in Table 5. A plot of nitrate concentrations with depth at Albuquerque Cluster 1, both those computed by the calibrated model and observed concentrations, is presented in Figure 5. The equivalent plot for Cluster 2 is presented in Figure 6.

The observed aqueous-phase concentrations shown in Figures 5 and 6 are of interest because they indicate a steep decline in nitrate levels within the top 5 to 10 feet of sediment. These observations suggest that the rate of nitrate penetration is hindered by the uppermost surface layer. Model calibration at the Cluster 2 location was based on a relatively small surface layer hydraulic conductivity of 0.1 ft/day and an infiltration rate of 1.80E-05 ft/day (0.2 cm/yr), the latter of which falls in the range of background recharge rates measured at SNL.

Table 5. Parameters Used in the Calibrated Models

	Santa Fe	Santa Fe	Taos	Taos	Albuquerque	Albuquerque
Parameter	Cluster 1	Cluster 2	Cluster 1	Cluster 2	Cluster 1	Cluster 2
Source						
Infiltration Rate (ft/day)	8.99E-05	7.37E-05	1.54E-04 ^a	1.43E-04 ^a	8.99E-05	1.80E-05
Source Concentration (mg/L)	2000	5500	500	1600	55250	93500
Unsaturated Sediment						
Saturated Hydraulic Conductivity (ft/day)	50	20	100	100	200	50
Porosity (unitless)	0.35	0.35	0.35	0.35	0.35	0.35
Residual Moisture Content (unitless)	0.04	0.04	0.04	0.04	0.04	0.04
van Genuchten's α (1/ft)	3	3	3	3	4.5	4.5
van Genuchten's β (unitless)	2.5	2.5	2.5	2.5	3.0	3.0
Longitudinal Dispersivity (ft)	10	10	10	10	10	10
Molecular Diffusion Coefficient (ft/day)	4.74E-04	4.74E-04	4.74E-04	4.74E-04	4.74E-04	4.74E-04
Shallow Surface Layer						
Thickness (feet)	5	5	7.5	7.5	12	12
Saturated Hydraulic Conductivity (ft/day)	0.5	0.5	8.9E-05	1.0E-04	0.4	0.1
Porosity (unitless)	0.4	0.4	0.4	0.4	0.42	0.45
Residual Moisture Content (unitless)	60'0	0.09	0.15	0.15	0.09	0.10
van Genuchten's α (1/ft)	1.0	1.0	-		_	
van Genuchten's β (unitless)	1.7	1.7	1.7	1.7	1.1	1.1
Longitudinal Dispersivity (ft)	10	10	10	10	10	10
Molecular Diffusion Coefficient (ft/day)	4.74E-04	4.74E-04	4.74E-04	4.74E-04	4.74E-04	4.74E-04

^a Infiltration rate calculated by the model.

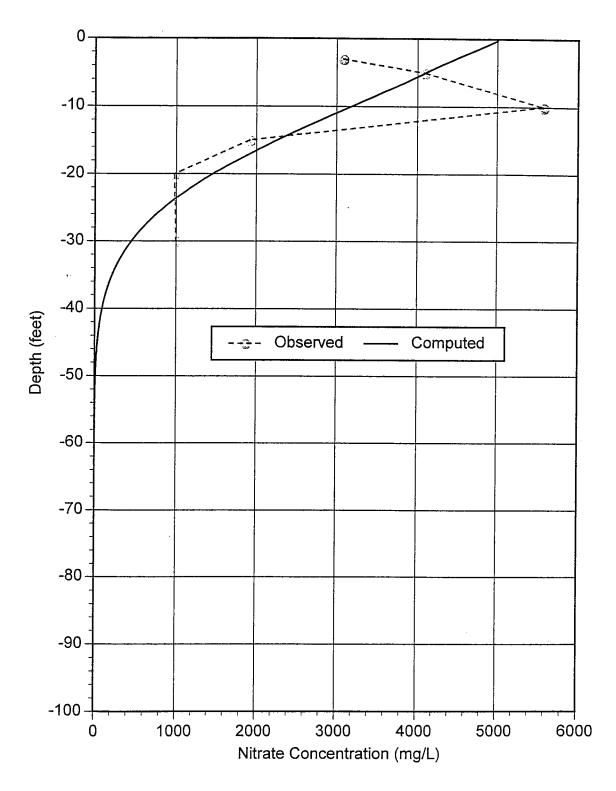


Figure 1. Observed and Computed Nitrate Concentrations in the Calibrated Model for Santa Fe Cluster 1.

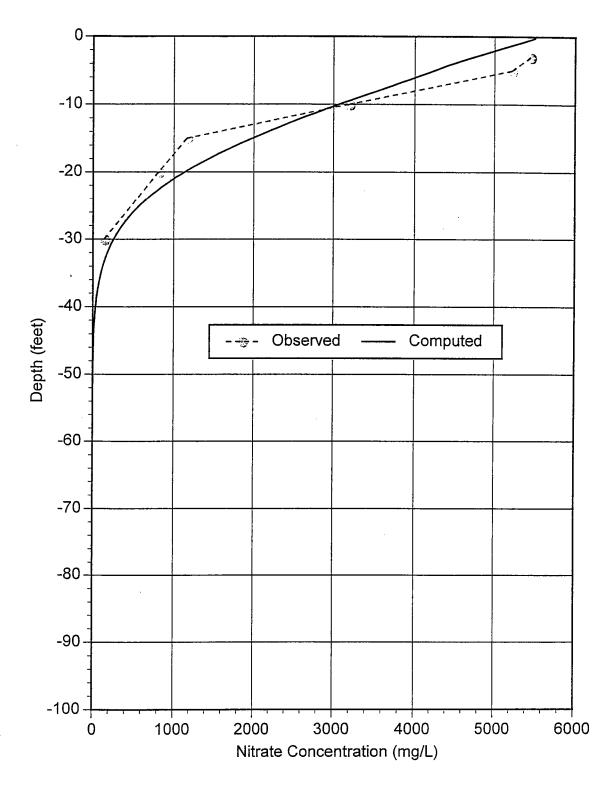


Figure 2. Observed and Computed Nitrate Concentrations in the Calibrated Model for Santa Fe Cluster 2.

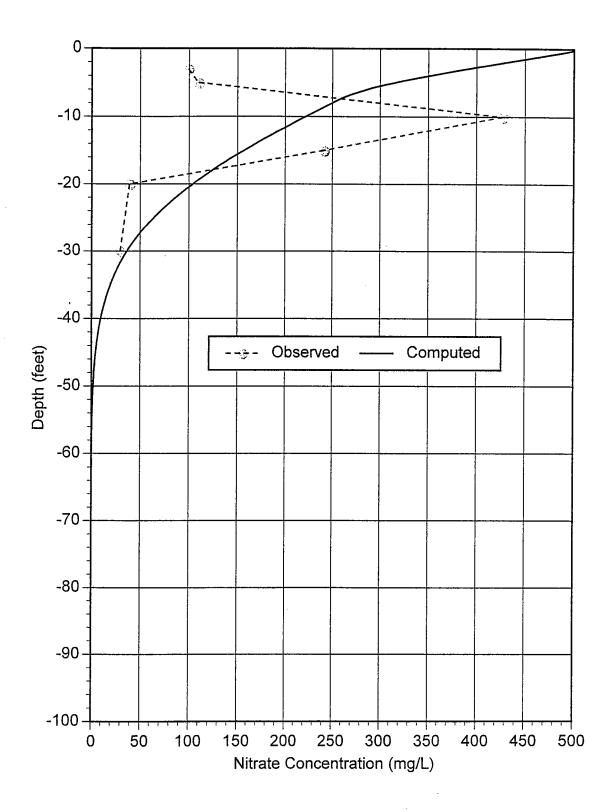


Figure 3. Observed and Computed Nitrate Concentrations in the Calibrated Model for Taos Cluster 1.

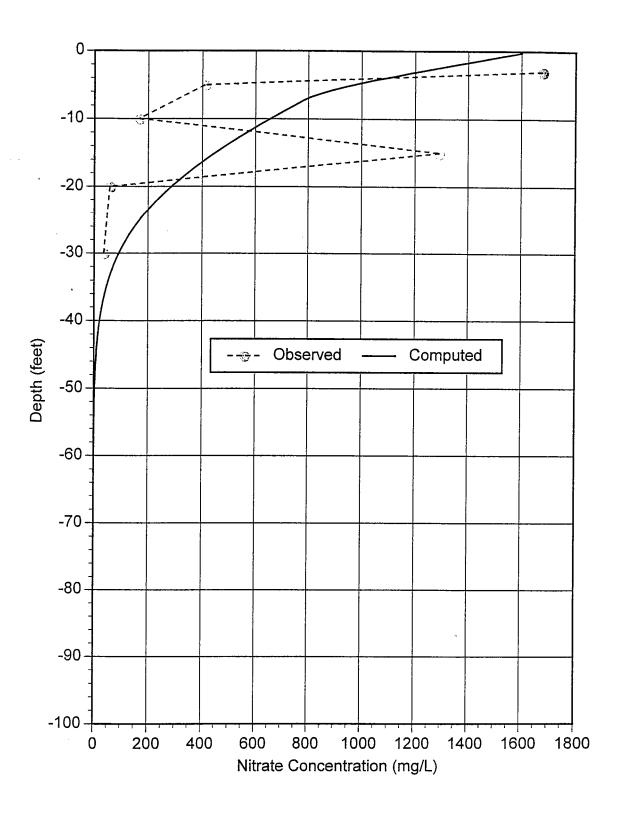


Figure 4. Observed and Computed Nitrate Concentrations in the Calibrated Model for Taos Cluster 2.

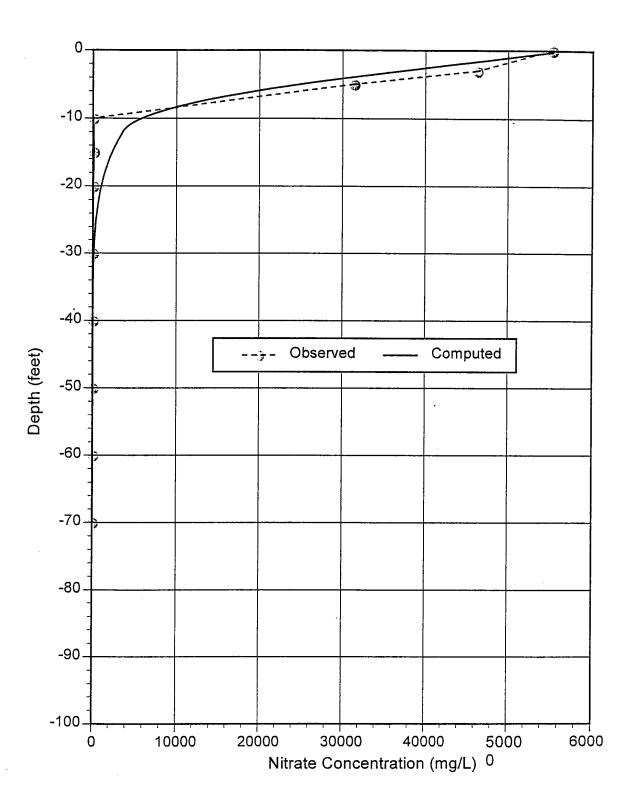


Figure 5. Observed and Computed Nitrate Concentrations in the Calibrated Model for Albuquerque Cluster 1.

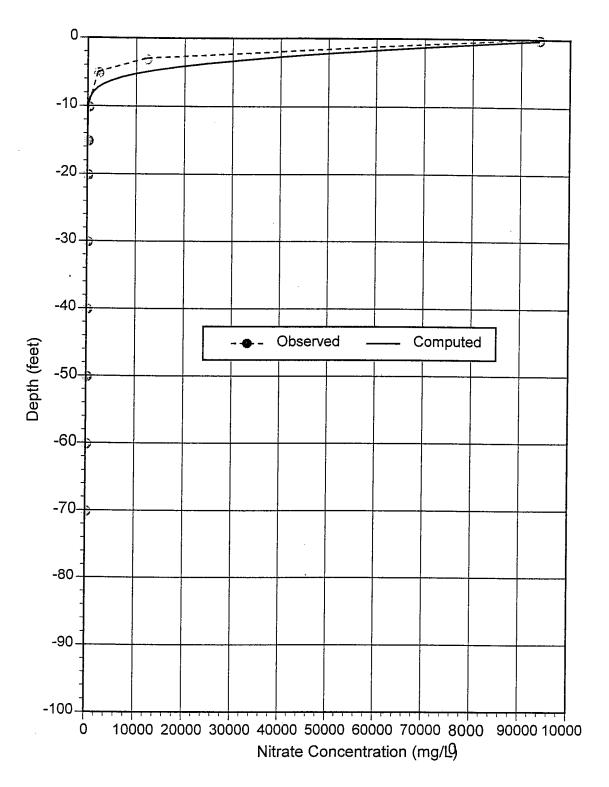


Figure 6. Observed and Computed Nitrate Concentrations in the Calibrated Model for Albuquerque Cluster 2.

8.0 PREDICTIVE SIMULATIONS

8.1 Predictive Model Development

DE&S performed three sets of predictive simulations. The first two were based on scenarios similar to those observed at the three field sites discussed in this report. Specifically, they involved systems containing two materials, with the uppermost 5 feet of sediment consisting of a relatively low permeability material, and the underlying sediment comprising a more permeable material. These first two types of predictive runs differed regarding the manner in which the uppermost boundary condition was handled, with the first approximating a sludge or septage land application, and the second representing septage impoundment. The third set of predictive simulations assumed a single soil type, thus removing the potential for a surface layer less permeable materials to affect flow and transport. These latter simulations were based solely on a land application waste disposal scenario; reasons for not examining a septage impoundment scenario with a uniform soil profile are presented in a subsequent section.

DE&S performed predictive simulations using five different soil types that were assumed to represent materials that are typically encountered in NM. These materials were used to represent the sediments underlying the uppermost low permeability soils in the simulations based on two materials, and a uniform domain of materials for the simulations based on a single soil type. The five soil types ranged from a relatively low permeability soil containing significant quantities of silt to that of a clean, coarse sand. The final selection of the representative soil types was made jointly by DE&S and representatives of the GWQB. A single set of boundary conditions representative of the infiltration and mass loading that would be expected at either a land application or an impoundment disposal site was applied to each representative soil type.

A total of 15 predictive simulations were performed. Subsequent sensitivity analyses based on the predictive simulations were used to ascertain the effects of changes in model input on model results. The sensitivity analyses make it possible to develop a range of possible model results, such as those corresponding to lower or higher mass loading rates, such that the GWQB could make use of a variety of modeling scenarios.

All of the predictive simulations were made using a normalized, or dimensionless, source concentration for nitrate. Such a normalized concentration is expressed mathematically as C_w/C_o , where C_o represents the actual aqueous-phase, source concentration. This approach makes it possible for users of the predictive model results to convert variable source concentrations into equivalent concentrations at depth below a disposal site. The total simulation time used for all of the predictive runs was 100 years. Graphical output of normalized nitrate concentration was developed at simulation times of 15, 25, 50, and 100 years.

In all cases, the finite-difference grid adopted for the predictive simulations had a total vertical extent of 100 feet. The choice of this depth was based on criteria established by the GWQB. For sites where the depth to groundwater is less than this depth, it was

anticipated that the results from the 100-foot deep predictions could be used to estimate the impacts on groundwater for the shallower conditions. If the depth to groundwater at a site is greater than 100 feet, and a predictive simulation representative of the site's upper 100 feet of materials shows no impact to groundwater, a conclusion of no impact could be considered logical for the deeper-groundwater case.

8.2 Land Application of Sludge or Septage

The hydraulic properties of the five soils used in the predictive simulations of 1-D nitrate transport below a land application disposal facility are presented in Table 6. Also listed are the properties assumed for the surface layer in the predictive model runs based on two materials. The shallow layer in all two-material simulations was given a depth of 5 feet. An infiltration rate of 8.99E-05 ft/day (1 cm/yr) was employed in all of the predictive simulations of land application disposal facilities. Dispersivity and the molecular diffusion coefficient were assumed to equal 10 feet and 4.74E-04 ft/day, respectively, in all materials and all simulations.

Table 6. Soil Hydraulic Parameters Used in the Predictive Simulations

Soil	Saturated Hydraulic Conductivity	Residual Moisture Content	Porosity	van Genuchten's	van Genuchten's
	(feet/day)	(unitless)	(unitless)	(1/feet)	(unitless)
Coarse Sand	200	0.04	0.35	4.5	3
Medium Sand	50	0.05	0.37	4.25	2.6
Loamy Sand	10	0.06	0.4	4.0	2.2
Sandy Loam	3	0.08	0.41	2.2	1.9
Silt Loam	0.5	0.1	0.45	0.6	1.4
Surface Layer – Land Application	0.2	0.1	0.45	0.6	1.4
Surface Layer – Impoundment	1.0E-04	0.1	0.45	1	1.7

Figures 7 through 11 present the resulting computed normalized concentrations from the simulations of a fine-grained surface layer overlying a more permeable sediment. As these figures show, the depth of penetration of the contaminant decreases as the saturated hydraulic conductivity of the sediment underlying the surface layer decreases. The

results of corresponding simulations in which the surface layer has been removed are illustrated in Figures 12 through 16. As expected, the depth of nitrate penetration increases in these simulations in comparison to the equivalent model runs that account for a surface layer.

8.4 Septage Impoundments

A 5-foot thick surface layer was assumed to exist in all of the predictive model runs for septage impoundments. The properties of the surface layer and the underlying sediments were the same as those applied in the land application model runs. The results from this latter set of simulations are presented in Figures 17 through 21.

8.5 Using Predictive Results for Site Evaluation

The manner in which the predicted concentration curves in Figures 7 through 21 can be used to assess the vertical penetration of nitrate can be illustrated with a simple example. In this example, it is assumed that the mass of nitrogen in a given volume of sludge destined for land application is known, and that the moisture content of the sludge after drying on the ground surface is also known. The aqueous-phase concentration of total nitrogen in the sludge is calculated by dividing the total nitrogen mass by the volume of water associated with the sludge. Then the equivalent concentration of nitrate, or source concentration C_0 , is calculated by multiplying the total nitrogen concentration in the aqueous phase by 0.75, or 75%. This step is taken under the assumption that 25% of the nitrogen will be lost to volatilization from ammonia and that the remaining ammonia is converted to nitrate via nitrification.

One of the sets of curves in Figures 7 through 16 is then selected as being representative of the site that is being evaluated. Since each of these sets is based on a background infiltration rate of 8.99E-05 ft/day (1 cm/yr), the nitrate concentrations calculated using them will be based on the same rate of downward seepage. To find the nitrate concentration at a depth of 10 feet below ground surface at 25 years, the value of C_w/C_o at the intersection of the 10-foot depth line with the 25-year curve is determined, and is then multiplied by the source concentration C_o . This same process can be repeated for any number of depth and time combinations, and the resulting concentrations compiled to assess the degree to which nitrate at problematic concentrations can be expected to penetrate.

8.6 Predicting Downward Transport at Other Sites

Though the three field sites discussed in this study have similar soil characteristics, and the long-term infiltration rates determined for each of them through calibration steps are close in magnitude to each other, it can be expected that the soil and infiltration characteristics of some other facilities will be significantly different. In such cases, the best approach to assessing the downward migration of nitrate with time will involve actual modeling of the site-specific conditions. The computer code used in this study, VS2DT, is easily applied to such a problem through its graphical user interface known as

VS2DI. The required inputs to the model for such an evaluation are the same as those that are discussed in Chapter 7 regarding model calibration. The primary factor affecting downward movement of nitrate with time will be the long-term seepage rate, which can be calculated in VS2DT by applying appropriate boundary conditions to the top of the simulation domain that is being used. In the case of land application, a prescribed pressure head, equivalent to the expected moisture content of the applied sludge, would be invoked at the top model boundary to allow the model to calculate the infiltration rate. For septage impoundments, a prescribed pressure head representative of the expected septage depth would be applied at the top boundary, and the model would again calculate the long-term infiltration rate.

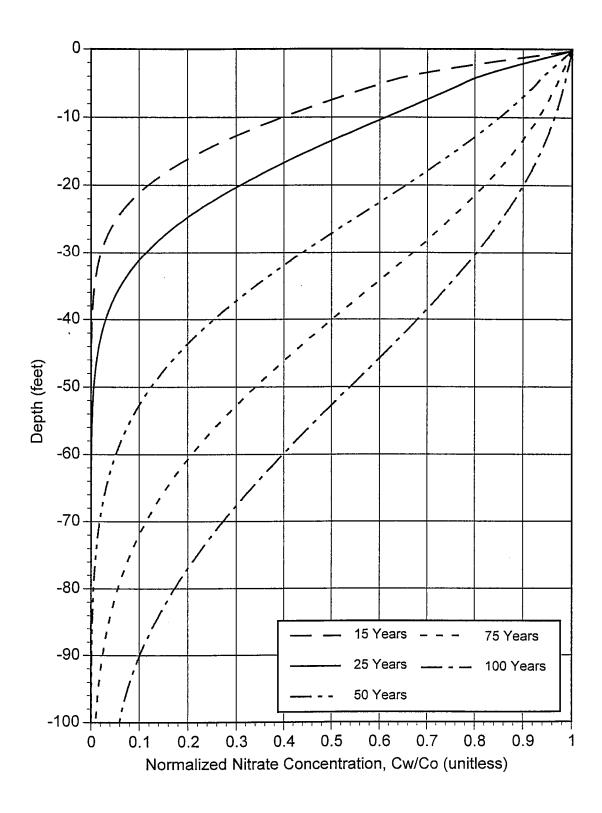


Figure 7. Predicted Normalized Concentration of Nitrate, for Land Application on a Fine-Grained Surface Layer Overlying Coarse Sand Sediments.

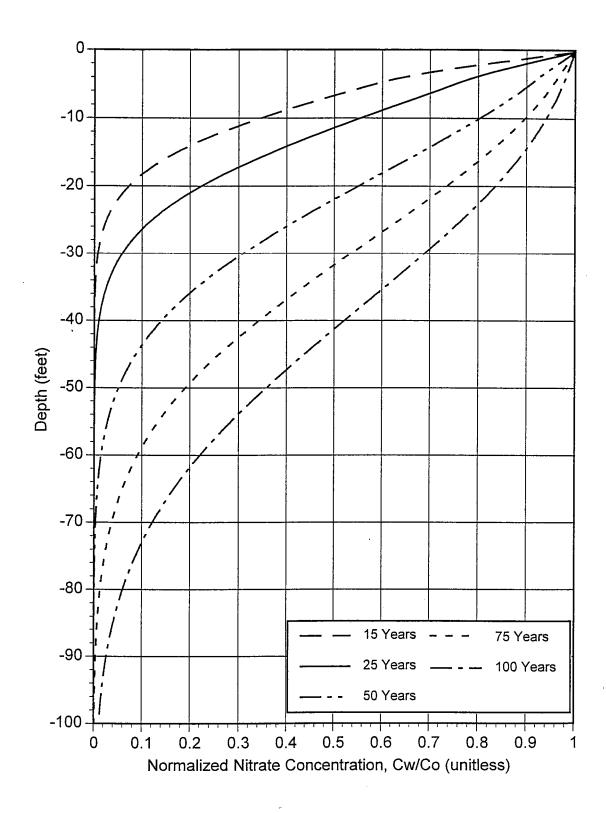


Figure 8. Predicted Normalized Concentration of Nitrate, for Land Application on a Fine-Grained Surface Layer Overlying Medium Sand Sediments.

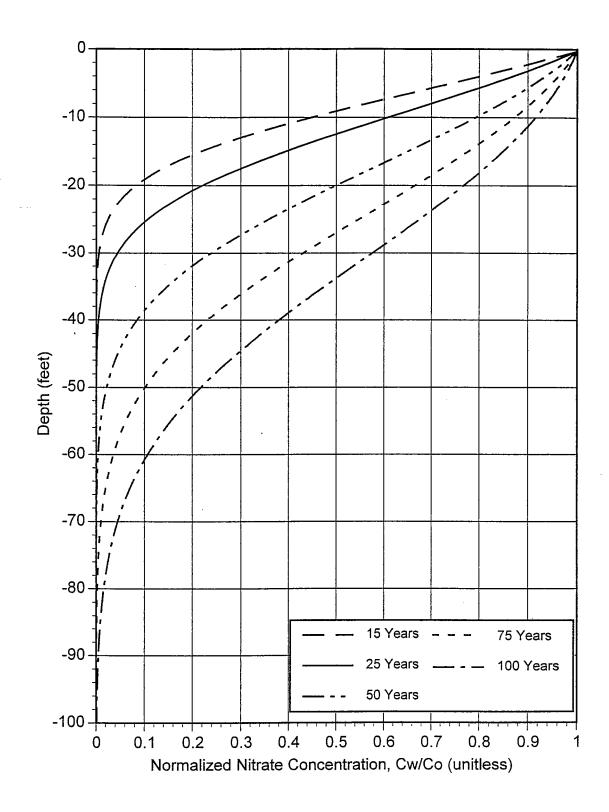


Figure 9. Predicted Normalized Concentration of Nitrate, for Land Application on a Fine-Grained Surface Layer Overlying Loamy Sand Sediments.

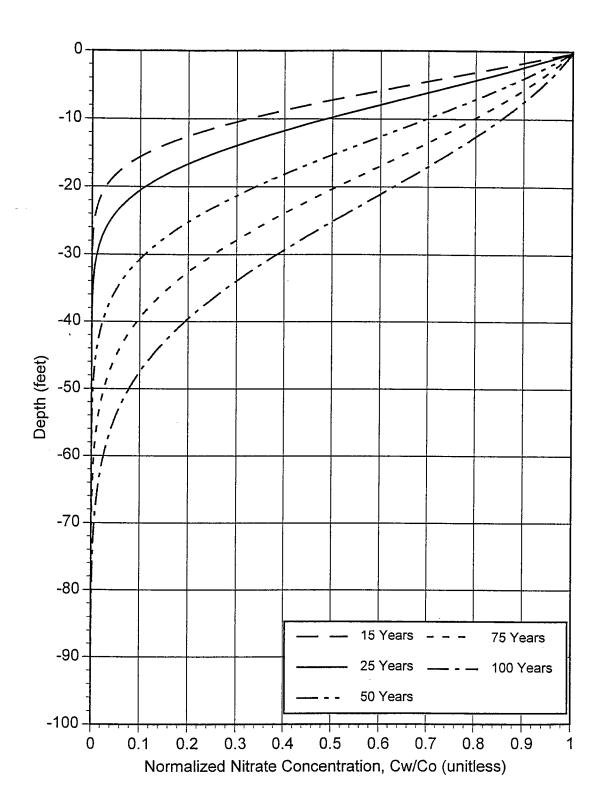


Figure 10. Predicted Normalized Concentration of Nitrate, for Land Application on a Fine-Grained Surface Layer Overlying Sandy Loam Sediments.

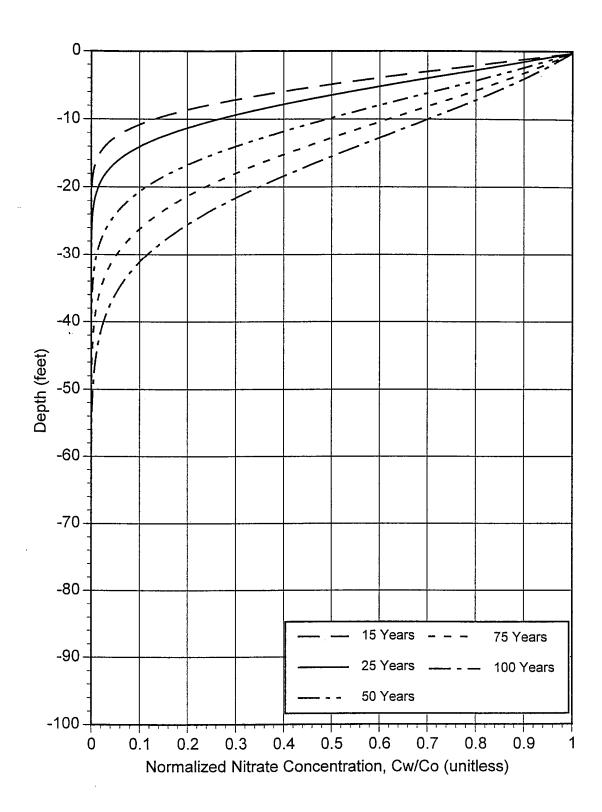


Figure 11. Predicted Normalized Concentration of Nitrate, for Land Application on a Fine-Grained Surface Layer Overlying Silt Loam Sediments.

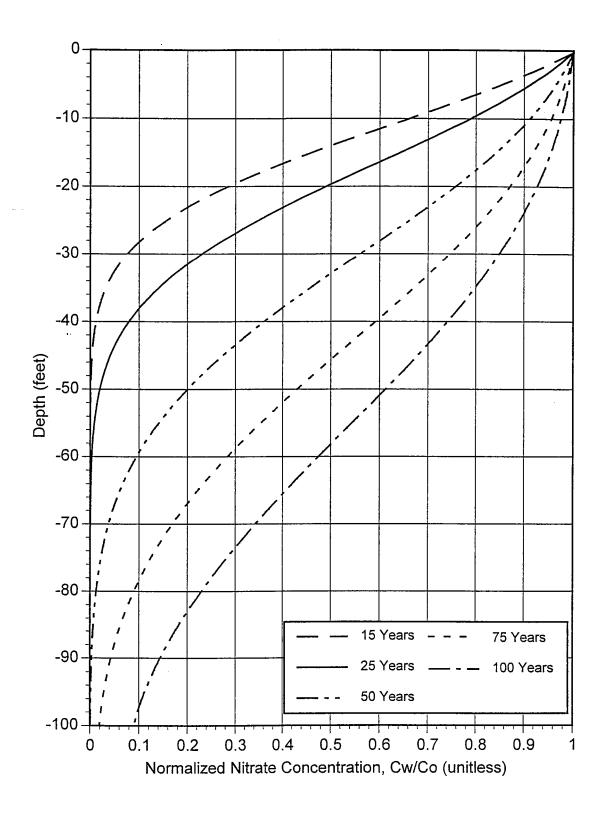


Figure 12. Predicted Normalized Concentration of Nitrate, for Land Application on Coarse Sand Sediments.

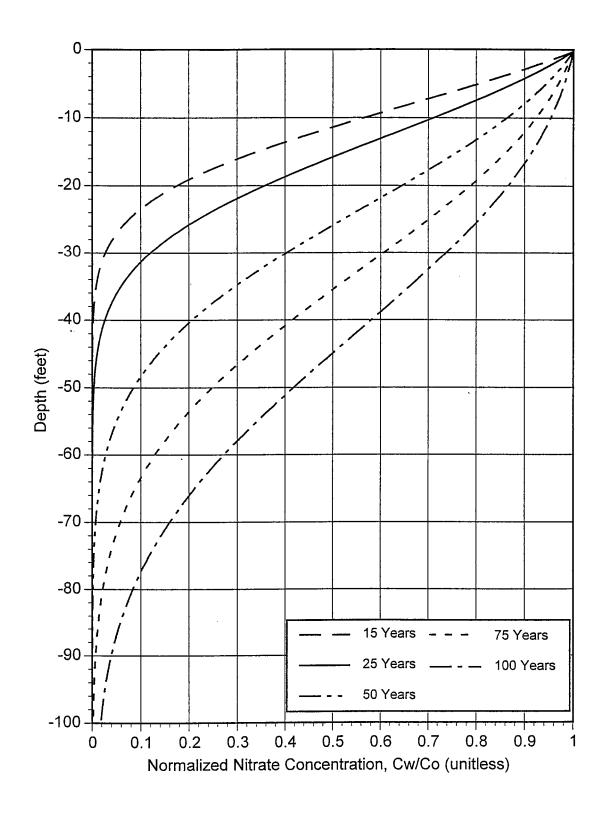


Figure 13. Predicted Normalized Concentration of Nitrate, for Land Application on Medium Sand Sediments.

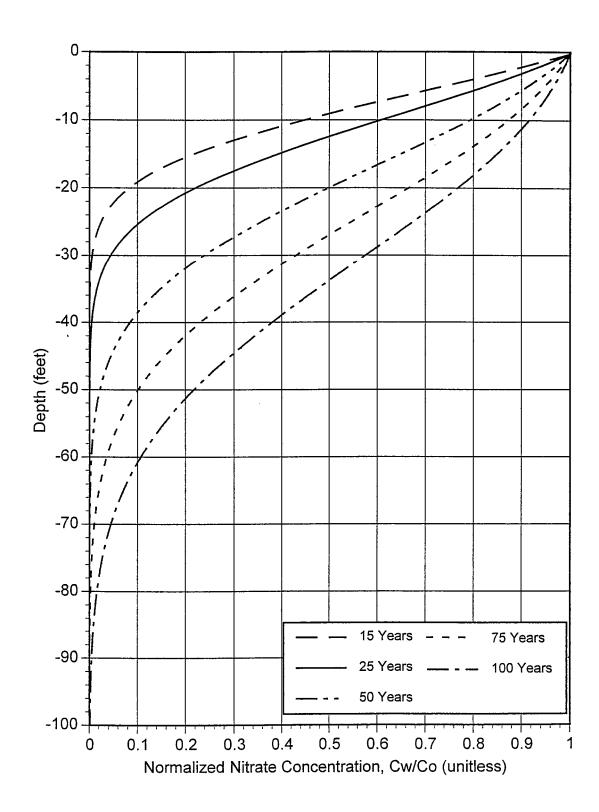


Figure 14. Predicted Normalized Concentration of Nitrate, for Land Application on Loamy Sand Sediments.

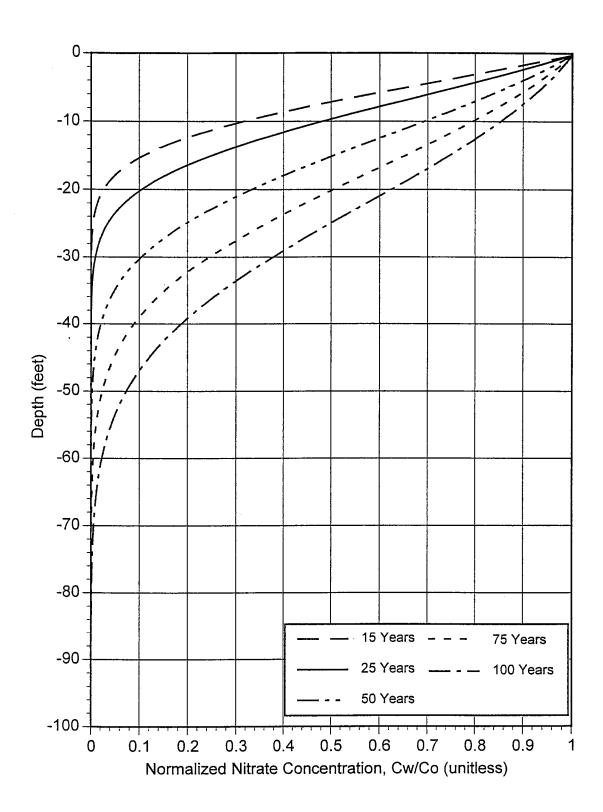


Figure 15. Predicted Normalized Concentration of Nitrate, for Land Application on Sandy Loam Sediments.

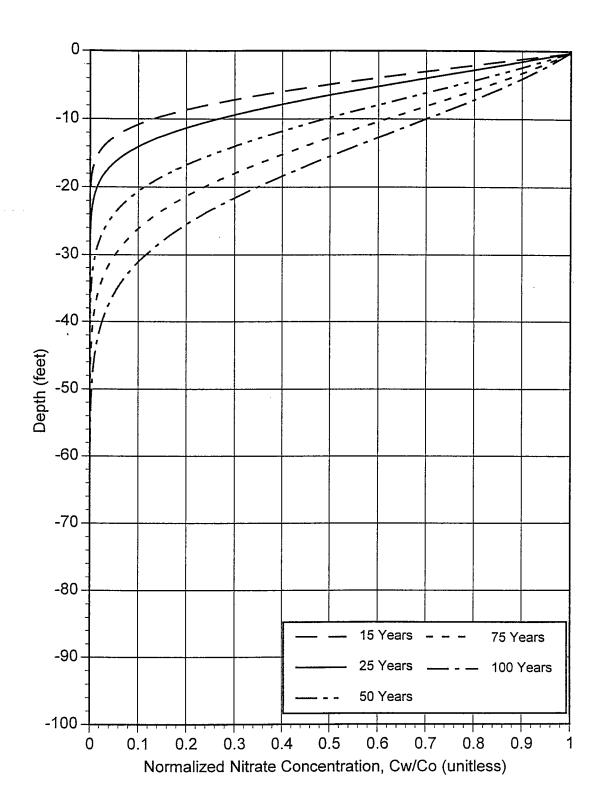


Figure 16. Predicted Normalized Concentration of Nitrate, for Land Application on Silt Loam Sediments.

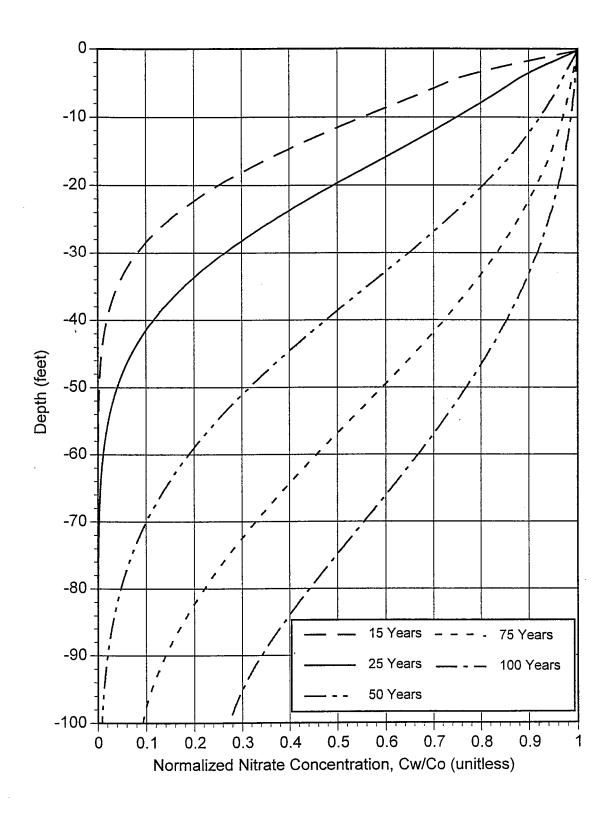


Figure 17. Predicted Normalized Concentration of Nitrate, for Septage Impoundment on a Fine-Grained Surface Layer Overlying Coarse Sand Sediments.

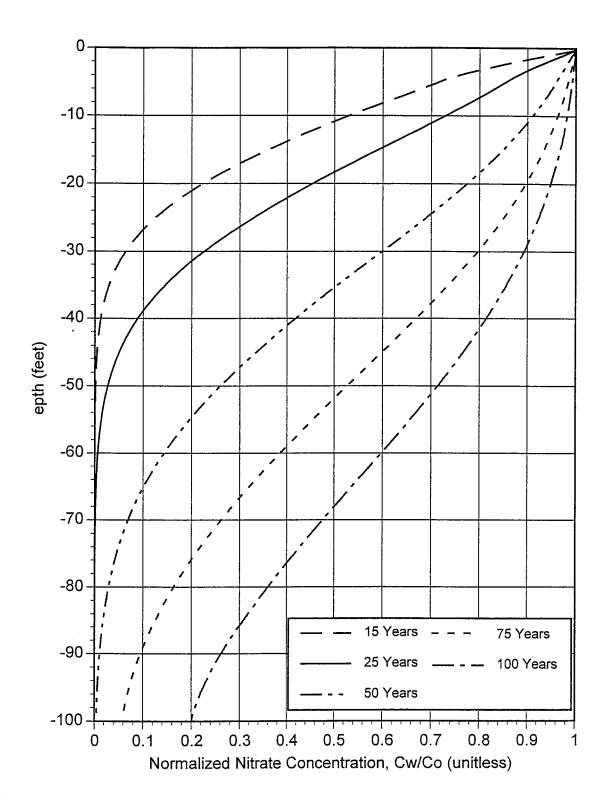


Figure 18. Predicted Normalized Concentration of Nitrate, for Septage Impoundment on a Fine-Grained Surface Layer Overlying Medium Sand Sediments.

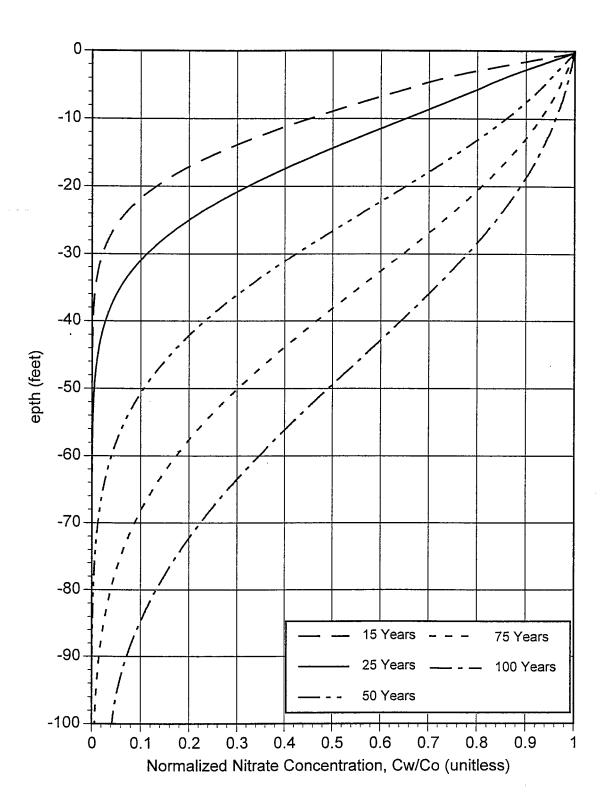


Figure 19. Predicted Normalized Concentration of Nitrate, for Septage Impoundment on a Fine-Grained Surface Layer Overlying Loamy Sand Sediments..

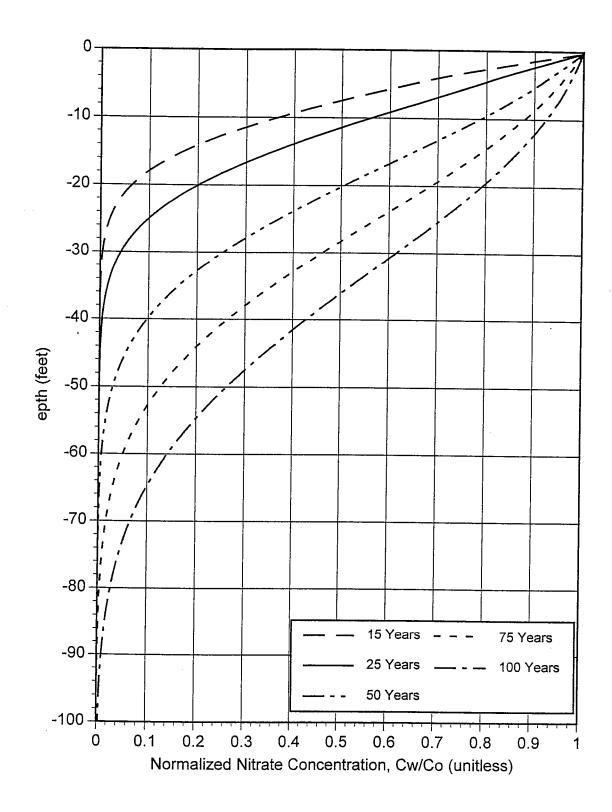


Figure 20. Predicted Normalized Concentration of Nitrate, for Septage Impoundment on a Fine-Grained Surface Layer Overlying Sandy Loam Sediments.

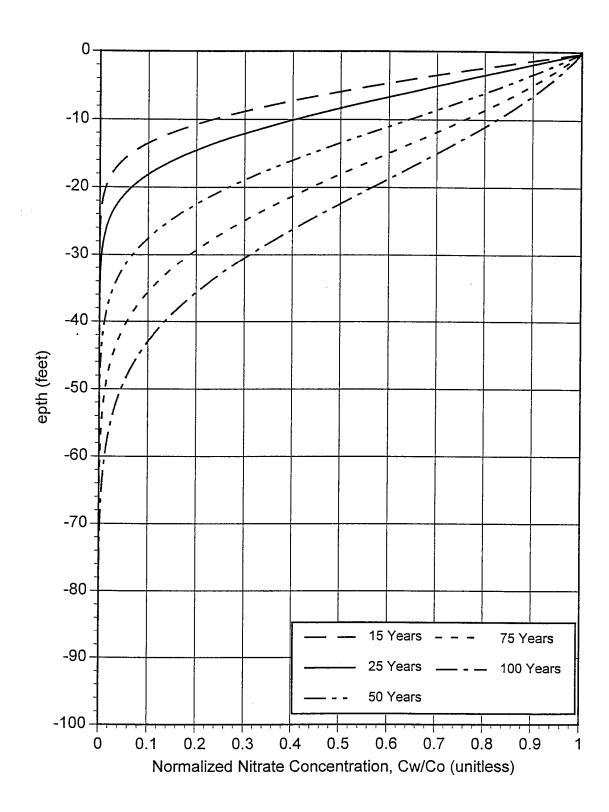


Figure 21. Predicted Normalized Concentration of Nitrate, for Septage Impoundment on a Fine-Grained Surface Layer Overlying Silt Loam Sediments.

9.0 SENSITIVITY ANALYSES

Sensitivity analyses were conducted by perturbing key input variables in both the calibrated and predictive models. There were potentially numerous variables that could be included in the sensitivity simulations; however, because of project constraints, it was important to limit the variables examined to those that were believed to have the greatest effect on model results.

Two types of variables were ultimately chosen for the sensitivity analyes: (1) saturated hydraulic conductivity and (2) infiltration rate at the ground surface, q, or factors that influence it. Dispersivity was not included in the perturbation simulations because DE&S has found during previous transport modeling investigations that this parameter typically has less influence on contaminant migration than do other transport inputs and the variables affecting flow. The van Genuchten parameters were also excluded from the sensitivity model runs because they appeared to have little influence on model results during calibration.

9.1 Perturbation Simulations

9.1.1 Calibrated Models

Three perturbation simulations were conducted using calibrated models. In the first simulation, the model of Cluster 2 at the Santa Fe facility was rerun using a saturated hydraulic conductivity of the main sediment (i.e., the materials below the surface layer) that was five times greater than the value used for calibration. In the second simulation, the long-term infiltration rate q in the Santa Fe Cluster 2 model was set at double the rate used in the calibrated model. In the third simulation, the model for Taos Cluster 1 was rerun using a septage depth, ψ_s , that was one-half the value used for calibration (i.e., septage depth = 1.5 feet). The results of these simulations are illustrated in Figures 22, 23 and 24, respectively.

The impacts of the first sensitivity run with the Santa Fe Cluster 2 model are not obvious. A five-fold increase the saturated hydraulic conductivity of the main sediment at the site produces concentrations (Figure 22) that are larger than those computed by the calibrated model (Figure 2), but the increase is slight. Moreover, the computed nitrate concentration profile in Figure 22 still appears to fit the observed nitrate concentration reasonably well. This result demonstrates that it is relatively difficult during model calibration to pinpoint what the actual sediment saturated hydraulic conductivity is, and that several values of sediment K_s could probably be used to produce reasonable calibration results.

In contrast, the computed concentration profile for Santa Fe Cluster 2 using an infiltration rate that is double the calibrated value (Figure 23) is far different from that produced by the calibrated model (Figure 2), and also departs significantly from the observed profile. In the latter perturbation simulation, the computed nitrate concentrations between the 10-and 30-foot depths exceed the calibrated model counterparts by 1000 mg/L or more.

These findings suggest that the infiltration rate occurring at a site plays a much bigger role than material properties in controlling the penetration depth of a nitrate plume.

Findings from the third perturbation simulation, in which septage depth ψ_s at Taos Cluster 1 was lowered from 3 to 1.5 feet, are similar to those developed from the first sensitivity simulation with the Santa Fe Cluster 2 model. That is, the computed nitrate concentrations (Figure 24) are somewhat smaller than the calibrated model counterparts (Figure 3), but the resulting match with observed concentrations is still reasonable. The reasonable match occurs although the computed seepage rate for the sensitivity run is 1.1E-04 ft/day, about 75% of the infiltration rate computed in the calibrated model. Again this observation illustrates that the parameters ultimately applied in a calibrated model are non-unique, and that several combinations of input variables will likely produce defensible calibration results. The fact that the calibrated model for Taos Cluster 1 uses the relatively large septage depth of 3.0 feet, and produces concentrations (Figure 3) that are larger than those computed in the sensitivity run (Figure 24), suggests that any predictive model runs based on parameters similar to those used in the calibrated model will likely produce conservatively large penetration depths for nitrate over time.

9.1.2 Predictive Model Sensitivity Runs

The predictive model sensitivity runs were made with the intent of illustrating how variations in saturated hydraulic conductivity and the downward seepage rate affect the depth to which nitrate penetrates the subsurface at several different times beyond the start of a facility's operations. Given the 15 different predictive simulations discussed in Chapter 8, and the numerous combinations of flow parameters that could be examined for sensitivity purposes, the number of sensitivity runs conducted could have become unwieldy. Consequently, DE&S chose to perform perturbation simulations for a single set of the soil properties listed in Table 6, for both a land application and a septage impoundment scenario. The chosen properties were thought to be most representative of the conditions observed at the three disposal facilities examined for this project. All simulations were based on a domain consisting of a relatively fine-grained surface layer overlying a coarser-grained sediment. The properties for a medium sand were selected to represent the coarser-grained material and the base-case properties of the surface layer corresponded to values shown in Table 6 for a land application site and a septage impoundment facility, respectively. As in previous analyses, a septage depth of 3 feet was assumed in all of the impoundment simulations.

The results of the various sensitivity runs with the predictive model are presented in two ways. First, the depth of nitrate penetration below ground surface at 15, 25, 50, 75, and 100 years is tabulated. The penetration depth is arbitrarily defined as the depth at which normalized concentration has a value of 0.01, or 1%. Table 7 shows the parameters that were perturbed for the land application model runs, the degree to which they were perturbed, and the corresponding sensitivity results in terms of nitrate penetration depth. Table 8 presents analogous results from the sensitivity runs for a septage impoundment scenario. Base-case results are presented in each table for comparison.

Results from the predictive model sensitivity runs are also shown in graphical form in Appendix A. A total of ten graphs are presented, each of which shows base-case model results and the computed normalized concentrations for each of the perturbation simulations at a specific time after facility startup. The graphical results of the simulations based on land application of sludge or septage (Figures A-1 through A-5) are significant because they clearly illustrate the strong influence of long-term infiltration rate q on the vertical penetration of dissolved nitrate over time. At any of the illustrated times, the normalized concentrations computed over the 20- to 30-foot depth range using an infiltration rate that is twice the base-case value is substantially larger than the computed base-case concentration.

As a whole, the figures in Appendix A provide a feasible range of normalized concentrations that could be expected at sites in New Mexico with conditions similar to those observed at the three field study locales.

Table 7. Sensitivity Results for Land Application Predictions

	Depth of Nitrate Penetration $(C_w/C_0 = 0.01)$ (feet)					
Time =	15 Yrs	25 Yrs	50 Yrs	75 Yrs	100 Yrs	
Sensitivity Simulation						
Base Case	29	40	63	82	>100	
Doubled Infiltration Rate (q x 2)	48	66	>100	>100	>100	
Halved Infiltration Rate (q/2)	19	26	41	53	65	
Five-fold Increase of Main Sediment Saturated Hydraulic Conductivity (K _s x 5)	30	41	65	86	>100	
Five-fold Decrease of Main Sediment Saturated Hydraulic Conductivity (K _s /5)	27	38	59	77	94	

Table 8. Sensitivity Results for Septage Impoundment Predictions

	Depth of Nitrate Penetration ($C_w/C_0 = 0.01$) (feet)					
Time =	15 Yrs	25 Yrs	50 Yrs	75 Yrs	100 Yrs	
Sensitivity Simulation						
Base Case	41	57	91	>100	>100	
Increase Septage Depth 1 Foot (ψ _s = 4 ft)	44	62	99	>100	>100	
Decrease Septage Depth 1 Foot (ψ _s = 2 ft)	37	52	82	>100	>100	
Five-fold Increase of Main Sediment Saturated Hydraulic Conductivity (K _s x 5)	43	59	95	>100	>100	
Five-fold Decrease of Main Sediment Saturated Hydraulic Conductivity (K _s /5)	38	53	84	>100	>100	

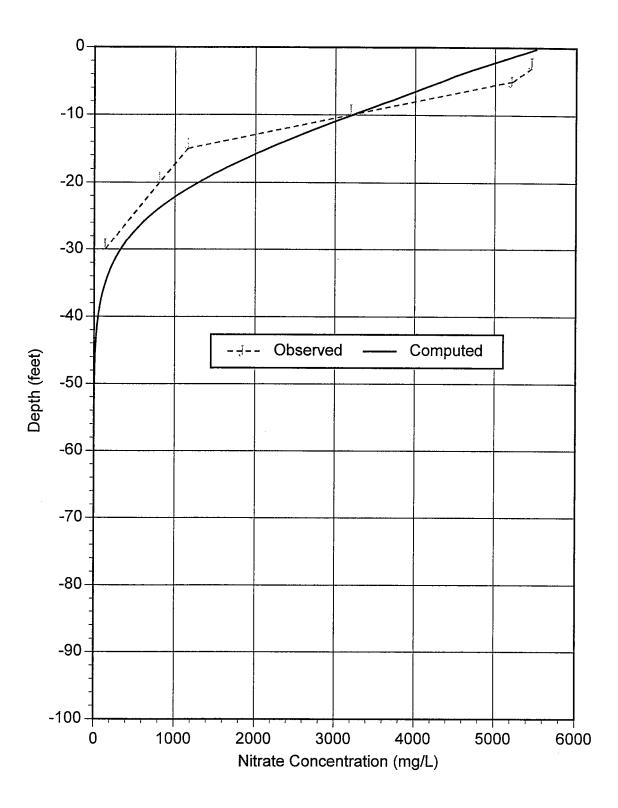


Figure 22. Predicted Nitrate Concentrations at Santa Fe Cluster 2 Using a Five-Fold Increase in the Main Sediment Saturated Hydraulic Conductivity.

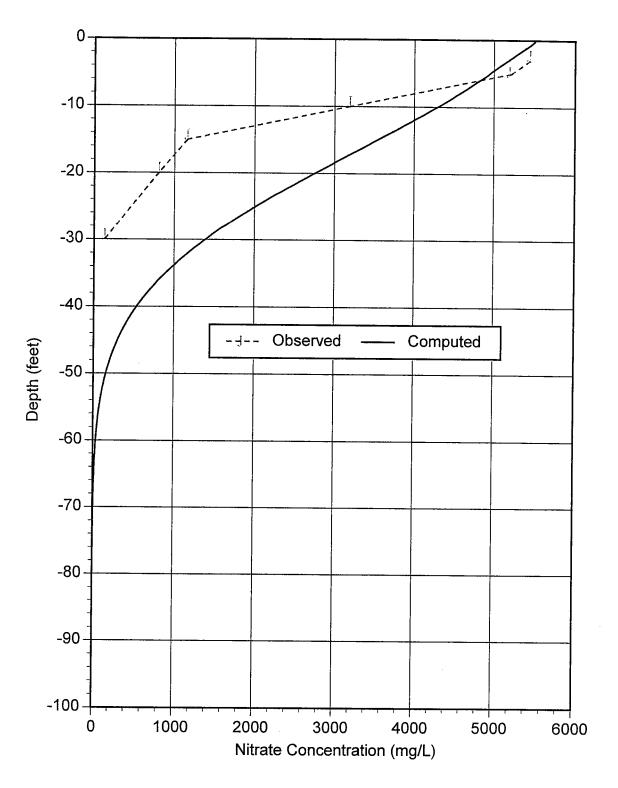


Figure 23. Predicted Nitrate Concentrations at Santa Fe Cluster 2 Using Twice the Calibrated Model Infiltration Rate.

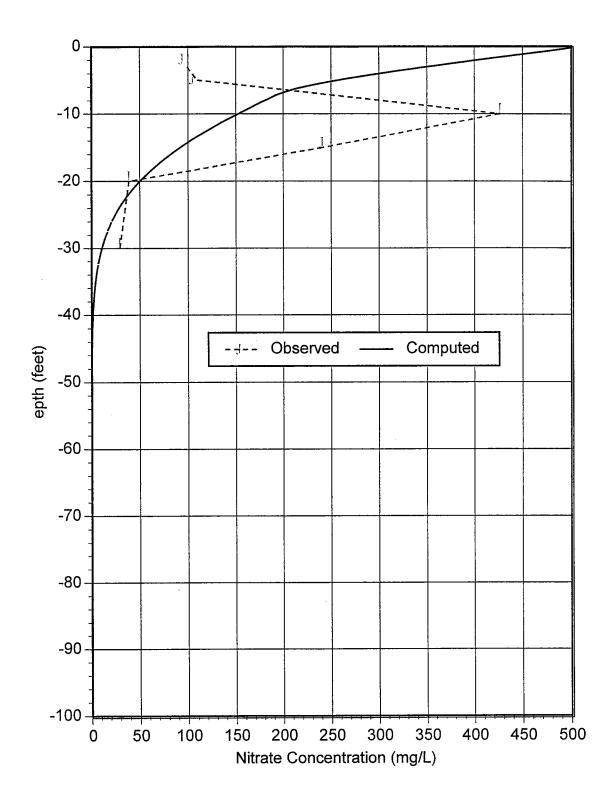


Figure 24. Predicted Nitrate Concentrations at Taos Cluster 1 Using Half the Calibrated Model Septage Depth ($\psi_s = 1.5$ feet).

10.0 CONCLUSIONS

- (1) The unsaturated flow and transport simulations performed under this study have resulted in feasible estimates of soil properties and long-term infiltration rates that could be expected at sludge and septage disposal facilities in New Mexico.
- (2) The models that have been calibrated using observed nitrate concentrations at the Santa Fe Sludge Disposal Facility, the Taos Impoundment Facility, and the Albuquerque Soil Amendment Facility, suggest that the long-term infiltration rate at each is relatively small, presumably the result of soil properties in a relatively fine-grained layer of surface soil. The infiltration rate at the Taos Facility appears to be limited by the presence of very low permeability materials in the surface layer, which is possibly the result of pore clogging by biological means or filtration of fine particles.
- (3) The most important parameter affecting downward migration rates of nitrate emanating from sludge and/or septage facilities is the long-term infiltration rate. The loading rate for nitrate, herein defined as the product of the infiltration rate and a nitrate source concentration in the aqueous phase, provides a key measure of the nitrate concentrations that can be expected below a site several years after it has begun operations.
- (4) Sensitivity analyses conducted with both calibrated and predictive models clearly illustrate that doubling of long-term infiltration rate can cause nitrate to migrate downward at a rate that is many times faster than the rate induced by a five-fold increase in saturated hydraulic conductivity of the main sediments through which nitrate migrates. Consequently, the more time that applied sludge or septage has to dry through evaporation, the more likely it is that the moisture levels in surface soils will be reduced, thus limiting the downward seepage rate and reducing downward migration of nitrate. This observation also means that downward penetration of nitrate can be reduced by (1) placing septage on a low-permeability surface layer, and (b) keeping low hydraulic pressure on the surface layer by minimizing septage depth, thereby limiting infiltration.
- (5) Several predictive simulations based on generic soil properties similar to those observed at the field investigation sites provide reasonable estimates of the depth to which aqueous-phase nitrate may penetrate the subsurface for periods of time exceeding the 13 to 16 years that the field sites have been in operation.
- (6) The calibrated models and predictive simulations in this study support the field investigation findings that nitrate has the potential to migrate to depths of about 20 to 30 feet after about 15 years of facility operation. Thus it would be imprudent to dispose of sludge or septage in an area where the water table was located at a relatively shallow depth.

- (7) Given that the two components of mass loading of nitrogen in the aqueous phase infiltration (downward seepage) rate and aqueous-phase concentration are to a large extent the determinants of nitrate concentration with depth below ground surface, a great deal of insight regarding the vertical extent of nitrate migration could be developed by (a) determining the type of surface soil at an active site and monitoring moisture contents within it, and (b) measuring the aqueous-phase concentration in the applied sludge or septage. The former parameters are descriptive of surface soil and could be used to estimate the long-term, downward seepage rate.
- (8) Several graphs of normalized nitrate concentration versus depth based on predictive simulations provide a means of estimating nitrate penetration and concomitant aqueous-phase concentrations for sites in New Mexico that are similar to the field sites studied under this project. Tables of results from sensitivity analyses based on the generic predictive simulations provide a range of estimated nitrate penetration depths and associated normalized concentrations that would be expected at similar New Mexico sites.
- (9) For sites that differ considerably from the three that have been characterized under this study, estimates of nitrate penetration in the subsurface and associated concentrations should be developed using a site-specific, unsaturated flow and transport model.

11.0 RECOMMENDATIONS

This report contains several aids and suggestions for estimating the downward transport of nitrate below land application and impoundment facilities in New Mexico for sludge and/or septage disposal. It is recommended that these methods be applied at disposal sites in New Mexico to assess their capacity to estimate the vertical penetration of nitrate in the subsurface and the decrease in nitrate concentration with depth below a facility. The application of the methods and an assessment of their efficacy at a newly proposed site that is subsequently put into operation would be very useful.

Because of the inherent variability and uncertainty in soil conditions, infiltration rates, impoundment rotations, land application frequencies, and several other factors that affect the downward migration of nitrogen species below disposal facilities, no single study can be used to estimate the effects of nitrate loading to and subsequent transport in the subsurface at all facilities. Thus it is helpful if site-specific conditions can be explicitly modeled whenever warranted by the data collected for a site. Accordingly, it is recommended that readers of this report become versed in the application of an unsaturated flow and transport model to actual sites. The finite-difference model applied in this investigation, VS2DT, is an example of a model that is capable of providing credible estimates of long-term nitrate migration given sludge or septage properties and information about the sediments upon or in which wastes are placed. The graphical user interface supplied with the model, VS2DI, makes it possible to develop preliminary predictions of downward nitrate transport within periods of several minutes to a few hours.

12.0 REFERENCES

- Canter, L.W., 1997. Nitrates in groundwater. CRC Press, Boca Raton, Florida, 263 p.
- Charbeneau, R.J., and D.E. Daniel, 1993. Contaminant transport in unsaturated flow. Chapter 15 in Handbook of Hydrology, D.R. Maidment, Editor in Chief.
- Finch, S.T., Jr., 1999. Evaluation of the migration of nitrogen compounds at the City of Santa Fe sludge disposal site near Santa Fe, New Mexico and at the S&R septage disposal site near Taos, New Mexico. John Shomaker and Associates, Inc. (JSAI), Albuquerque, NM.
- Finch, S.T., Jr., 2000. Evaluation of the migration of nitrogen compounds at the City of Albuquerque soil amendment facility near Albuquerque, New Mexico. John Shomaker and Associates, Inc. (JSAI), Albuquerque, NM.
- Hantzsche, N.N., and E.J. Finnemore, 1992. Predicting ground-water nitrate-nitrogen impacts. Ground Water, 30(4), pp. 490-499.
- Healy, R.W., 1990. Simulation of Solute Transport in variably saturated porous media with supplemental information on modifications to the U.S. Geological Survey's computer program VS2D. U.S. Geological Survey, Water-Resources Investigations Report 90-4025, 125 p.
- Healy, R.W., and Ronan, A.D., 1996. Documentation of computer program VS2DH for simulation of energy transport in variably saturated porous media -- modification of the U.S. Geological Survey's computer program VS2DT: U.S. Geological Survey Water-Resources Investigations Report 96-4230, 36 p.
- Hsieh, P.A., W. Wingle, and R.W. Healy, 2000. VS2DI--A graphical software package for simulating fluid flow and solute or energy transport in variably saturated porous media: U.S. Geological Survey Water-Resources Investigations Report 99-4130, 16 p.
- Lappala, E.G., R.W. Healy, and E.P. Weeks, 1987. Documentation of computer program VS2D to solve the equations of variably saturated porous media. U.S. Geological Survey, Water-Resources Investigations Report 83-4099, 184 p.
- Leij, F.J., W.J. Alves, M.Th. van Genuchten, and J.R. Williams, 1996. User's manual of UNSODA unsaturated soil hydraulic database. United States Environmental Protection Agency, National Risk Management Research Laboratory, EPA/600/R-96/095, 103 p.

- McCord, J.T., and D.B. Stephens, 1987. Lateral moisture movement on sandy hillslopes in the apparent absence of an impeding layer. Hydrologic Processes, vol. 1, no. 3, pp. 225-238.
- Phillips, F.M., J.L. Mattick, and T.A. Duval, 1988. Chlorine-36 and tritium from nuclear weapons fallout as tracers for long-term liquid and vapor movement in desert soils. Water Resources Research, vol. 24, no. 11, pp. 1677-1691.
- Rawls, W.J., L.R. Ahuja, D.L. Brakensiek, and A. Shirmohammadi, 1993. Infiltration and soil water movement. Chapter 5 in the Handbook of Hydrology, D.R. Maidment, editor in chief, McGraw-Hill.
- Sandia National Laboratories (SNL), 1996. Site-wide hydrogeological characterization report, calendar year 1995, annual report.
- Simunek, J., and M. Th. van Genuchten, 1994. The CHAIN_2D code for simulating the two-dimensional movement of water, heat, and multiple solutes in variably-saturated porous media. U.S. Department of Agriculture, U.S. Salinity Laboratory, Riverside, California, Research Report No. 136, 194 p.
- Stephens, D.B., and R.G. Knowlton, Jr., 1986. Soil-water movement and recharge through sand at a semi-arid site in New Mexico. Water Resources Research, vol. 22, pp. 881-889.
- U.S. Environmental Protection Agency (EPA), 1994. Guide to septage treatment and disposal. EPA/625/R-94/002, 59 p.
- U.S. Environmental Protection Agency (EPA), 1995. Surface disposal of sewage sludge and domestic septage Office of Research and Development, Washington, D.C., EPA/625/R-95/002.
- U.S. Soil Conservation Service (SCS), 1977. Soil survey of Bernalillo County and Parts of Sandoval and Valencia Counties, New Mexico. U.S. Department of Agriculture, 114 p.

APPENDIX A

PREDICTIVE SIMULATION SENSITIVITY RESULTS

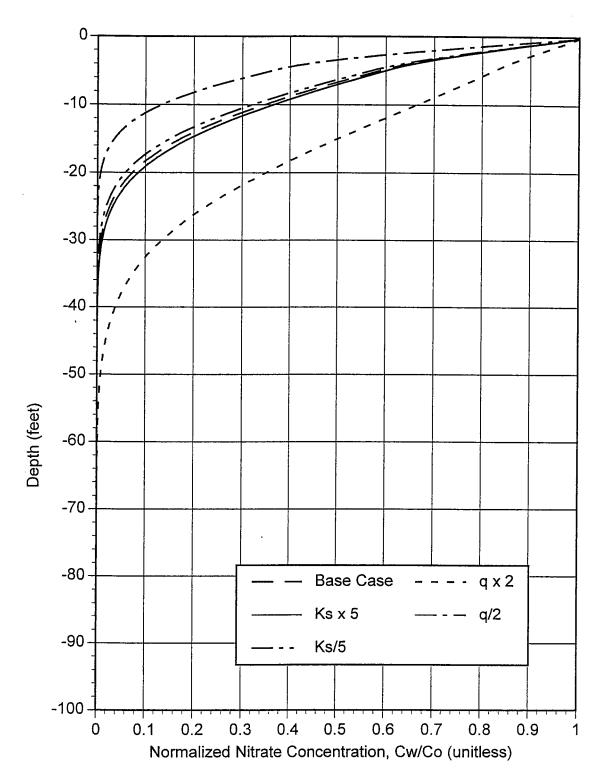


Figure A-1. Results of Predictive Model Sensitivity Simulations for Land Application at 15 Years After Facility Startup.

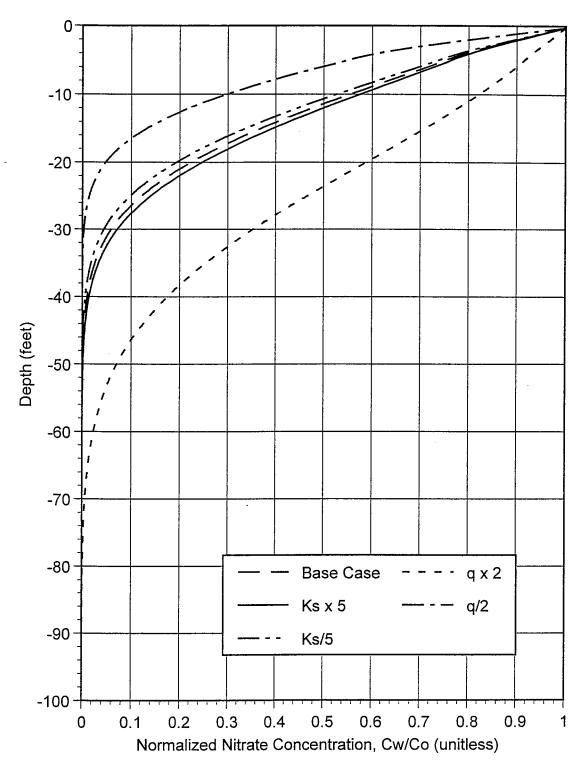


Figure A-2. Results of Predictive Model Sensitivity Simulations for Land Application at 25 Years After Facility Startup.

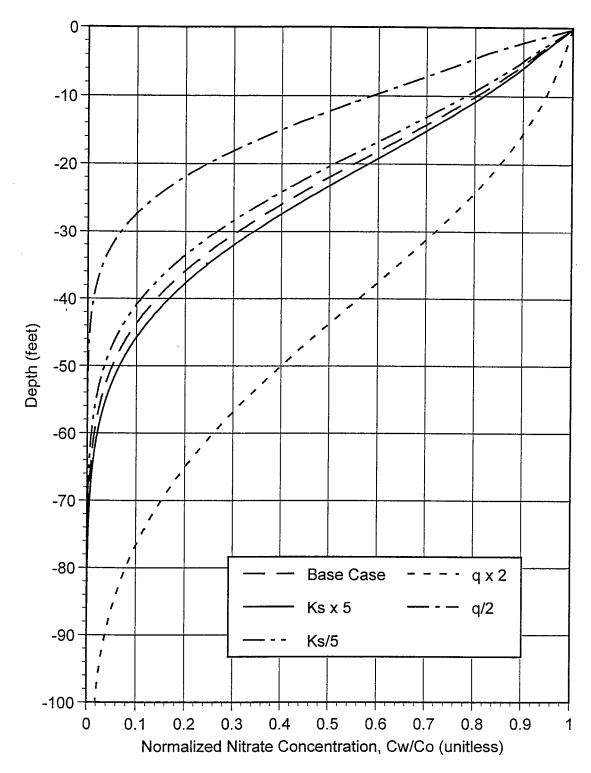


Figure A-3. Results of Predictive Model Sensitivity Simulations for Land Application at 50 Years After Facility Startup.

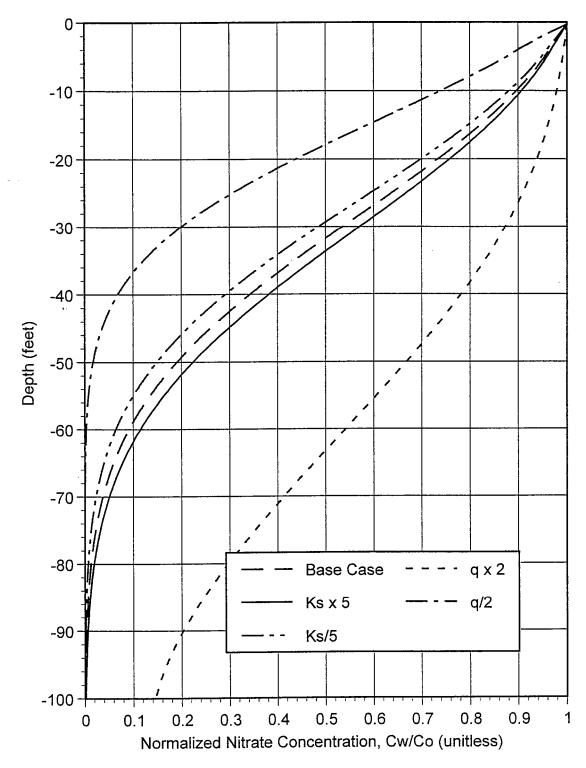


Figure A-4. Results of Predictive Model Sensitivity Simulations for Land Application at 75 Years After Facility Startup.

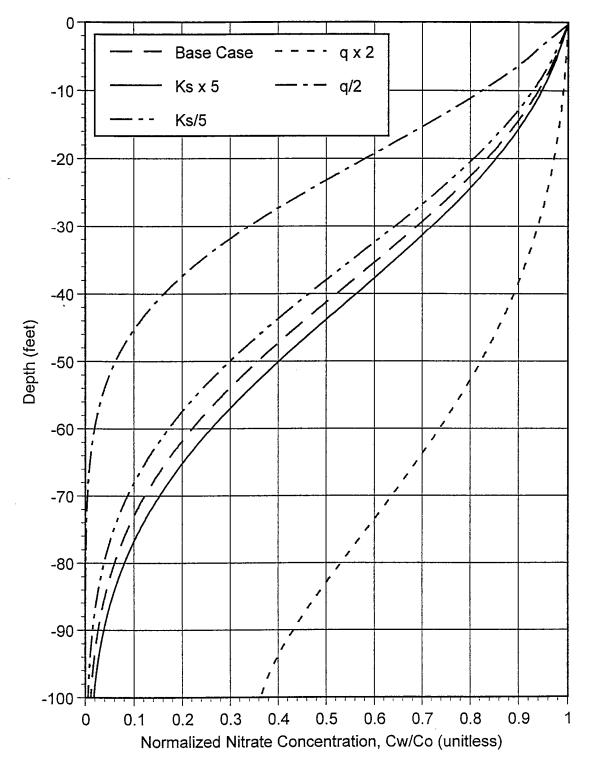


Figure A-5. Results of Predictive Model Sensitivity Simulations for Land Application at 100 Years After Facility Startup.

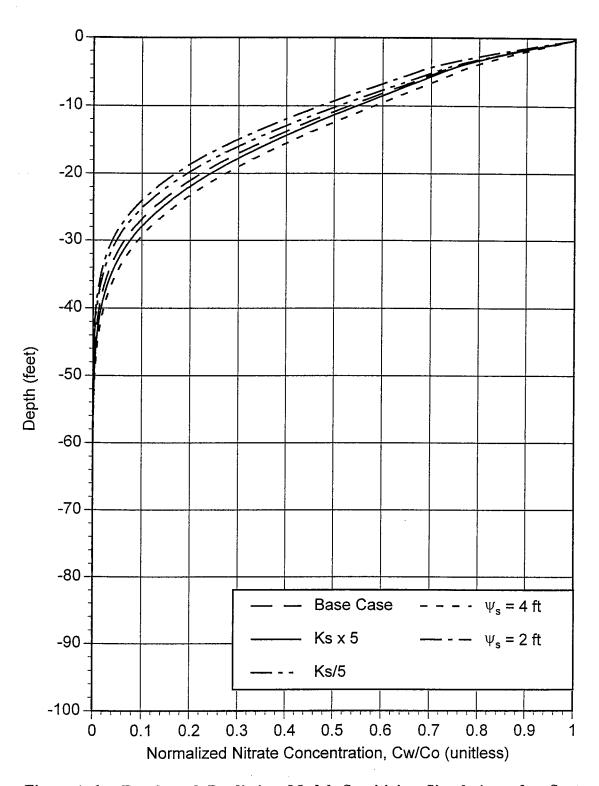


Figure A-6. Results of Predictive Model Sensitivity Simulations for Septage Impoundment at 15 Years After Facility Startup.

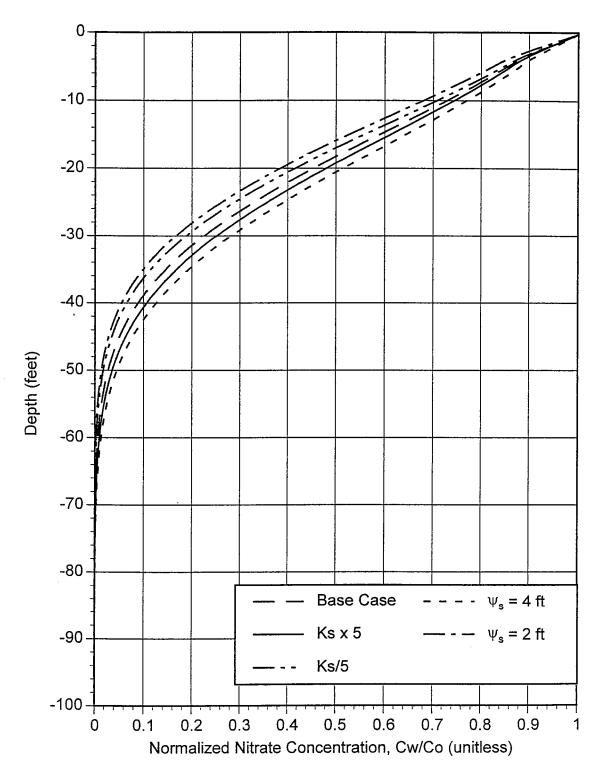


Figure A-7. Results of Predictive Model Sensitivity Simulations for Septage Impoundment at 25 Years After Facility Startup.

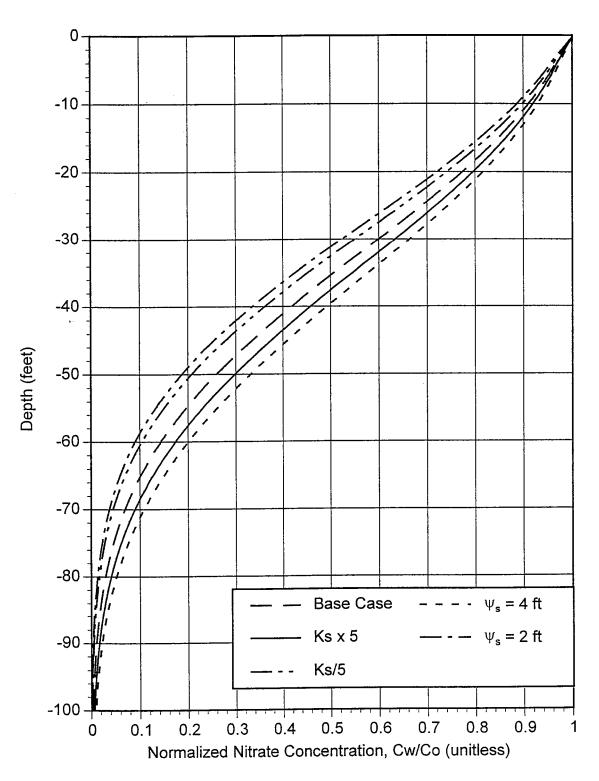


Figure A-8. Results of Predictive Model Sensitivity Simulations for Septage Impoundment at 50 Years After Facility Startup.

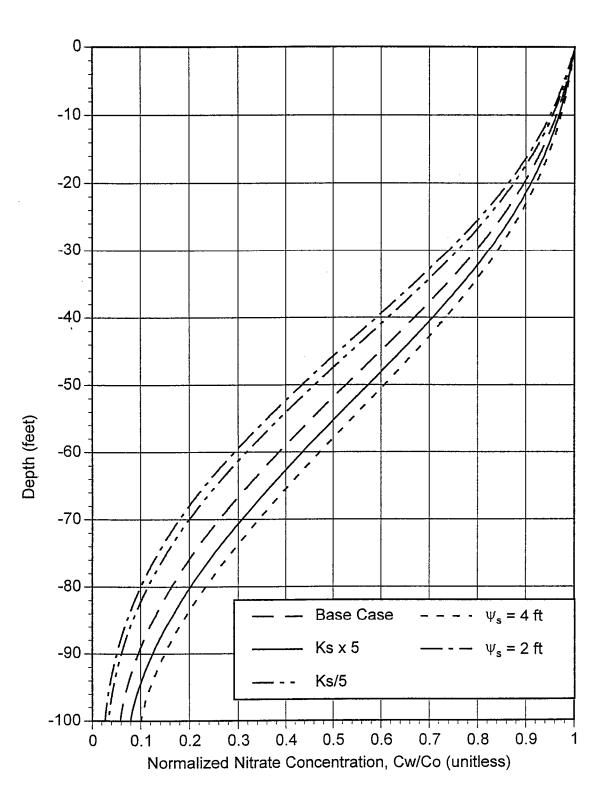


Figure A-9. Results of Predictive Model Sensitivity Simulations for Septage Impoundment at 75 Years After Facility Startup.