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REEVALUATION OF LARGE-SCALE DISPERSIVITIES FOR A WASTE CHLORIDE PLUME: EFFECTS OF TRANSIENT FLOW

DANIEL J. GOODE & LEONARD F. KONIKOW
U.S. Geological Survey, Reston, Virginia 22092, USA

ABSTRACT This paper investigates the effects of transient groundwater flow on dispersion of a waste chloride plume in the basaltic aquifer beneath the Idaho (USA) National Engineering Laboratory. In an early application of numerical modeling techniques to the two-dimensional simulation of field-scale plumes, previous investigators identified longitudinal and transverse dispersivities using an independently calibrated steady-state flow model and matching contours of observed and simulated concentrations. The unusual result of calibrated transverse dispersivity (140 m) being significantly larger than longitudinal dispersivity (90 m) has been attributed to spatial heterogeneity, the fractured nature of the aquifer, and to the use of a two-dimensional model. New calibrations of the solute-transport model are performed on point concentration observations using a flow model incorporating transient recharge conditions that cause significant fluctuations in velocity. Under transient flow conditions, lowest calibration errors are achieved with significantly larger dispersivities than previously hypothesized, and with the longitudinal component larger than the transverse component. Unfortunately, the sensitivity of the model calibration error to dispersivity is low. Incorporating transient flow in this two-dimensional porous-media model does not significantly improve our understanding of the processes controlling chloride transport at this site.

INTRODUCTION

A large-scale chloride plume from injection well disposal has developed in the basalt aquifer beneath the Idaho National Engineering Laboratory (INEL). Robertson et al. (1974) provide background information on the site and its hydrologic conditions, including waste disposal practices and observed groundwater contamination. This information has been continually updated by U.S. Geological Survey reports, including those by Lewis & Goldstein (1982) and Pittman et al. (1988).

In one of the first comprehensive numerical transport-modeling studies, Robertson (1974) calibrated a two-dimensional flow and transport model using data from the early 1950's through 1972 and used the calibrated model to predict solute spreading to 2000. The calibrated longitudinal (α_L) and transverse dispersivities (α_T), about 90 and 140 m, respectively, were based on simulations assuming steady flow and no recharge in Big Lost River, a losing river adjacent to the contamination plumes. The characteristic of $\alpha_T > \alpha_L$ is theoretically unexpected and unique among field-scale case studies. Lewis & Goldstein (1982) compared Robertson's predictions with observed concentrations in 1980, noting differences in the spreading and rate of front movement and discussing possible reasons for these differences, including recharge fluctuations.

Duffy & Harrison (1987) examined the relation between temporal fluctuations in tritium concentration at the injection well and at near-field (<500 m downstream) observation wells, and applied a spectral method to estimate α_L. The method assumes concentration fluctuations are damped and filtered reflections of mass flux fluctuations at the injection well, the flow field is steady, and transverse dispersion is neglected. Values of α_L derived by Duffy & Harrison ranged from 40 to 125 m for different wells, and averaged 88 m. Duffy & Harrison also examined the effect of radial advection from the injection well on the transverse spreading of the plume, estimating that "the width of the advective zone is of the order of 1.2 km and explains only a portion of the width of the plume." They concluded that "horizontal, transverse, dispersive mixing, as originally proposed by Robertson (1974), still contributes significantly to the unique shape of this plume."

Fryar & Domenico (1989) fit an approximate analytical model of two-dimensional transport to tritium concentrations at wells located 1410 to 4620 m downgradient from the injection well at INEL. Although their model assumed uniform, steady flow, it included a finite-width source that approximated advective spreading in the near-well radial flow field. The source widths resulting from calibration ranged from 1900 to 2400 m for different sets of wells, and averaged 2200 m. Calibrated α_T ranged from 49 to 100 m, averaging 81 m. Fryar & Domenico considered these well locations too close to the injection well to estimate α_L.

Recent theoretical investigations indicate that transient flow conditions that are ignored during calibration of a solute-transport model may lead to inaccurate estimates of α_L and α_T, particularly for the transverse component. This effect is most likely to be significant in aquifers that respond relatively quickly to hydraulic boundary and recharge conditions having significant fluctuations, and that have a (true) α_T much smaller than α_L (Goode & Konikow, 1988). Kinzelbach & Ackerer (1986) illustrated the ability of a steady-flow model to incorporate the dispersive effects of transient flow on solute transport by increasing α_T. The plumes at INEL may exhibit the effects of a transient flow field because the aquifer system has low storativity, and hence responds quickly to changing hydraulic stresses, and because the variations in annual recharge through Big Lost River are significant relative to flow rates in the aquifer.

In this paper, we examine the effects of large-scale transient flow conditions caused by fluctuating recharge from Big Lost River on Robertson's (1974) transport model calibration. We re-calibrate Robertson's transport model using observed well concentrations in 1969 and compare calibration of α_L and α_T under steady and transient flow. The emphasis of our study is the relation between transients in the flow field and large-scale dispersivities identified through model calibration; hence, we do not consider conceptual models including other processes, such as vertical flow or small-scale heterogeneity, that may significantly affect solute spreading at INEL.

FLOW MODEL CALIBRATION

Following Robertson (1974), subsurface flow at INEL is modeled through a governing equation assuming two-dimensional horizontal flow, transmissivity constant in time, and storativity constant and uniform in space. This equation is solved using implicit finite-differences in time and standard 5-point block-centered finite-differences for spatial derivatives as implemented in the computer program of Konikow & Bredehoeft (1978). We employ two linked grids: a large-scale grid with uniform square blocks 5150 by 5150 m covering the entire area simulated by Robertson and a small-scale grid with uniform square blocks 430 by 430 m covering the area simulated for future projections of solute transport by Robertson (1974, shaded part of his Fig. 16). The fixed-head boundary conditions of Robertson are employed for the large-scale grid. Internal block-interface fluxes from the large-scale grid are interpolated as flux boundary conditions for the small-scale grid, with a specified-head node at the southeastern corner of the small-scale grid providing the model datum. In this way, inconsistencies in the different scale simulations would be shown by differences in the head contours.

In the simulations presented here, we use model transmissivities from Robertson's (1974) second ("future projection") data set. The aquifer is highly permeable and model transmissivities range from about 10^3 to 10^5 m^2/d. We use spatially weighted averages of these values for the large-scale grid. Each of the smallest blocks in Robertson's model corresponds to 9 blocks in our small-scale model, hence we assign these block transmissivities to each of the corresponding 9 blocks in our small-scale model. Robertson's Figure 7 is a contour map of transmissivity showing a low-transmissivity zone downgradient of the injection well location. Preliminary simulations of solute transport with no dispersion (α_L=α_T=0) and no recharge indicated that this zone causes spreading of the advection-only plume. A steady-state flow simulation with the long-term average recharge in Big Lost River resulted in a narrower plume under advection alone because streamlines from the injection well did not pass through the low-transmissivity zone. It is not apparent how this zone was identified given that no wells were known to be present in the zone. Because of the need to focus our investigation on the spreading effect of transient flow, and because of the lack of evidence for this low-transmissivity zone, we removed this zone for these simulations. The values of transmissivity in these blocks and in several adjacent blocks were replaced by their combined average value. This slight modification in the transmissivity field did not significantly affect computed heads.

Robertson (1974) considered the early 1965 head distribution observed at INEL as near steady-state and used these data to calibrate a steady-state model of flow in the aquifer by trial and error. Because flow in Big Lost River was relatively low in the years before 1965, and because heads were near record lows in late 1964, no recharge in Big Lost River was included in the steady-state flow calibration. Potentiometric heads resulting from our steady-state flow simulation assuming no recharge are essentially the same as the head contours presented by Robertson (1974, Fig. 8).

Using the steady-state (no recharge) calibration as an initial condition, Robertson (1974) calibrated a single storativity value of 0.1 for the entire aquifer by simulating the increase in head caused by record recharge in Big Lost River during 1965. Although not described in detail in his report, we assume that this recharge had the same spatial distribution as the recharge used in projections of future simulations; that is, 56% infiltrated at, or upstream from the Diversion Area and 44% infiltrated along the channel or in the playas north of the injection well. (The Diversion Area (Fig. 1) is a flood control basin used to regulate Big Lost River discharge onto INEL.) The volume of the recharge event used for calibration is not reported, but it is stated that the annual recharge volume of 1.6×10^8 m^3, used in future projections, was about 1/2 the 1965 recharge volume, implying that the simulated recharge volume was about 3.2×10^8 m^3.

For our simulations, we modified both the spatial distribution and the magnitude of Big Lost River recharge on the basis of more recent observations. Pittman <u>et al.</u> (1988) present annual Big Lost River discharges at the INEL Diversion Dam for 1965 through 1985. Data are available on annual discharge upstream from INEL on Big Lost River at Mackay Dam dating back to the early 1900's. Regression of the discharge at INEL against the Mackay Dam discharge for the period 1965 through 1985 yields the following regression equation: (INEL discharge) ≈ 1.06 (Mackay discharge) - 2.43×10^8 m^3, for which $r^2 = 0.801$. This regression equation is used to estimate annual discharge prior to 1965 at INEL from Mackay Dam discharge data. For 1965 and later, measured discharge at INEL is used directly. Pittman <u>et al.</u> (1988) also present data indicating that, from 1965 through 1985, an average of about 40% of the annual discharge of Big Lost River entered the Diversion Area. For the transient flow simulations, we distribute the recharge as follows: 40% in the Diversion Area, 30% in the channel from the Diversion Area to the playas in the north, and 30% in the playas.

Using our modified recharge parameters, we approximately reproduce Robertson's (1974) transient-flow calibration results. Figure 1 shows the increase in heads in the aquifer after 1 yr of simulation using the large-scale grid with a constant recharge rate of 2.07×10^8 m^3 yr^{-1}, about 65% of the rate apparently used by Robertson. However, the rate apparently used by Robertson is also larger than the total discharge for Big Lost River at the Diversion Dam subsequently reported by Pittman <u>et</u>

al. (1988). These contours (Fig. 1) are very similar to the observed head rise and simulation presented by Robertson. Some of the differences are probably attributable to our grid spacing, which is larger than that used by Robertson, for the large-scale grid..

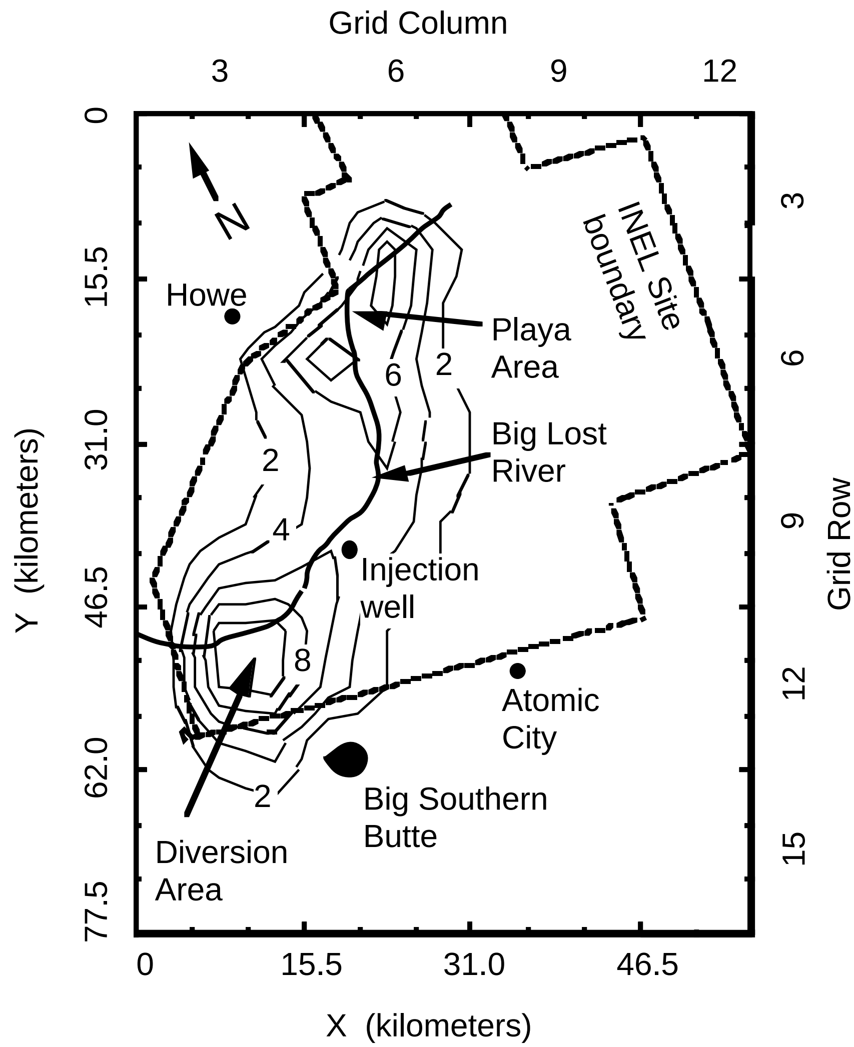

FIG. 1 Contours of head increase (solid lines, in feet, 1 ft = 0.3048 m, contour interval is 2 ft) for transient flow calibration. Also shown are several features of the INEL facility and environs.

The recharge to the aquifer in our simulation is 80% of the estimated Big Lost River discharge, and this relation is used for our transient simulations of flow. However, based on hydrographs of wells near Big Lost River, we distribute the annual recharge during 6 months of the year only for our transient simulations, and specify no recharge for the remaining 6 months. Figure 2 shows the assumed histogram of annual recharge volumes (occurring in 6-month periods) and specific discharge magnitude and direction in the aquifer simulated for 1953 through 1980 at a model block about 200 m downgradient from the injection well. As noted by Robertson, the flow-field was relatively steady during the years just prior to 1965 when the near-record recharge event occurred. The groundwater flow direction fluctuates by up to 20 degrees at this location following high recharge in Big Lost River, and transient effects continue more than 1 year after recharge fluctuations. The response in succesive years with high (or low) recharge is cumulative.

In summary, we reproduce Robertson's (1974) steady flow calibration without difficulty using his transmissivities mapped to our large- and small-scale grids. However, the volume of recharge used for our transient flow simulation appears to be significantly smaller than that used by Robertson. The value used in our simulation appears more consistent with Big Lost River discharge values subsequently reported by Pittman et al. (1988). We have not independently calibrated our transient-flow model. This flow model is generally consistent with that used by Robertson, and it approximates the transient hydraulic response of the aquifer. This model provides a basis for our preliminary re-calibration of Robertson's solute-transport model that incorporates transient-flow conditions.

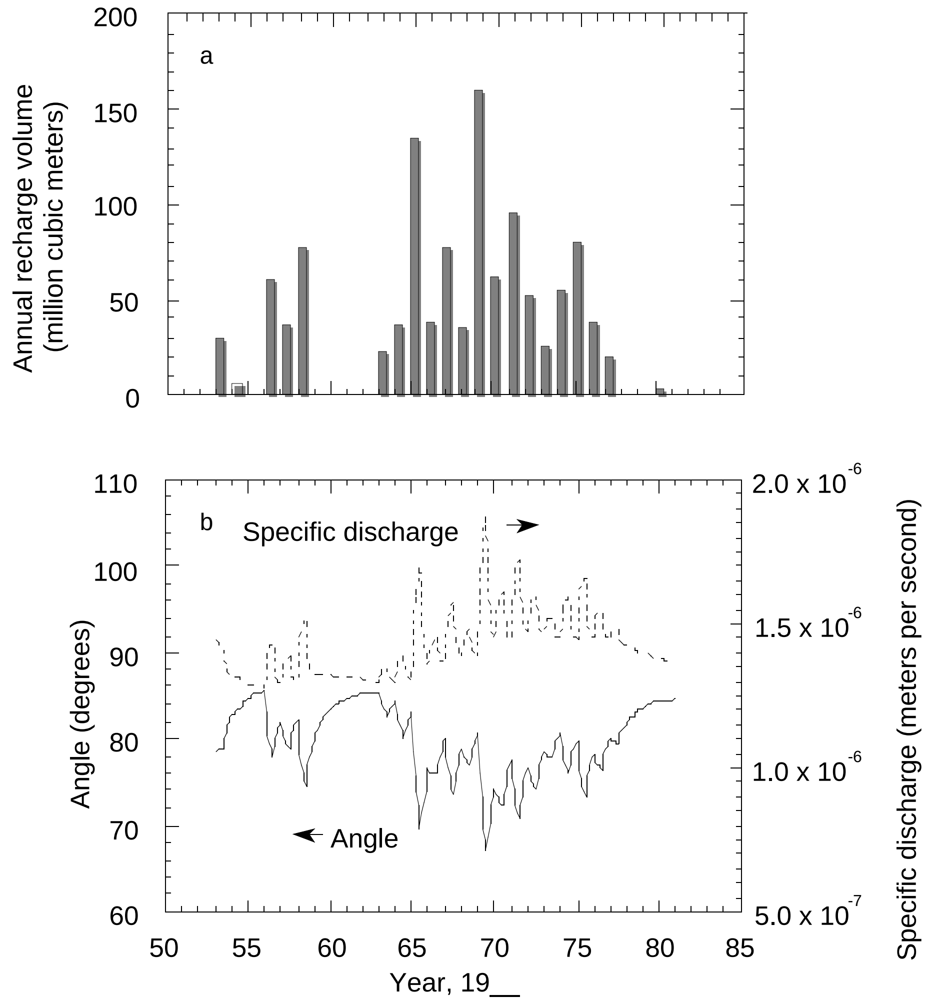

FIG. 2 Hydraulic transients at INEL: (a) Histogram of annual recharge volumes from Big Lost River; (b) Angle of flow and specific discharge simulated about 200 m downgradient from injection well.

CONCENTRATION DATA USED FOR CALIBRATION

We define model calibration error as the simulated concentrations after 16 yrs of injection minus the observed concentrations in 1969 (Bagby et al., 1985) at 28 model blocks (Table 1). As previously discussed by Robertson (1974), Duffy & Harrison

(1987), and Fryar & Domenico (1989), the observed well concentrations do not vary in a manner that is fully consistent with current conceptual models of transport at the site. For example, the observed concentrations at CFA-1 and CFA-2 are exceeded by only two wells (67 & 77), despite the fact that many of the other observation wells are closer to the injection well. Instead of using these data directly, Robertson (1974) matched contours of model results to contours of the observations that were drawn by hand. Thus, the observed concentrations were transformed into a plume shape, more consistent with the conceptual model of transport, by applying hydrogeologic judgement and interpretation. Duffy & Harrison (1987) focused on near-field wells because tritium concentrations at wells farther downgradient did not fluctuate in a manner consistent with fluctuations at the injection well. Fryar & Domenico (1989) did not use observed tritium concentrations at two wells. Well 36 was thought to be in a "poorly connected zone" and concentrations at well 20 were considered erratic, possibly indicating measurement errors (Fryar & Domenico, 1989).

TABLE 1 Observed concentrations in 1969 used for calibration.

Grid block col.	row	concentration (mg/L)	INEL well ID	comments
41	22	63.	CFA-1	
40	24	67.	CFA-2	
49	23	20.	EOCR	
30	31	15.	EBR-I	actual C=14. mg/L
50	24	21.	OMRE	
52	22	16.	Site 9	
43	18	30.	20	
38	18	56.5	37 and 38	
37	17	24.5	34 and 36	
36	16	15.	35 and 39	actual C=12.5 mg/L
39	16	50.	57	
41	15	97.	67	
34	13	16.	76	
40	18	73	77	
42	13	26.	82	
43	30	15.	83	actual C=11. mg/L
34	15	15.	84	actual C=13. mg/L
37	20	24.	85	
36	7	15.	Fire Station	
53	15	20.	SPERT 1	
27	22	15.	Hwy-3	6. mg/L in 1977
44	7	15.		artificial background
50	10	15.		artificial background
50	29	15.		artificial background
44	34	15.		artificial background
37	32	15.		artificial background
26	28	15.		artificial background
28	16	15.		artificial background

We also found it necessary to exclude certain observed concentration data to yield meaningful calibration results. In particular, the data in Table 1 do not include concentrations at several wells located very near the injection well that indicated relatively low chloride concentrations, ranging from 13 to 38 mg/L. Given our conceptual model, which includes a constant source concentration from 1953 through 1969, the inclusion of these data results in high root-mean-squared (RMS) calibration errors. These RMS errors are larger than the standard deviation of the observed data, indicating that attempting to model the transport process (with the simulated flow field) is worse than simply assuming that concentration is uniform in space at the mean value of the observations. In addition to ignoring these near-field observations, we imposed a minimum background chloride concentration of 15 mg/L (see Pittman et al., 1988) and added seven artificial background observations at dispersed locations beyond any wells indicating contamination. These artificial data serve to offset the clustering of observation wells near the source of contamination and increase the relative RMS errors for very large dispersivities.

TRANSPORT CALIBRATION IN STEADY FLOW

Robertson (1974) applied a method of characteristics model of two-dimensional solute transport (Bredehoeft & Pinder, 1973) to the chloride and tritium plumes at INEL and calibrated α_L=90 m and α_T=140 m, by trial and error. Apparently, the calibrated steady-flow model with no Big Lost River recharge was used for these simulations, and the source flow rates and concentrations were constant for the entire simulation period.

The results of our simulation of the chloride plume with the method of characteristics model of Konikow & Bredehoeft (1978) using constant source flow rate (1.13×10^6 m^3 yr^{-1}) and concentration (550 mg/L) at the injection well and α_L=90 m and α_T=140 m are very similar to the results presented by Robertson (1974, Fig. 12). The secondary injection well considered by Robertson is not included in these simulations because it does not appear to significantly affect long-term chloride concentrations (see Fig. 32 of Pittman et al., 1988).

The major difference in the model parameters used here and those of Robertson is that the source concentration is over twice as high as his value. Because these simulations differ significantly only in the magnitude of the source concentrations, and because our simulations are using essentially an improved version of the computer program used by Robertson, we conclude that the program used by Robertson generated some numerical errors in simulation of the dilution and mixing at the injection well. These errors are probably associated with the method used to generate new particles at sources. Significant improvements in the numerical algorithms, including those for source terms, are reflected in the model of Konikow & Bredehoeft (1978) and its updates (e.g., Goode & Konikow, 1989).

In order to focus on the effects of transient flow on the dispersion process, we use an alternative simulation for steady flow in which the long-term (1953 through 1969) average recharge value is specified in Big Lost River. The average velocity under transient recharge conditions is different than the steady-state velocity if no recharge is assumed. However, the steady-state velocity for a simulation with the average recharge is essentially the same as the average velocity under transient recharge conditions. Thus, the temporal differences between this steady-flow velocity and transient velocities will be limited primarily to fluctuations about the mean. Because recharge in Big Lost River increases the magnitude of specific discharge downgradient from the injection well (Fig. 2), the porosity must be increased to yield similar velocities to the case of no recharge. For the same reason, the source concentration must be increased. For the long-term average recharge used here, porosity was increased from 0.1 to 0.13 and source concentration was increased to 700 mg/L to yield velocities and concentration contours that are similar to those for the no-recharge case. As might be expected, the differences between these simulations and those above for the case of no recharge indicate a shift in the flow direction away from Big Lost River because of recharge.

We conducted numerous calibration runs using the steady-flow model having long-term average recharge in Big Lost River. Figure 3 shows the variation of the RMS calibration error as a function of α_L and α_T. Because the transport solution is linearly proportional to the source concentration, the source concentration that yields the minimum RMS error for a given α_L and α_T can be determined directly after one simulation. Hence, the RMS errors in Fig. 3 are for simulations using the source concentration that yields the minimum RMS error for the particular values of α_L and α_T shown. These source concentrations ranged from 330 to 760 mg/L and increase with increasing dispersivity. A simulation assuming steady flow and no recharge in Big Lost River and using the calibrated dispersivities of Robertson (1974) yields an RMS error of 17 mg/L. Finally, the RMS errors for steady-state flow simulations using the parameter estimates by Duffy & Harrison (1987), $\alpha_L \approx 88$ m, and Fryar & Domenico (1989), $\alpha_T \approx 81$ m, would be similar to those shown for the case of $\alpha_L = \alpha_T = 90$ m.

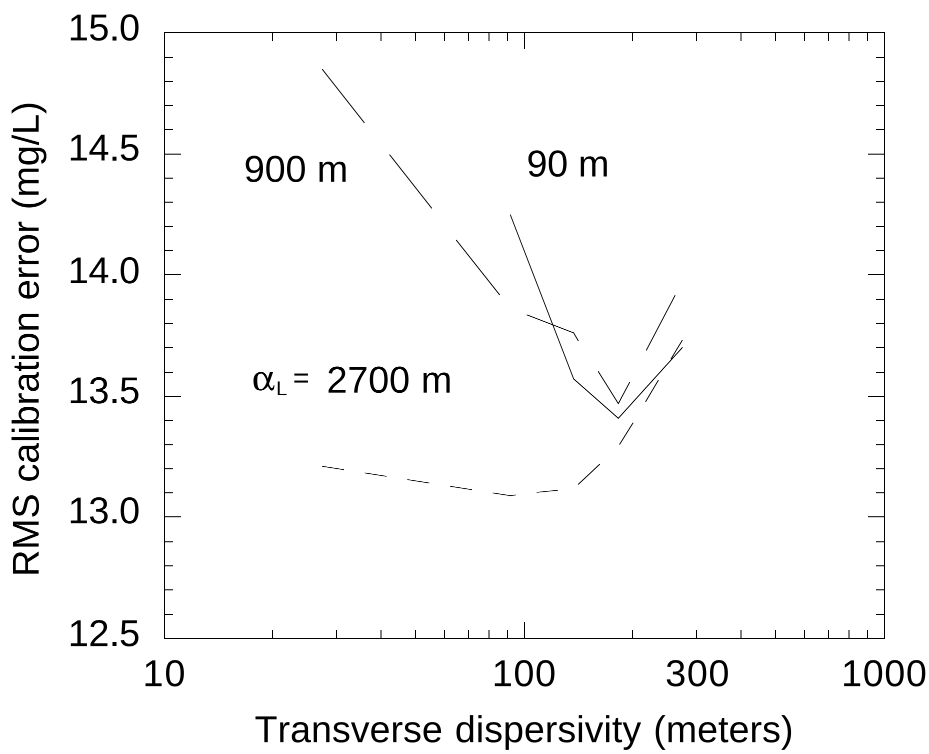

FIG. 3 Root-mean-square calibration error as a function of transverse dispersivity for several values of longitudinal dispersivity, assuming steady-state flow and average recharge in Big Lost River.

The RMS calibration error for this model shows a nonlinear variation with respect to α_L. For $\alpha_L = 90$ m, minimum RMS error is achieved with $\alpha_T = 180$ m, similar to Robertson's (1974) result that $\alpha_T > \alpha_L$. However, simulations with $\alpha_L = 900$ m have very similar error and would provide an equally suitable match having the characteristic $\alpha_L > \alpha_T$. Furthermore, these results indicate that smallest RMS error is achieved with much larger α_L than that used by Robertson, or identified by Duffy & Harrison (1987). We achieved minimum RMS error using $\alpha_L = 2700$ m and $\alpha_T = 90$ m. For this case, RMS error appears relatively insensitive to α_T over a range from about 30 to 140 m. As noted above, these RMS errors are large relative to the standard deviation of the observations in Table 1, which is 22 mg/L, indicating that the model does not explain a significant portion of the variability in the observations.

TRANSPORT CALIBRATION IN TRANSIENT FLOW

The calibration of the solute-transport model under transient flow conditions was performed in the same manner as the calibration for steady-flow conditions. Figure 4 shows the variation of RMS error with α_L and α_T. As above, these simulations use the source concentration that results in minimum RMS error for a given α_L and α_T. These results (Fig. 4) are very similar to the calibration under steady-flow conditions. In this case, RMS errors decrease with increasing α_L. Again, the lowest RMS errors are achieved with larger α_L than used by previous investigators. Furthermore, for higher values of α_L, lower calibration error is achieved with $\alpha_L > \alpha_T$, which is typical of most field-scale studies.

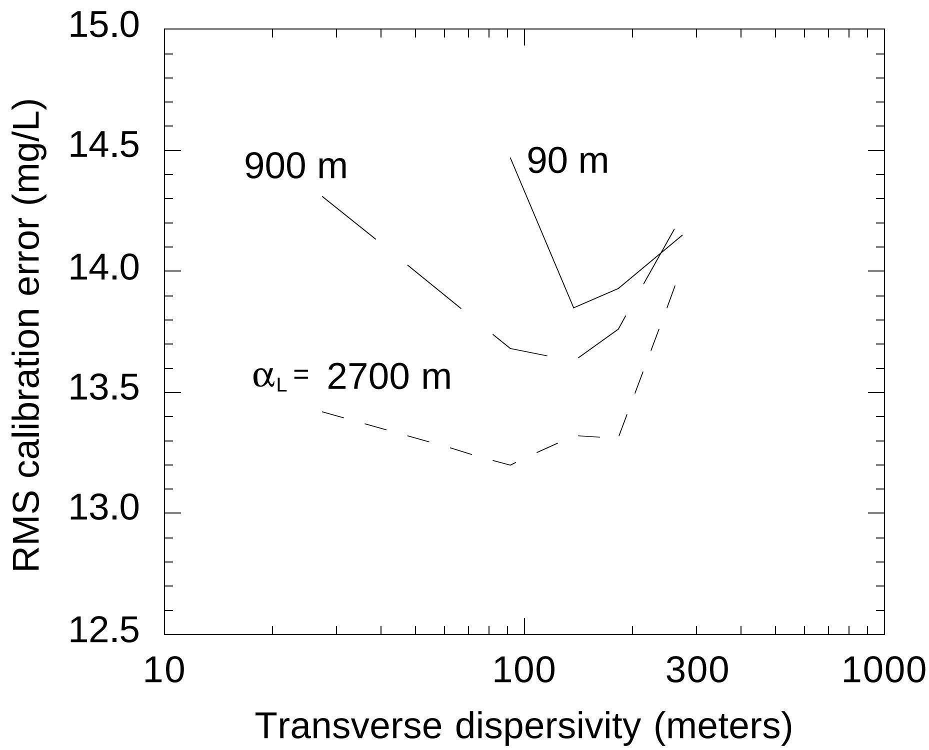

FIG. 4 RMS calibration error as a function of transverse dispersivity for several values of longitudinal dispersivity, assuming transient flow and Big Lost River recharge shown in Fig. 2a.

These simulations indicate that the calibration errors achieved with a steady-state flow model are very similar to those achieved with a transient flow model. As the magnitude of α_L increases, the differences between the models decreases. This is caused by, in part, the decreasing relative importance of velocity fluctuations when transport is dominated by dispersion. The effect of hydraulic transients on calibrated dispersivities is likely to be small if the true α_L and α_T are of the same order (Kinzelbach & Ackerer, 1986; Goode & Konikow, 1988). The results here indicate that even for the case of $\alpha_L > \alpha_T$, there is relatively little difference between simulations assuming steady flow and those assuming transient flow. These preliminary results, of course, depend on the observed data used in the calibration procedure, and current efforts are underway to improve the calibration data set of 1969 and to calibrate the model using more recent observations.

CONCLUSIONS

We reevaluated Robertson's (1974) solute-transport model calibration for plumes at INEL to investigate the possible effects of transient flow conditions on the large calibrated value of transverse dispersivity. Using Robertson's transmissivities, our simulations of flow agree well with his simulations for steady-state flow, and by using somewhat lower recharge to the aquifer we approximately match his transient flow calibration. Our results indicate that RMS calibration error, determined from a small number of well concentrations, is relatively insensitive to dispersivity over a wide range of values. Lowest RMS errors are achieved here using significantly larger α_L than used previously, and using a dispersivity tensor that has the typical characteristic $\alpha_L > \alpha_T$. For this calibration data set, there is little difference between RMS errors for steady and transient flow simulations. Thus, explicitly accounting for the effects of transient flow conditions does not significantly improve model fit.

REFERENCES

Bagby, J. C., White, L. J., & Jensen, R. G. (1985) Water-quality data for selected wells on or near the Idaho National Engineering Laboratory, 1949 through 1982. USGS Open-File Rep. 84-714 (DOE/ID-22068).

Bredehoeft, J. D., & Pinder, G. F. (1973) Mass transport in flowing ground water. Wat. Resour. Res. 9 (l), 194-209.

Duffy, C. J., & Harrison, J. (1987) The statistical structure and filter characteristics of tritium fluctuations in fractured basalt. Wat. Resour. Res. 23 (5), 894-902.

Fryar, A. E., & Domenico, P. A. (1989) Analytical inverse modeling of regional-scale tritium waste migration. J. of Contaminant Hydrol. 4, 113-125.

Goode, D. J., & Konikow, L. F. (1988) Can transient flow cause apparent transverse dispersion? (abstract). Eos Trans. AGU 69 (44), 1184-1185.

Goode, D. J., & Konikow, L. F. (1989) Modification of a method-of-characteristics solute-transport model to incorporate decay and equilibrium-controlled sorption or ion exchange. USGS Wat.-Resour. Investigations 89-4030.

Kinzelbach, W., & Ackerer, P. (1986) Modelisation de la propagation d'un contaminant dans un champ d'ecoulement transitoire. Hydrogeologie, 2, 197-205.

Konikow, L. F., & Bredehoeft, J. D. (1978) Computer model of two-dimensional solute transport and dispersion in ground water. USGS Techniques of Wat.-Resour. Investigations Book 7, Chapter C2.

Lewis, B. D., & Goldstein, F. J. (1982) Evaluation of a predictive ground-water solute-transport model at the Idaho National Engineering Laboratory, Idaho. USGS Wat. Resour. Investigations 82-25.

Pittman, J. R., Jensen, R. G., & Fischer, P. R. (1988) Hydrologic conditions at the Idaho National Engineering Laboratory, 1982 to 1985. USGS Wat.-Resour. Investigations 89-4008.

Robertson, J. B., Schoen, R., & Barraclough, J. T. (1974) The influence of liquid waste disposal on the geochemistry of water at the National Reactor Testing Station, Idaho, 1952-1970. USGS Open-File Rep. IDO-22053.

Robertson, J. B. (1974) Digital modeling of radioactive and chemical waste transport in the Snake River Plain Aquifer at the National Reactor Testing Station, Idaho. USGS Open-File Rep. IDO-22054.