A COMPARISON BETWEEN SIMPLE AND DETAILED METHODS FOR ANALYZING RELEASES OF RADIONUCLIDES TO GROUND WATER FROM LOW-LEVEL WASTE FACILITIES*

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ABSTRACT

A performance assessment methodology has been developed for use by the U.S. Nuclear Regulatory Commission in evaluating license applications for low-level waste disposal facilities. The methodology has been designed to be modular in structure, so that either simple or more complex analyses can be used, as appropriate. This paper compares results from a simple ground-water transport analysis implemented in the computer code PAGAN to results from VAM2D, which is used in the methodology for more complicated analyses. It is shown that the two approaches are in excellent agreement when the conceptual model is compatible with the assumptions in the simple approach. When the two codes are compared for a more complicated situation, the simpler approach tends to be conservative.

INTRODUCTION

A performance assessment methodology has been developed for use by the U.S. Nuclear Regulatory Commission (NRC) in evaluating license applications for low-level waste disposal facilities (1). The methodology has been designed to be modular in structure, which greatly increases the flexibility of the methodology in handling a variety of disposal conditions. For each module in the methodology, the user can choose either a simple or a more complicated approach. The concept is to use reasonably simple modeling approaches, and graduate to more complicated approaches only if the site merits the additional detail (2). It is desirable in this methodology for the simpler approach to be the more conservative of the two approaches. If this is the case, one can generate confidence that the simpler model bounds the behavior of the more complicated model.

One of the key components of low-level waste performance assessment is the analysis of the ground-water pathway (3). The approach used in the low-level waste performance assessment methodology for simple analyses of ground-water concentrations is embodied in a personal-computer based computer code named PAGAN, Version 1.1 (Performance Assessment Ground-water Analysis for low-level Nuclear waste). PAGAN contains a simple model for releases from a disposal unit that is based on a cascade of mixing cells, and includes leach mechanisms that can be used to analyze either surface-contaminated wastes or diffusion-controlled releases (4, 5). The results from this source-term model provide input to a simple model for transport in an aquifer. Details of the models implemented in PAGAN are discussed in detail by Kozak et al. (4), and a user's guide to the code is given in Chu et al. (5).

The approach used in the methodology for more complicated analyses is to use either VAM2D (6) or FEMWATER/BLT (7). VAM2D is a two-dimensional finite-element computer code for the analysis of both flow and transport in both vadose and saturated zones. It has considerable flexibility in the types of boundary conditions that can be specified, and contains numerical methods that converge for a wide variety of nonlinear problems. FEMWATER/BLT is also a two-dimensional code for analyzing flow and transport in both vadose and saturated zones. In addition, the package includes comparatively sophisticated methods for the analyzing the breach rate of waste containers, and the leach rate of radionuclides from waste forms. However, the numerical methods used in FEMWATER have been found to be somewhat less robust in analyzing vadose-zone flow than are those used in VAM2D (4).

Kozak et al. (4) conducted a comparisons between the models in PAGAN and VAM2D, as well as between PAGAN and FEMWATER/BLT. The intent of this study was to compare the simple and complicated approaches to ground-water transport for an overall analysis of a low-level waste disposal trench. The conceptual model used in this comparison was of a disposal trench over an unconfined aquifer. In each case tested, the models in PAGAN exhibited less dispersion and higher (hence more conservative) ground-water concentrations than either VAM2D or FEMWATER/BLT. It was concluded that the differences were due to two effects that were accounted for in the more complicated analyses, but not in PAGAN. These effects were (a) dilution at the water table due to recharge, and (b) dispersion in the unsaturated zone.

The purpose of the present contribution is to test this conclusion by comparing results from PAGAN to results from VAM2D for a conceptual model in which the two

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complicating effects are absent. In essence, these analyses can be considered a benchmarking exercise. The results of the exercise are intended to increase confidence in both codes. In order to conduct a benchmarking exercise, it is necessary to compare the assumptions made in the two codes, to ensure that the assumptions are compatible for the conceptual model. Consequently, the assumptions in the two codes are briefly given here.

PAGAN, VERSION 1.1

PAGAN, Version 1.1 has the capability to model the source term, vadose-zone transport, and aquifer transport of radionuclides from a waste disposal unit. Version 1.1 primarily differs from Version 1.0 in its treatment of dispersivity. In Version 1.0 dispersivity was defined as the dispersion coefficient divided by Darcy velocity. This definition, while not incorrect, is not standard. It is standard to define dispersivity as dispersion coefficient divided by pore velocity (Darcy velocity over porosity); Version 1.1 of PAGAN defines dispersivity in standard fashion. Source-term releases are described using the mixing-cell cascade source-term model, and vadose-zone transport is treated as a simple delay time between the bottom of the disposal unit and the water table. These aspects of the code will not be of concern in this analysis, and will not be discussed further in this paper. Further details on these aspects of the code are available in prior reports on the performance assessment methodology (4, 5).

Aquifer transport is modeled using the conventional convective-dispersion equation. The Darcy velocity in the aquifer is assumed to be one-dimensional, uniform, and constant; the aquifer is assumed to be homogeneous and isotropic, and of arbitrary but uniform thickness. An arbitrary rectangular (plan view) source is considered at the top boundary of the aquifer (at the water table for an unconfined aquifer). The solution allows three-dimensional dispersion and one-dimensional convection. Simple radioactive decay and linear (K_d) sorption are accounted for in the source and in the aquifer. The code calculates the maximum concentration in the plume at a particular distance; that is, the centerline concentration at the top of the aquifer. The concentration is not averaged over any depth, nor are dilution effects in the pumping well accounted for. These are intended to be conservative assumptions about the concentration available for consumption at a well. The solution to the convective-dispersion equation in the aquifer is effected by a numerical integration of an analytical Green's function. The integrand consists of the product of the Green's function times the source rate given by the mixing-cell cascade source-term model, as described in Kozak et al. (4).

VAM2D

VAM2D is a two-dimensional, finite-element code for the analysis of both flow and transport in both saturated and vadose zones. Radionuclide transport is simulated using the conventional convective-dispersion equation. The user can either solve for the flow field to be used in the convective-dispersion equation, or can specify a flow field. VAM2D accounts for two-dimensional dispersion, and the dispersion is specified as a combination of molecular diffusivity and mechanical dispersion. The user can analyze linear (K_d) sorption, simple radioactive decay, or chain decay up to four-member chains. Radionuclide sources can be specified as constant flux, constant concentration, transient flux, or transient concentration types. Details about VAM2D, its numerical methods, and capabilites are available in Huyakorn et al. (6).

TEST CASE DESCRIPTION

The benchmarking analyses were performed for a confined, homogeneous, isotropic aquifer. The aquifer properties were arbitrarily chosen to be porosity 0.3, Darcy velocity 2.3 m/yr, aquifer depth 25 m. A 16 m long (in the dimension parallel to the aquifer flow direction) radionuclide source was imposed at the upper surface of the aquifer, as shown in Fig. 1. The radionuclide release rate was specified to be a constant flux.

The VAM2D finite-element grid used in the analysis of this problem is shown in Fig. 1. The overall domain is 2500 centimeters deep by 23000 centimeters in lateral extent. There are 51 nodes in the horizontal direction and 6 in the vertical direction. The top and bottom surfaces are specified as no flux, and a uniform Darcy flow field (from left to right) was imposed throughout the domain. The

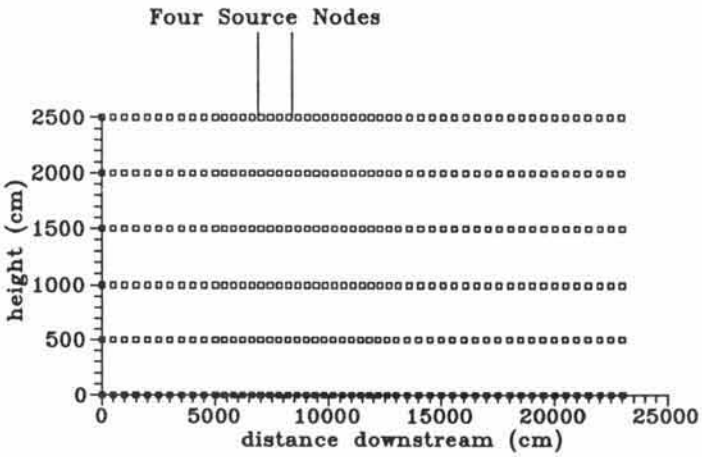

Fig. 1. VAM2D Finite-Element Grid (vertical exaggeration 5:1).

radionuclide source nodes were specified to be the four nodes centered around 76 meters downstream from the left boundary of the domain, at the top of the domain.

As discussed in Kozak et al. (4), to put the two-dimensional VAM2D solution and the three-dimensional PAGAN solution on the same basis, one must be careful to account for two effects in the release rate. First, the two-dimensional solution implicitly assumes that negligible effects occur in the third dimension, which means that the source width (perpendicular to the aquifer flow) used in PAGAN must be specified to be large. In this way any end effects from the third dimension of the source are eliminated. In the analyses described in this paper, the source width was set to 10,000 meters. Second, fluxes in the VAM2D simulations are specified per centimeter width of the source. To put the two analyses on the same flux basis, a VAM2D discharge rate per unit length of the source must be multiplied by 10^6 for use in PAGAN with a 10,000 meter wide source. For the analyses to be discussed here, the initial flux for all cases was chosen to be 0.1533 Ci/m^2/yr. This flux is subject to radioactive decay in both analyses.

Dispersivity is defined differently in the two codes. As discussed above, in PAGAN Version 1.1 the dispersion coefficient (either transverse or longitudinal) is the product of the dispersivity and the pore velocity. In VAM2D the definition of dispersion coefficient includes a term for apparent molecular diffusivity (6). Consequently, the dispersion coefficients from the two codes were put on the same basis by setting the apparent molecular diffusivity in the VAM2D equations to zero.

RESULTS

As discussed above, PAGAN analyzes the evolution in time of the centerline concentration at the top of the aquifer. The comparisons were made between the spatial profiles of the appropriate concentration at several times.

Comparisons were made between PAGAN and VAM2D for three cases that will be described here. First, a comparison was made between the codes using tritium (H-3) to examine the concentration profile 50 years from the beginning of the release. This comparison tests the treatment of decay in both the source and the aquifer using the two codes. The second comparison tested a larger value of dispersivity, sufficiently large that the no-flux boundary condition at the bottom of the aquifer affected the results. The third case compares the two codes for a case of simultaneous high dispersivity and high retardation. The parameters of interest in these three cases are shown in Table I. The results described here are representative of a larger set of analyses that produced similar or closer comparisons between the two codes.

TABLE I

Summary of Parameter Variations

Case Number	Longitudinal Dispersivity (α_L)	Transverse Dispersivity (α_T)	Retardation Factor (R)
1	2.0 meters	0.4 meters	1.0
2	20.0 meters	4.0 meters	1.0
3	20.0 meters	4.0 meters	2.225

Case 1: Base Case H-3 Transport

The base-case analysis involves analyzing the concentration distribution as a function of downstream distance at several times following the start of release of H-3 into the aquifer. Dispersivities are $\alpha_L = 2$ meters and $\alpha_T = 0.4$ meters.

The purpose of the first comparison study is twofold. First, the case compares the treatment of convective dispersion between the two codes for a case in which the aquifer is fairly deep compared to the extent of dispersion. That is, the no-flux boundary at the bottom of the aquifer has little effect on the solution. Second, the case compares the treatment of radioactive decay in both the source release rate and in the aquifer.

Concentration contours at 50 years generated using VAM2D are shown in Fig. 2 for this case. The contours were produced by kriging nodal concentrations produced by VAM2D. Concentrations at the lower boundary are about an order of magnitude lower than the concentrations at the aquifer top, which supports the notion that the lower boundary does not strongly affect the solution.

The comparison between VAM2D and PAGAN concentration distributions at the upper boundary at 50 years is shown in Fig. 3. There is excellent agreement between the two analyses for all downstream distances. Concentration profiles were compared at other simulation times for this case, and all showed similarly close agreement.

Case 2: High Dispersivity H-3 Transport

The purpose of this analysis is to compare the codes for a case in which the contaminant plume interacts strongly with the lower boundary of the aquifer. Hence for this case both longitudinal and transverse dispersivities have been increased by a factor of ten: $\alpha_L = 20$ meters, and $\alpha_L = 4$ meters.

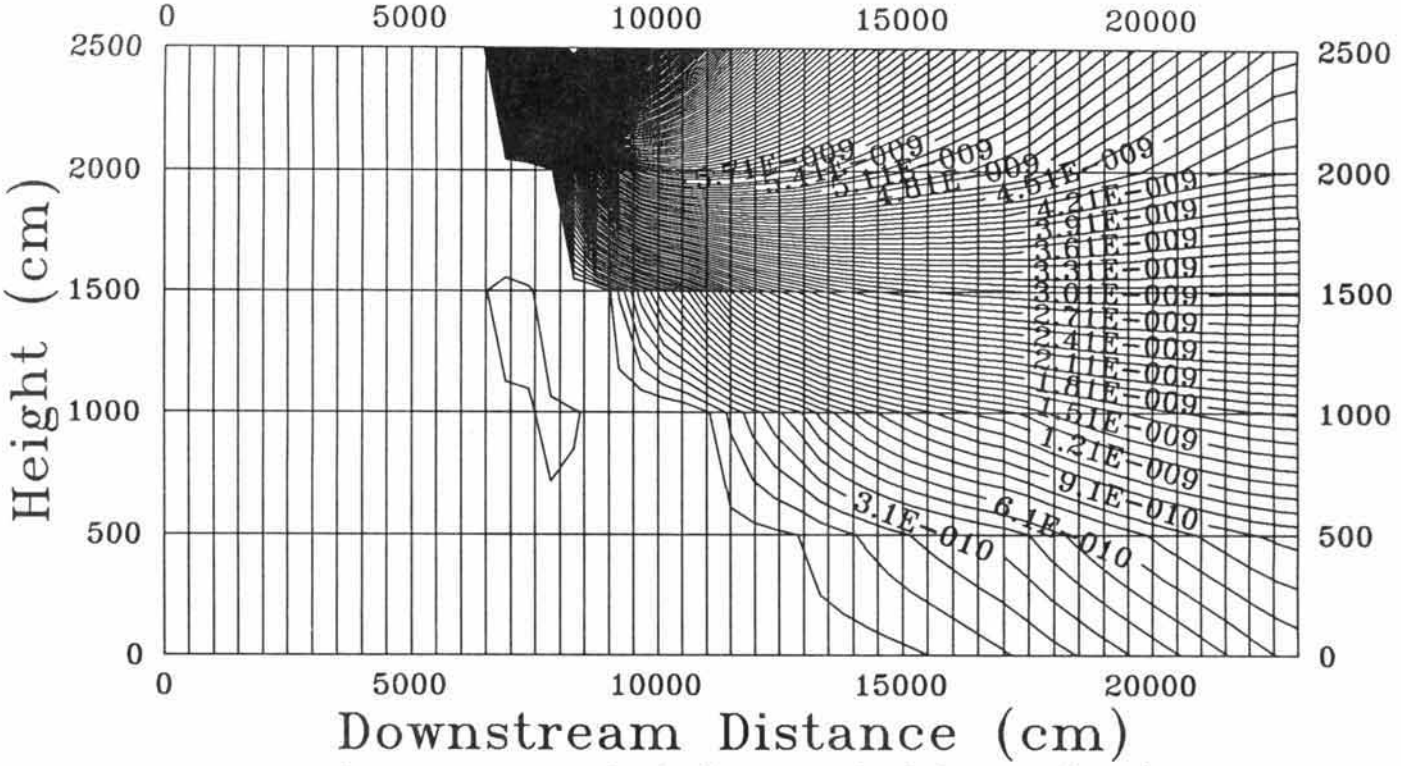

Fig. 2. Case 1 concentration (g/cc) at 50 years (vertical exaggeration 5:1).

Concentration contours generated using VAM2D at 50 years are shown in Fig. 4. Concentrations at the lower boundary are almost identical to the concentrations at the upper boundary, which indicates that the plume has sufficiently dispersed to fill the aquifer with an approximately vertically uniform concentration. It is clear from this figure that there is strong interaction between the bottom boundary and the contaminant plume.

A comparison between VAM2D and PAGAN concentration profiles at 50 years is shown in Fig. 5. As in Case 1, there is excellent agreement between the results from the two codes, although there is some deviation between the curves near the peak. This difference occurs for the nodes at which radionuclides are injected, and is the result of the drastically different way in which the source is treated in the two codes. In PAGAN the source is treated as an area-averaged flux, while in VAM2D the radionuclides are released concentrated at discrete nodal points. It is therefore not surprising that VAM2D predicts higher concentrations at the source nodal points. Nevertheless, the differences in concentration are relatively minor (less than about 10 percent for all cases studied). As in the Case 1 results, the curves shown in Fig. 5 are typical of other simulation times.

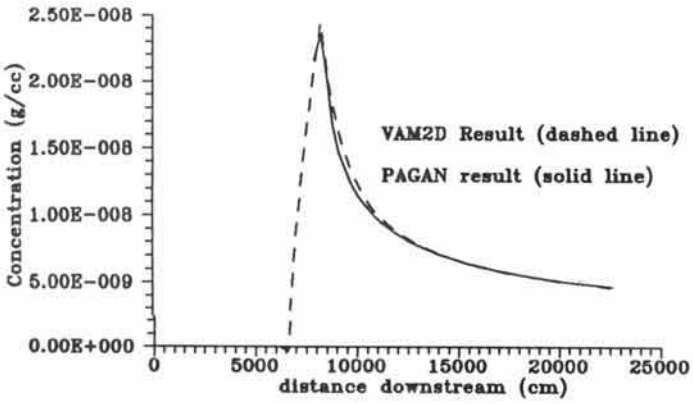

Fig. 3. Case 1 concentration along upper surface at 50 years.

Case 3: High Dispersivity and High Retardation H-3 Transport

The purpose of this analysis is to compare the treatment of retardation in the two codes. The values for dispersivity used are α_L = 20 meters and α_T = 4 meters, and a sorption coefficient, K_d, equal to 0.3 cc/g. The bulk density of the soil is assumed to be 1.75 g/cc, and the retardation factor, R, is calculated from

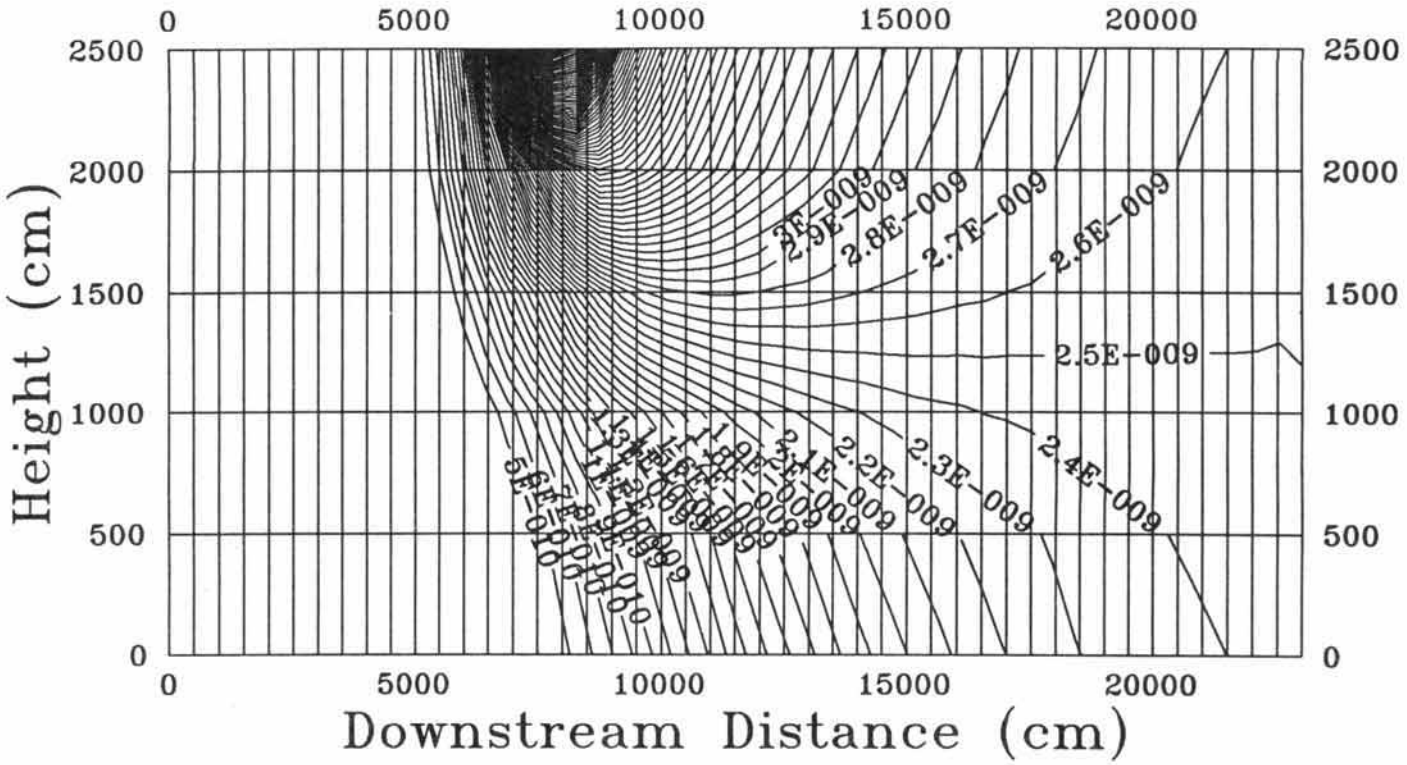

Fig. 4. Case 2 concentration (g/cc) at 50 years (vertical exaggeration 5:1).

$$R = 1 + \rho\,(1-\varepsilon)K_d/\varepsilon, \qquad \text{(Eq. 1)}$$

where ρ is the soil bulk density, and ε is the porosity. Using the appropriate values for the variables leads to a retardation factor equal to 2.225. As in Case 2, there is strong interaction between the contaminant plume and the lower boundary of the domain in this analysis.

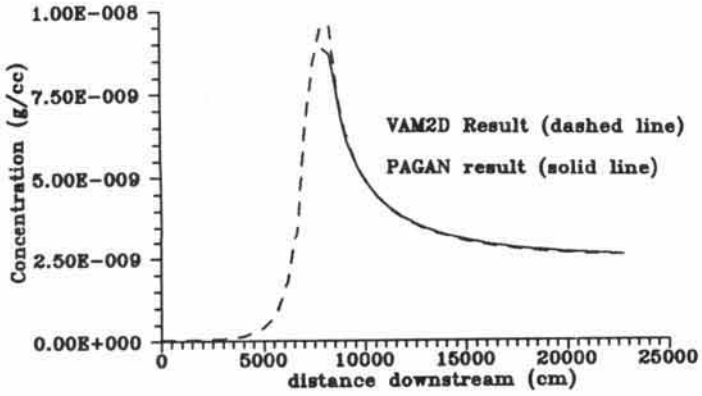

Fig. 5. Case 2 concentration along upper surface at 50 years.

The comparison between VAM2D and PAGAN concentration distributions at 10 years is shown in Fig. 6. The two analyses deviate slightly, with the PAGAN analysis predicting higher concentrations, and the concentration profiles are in reasonable agreement. A similar comparison is shown in Fig. 7 for the concentration profiles at 50 years, with similar results.

CONCLUSIONS

PAGAN and VAM2D have been compared for a conceptual model in which the assumptions are consistent between the two modeling approaches. The cases that were examined compared the two codes in their treatment of convective dispersion, decay in both the aquifer and the source, the treatment of no-flux boundary at the bottom of the aquifer, and the treatment of retardation. For unretarded tritium the analyses were in excellent agreement for all times and locations downstream from the edge of the source. Concentrations in the source region were within reasonable agreement, with PAGAN predicting slightly lower concentrations. These differences are attributed to the drastically different way in which the source is modeled using the two solution methods. For retarded tritium the

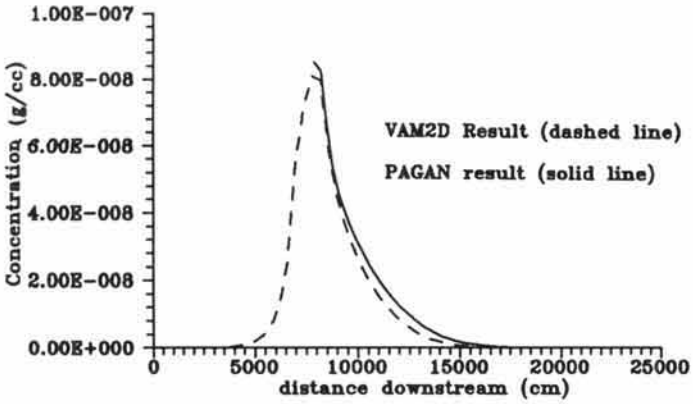

Fig. 6. Case 3 concentration along upper surface at 10 years.

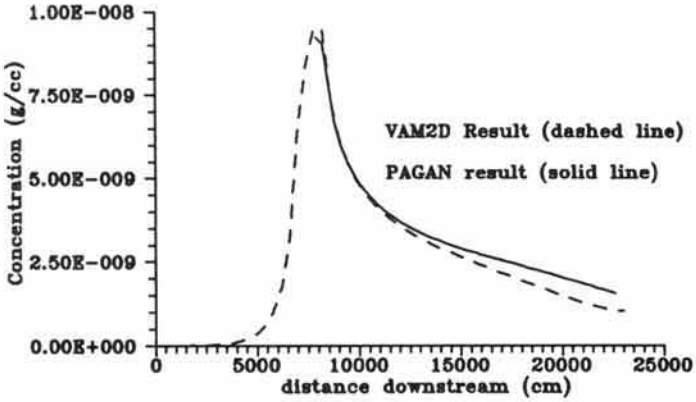

Fig. 7. Case 3 concentration along upper surface at 50 years.

agreement between PAGAN and VAM2D was good, with PAGAN predicted slightly higher concentrations and earlier breakthrough times. The difference between the two codes for the retarded solute is considered to be acceptable.

These results support the assertion made by Kozak et al. (4) that differences between the two codes in an earlier comparison were due to differences in the treatment of dispersion in the vadose zone and aquifer dilution due to recharge. Furthermore, the results provide additional confidence that the two computer codes provide accurate solutions to the governing equations.

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