Stochastic simulation of transmissivity fields conditional to both transmissivity and piezometric head data—3. Application to the Culebra Formation at the Waste Isolation Pilot Plan (WIPP), New Mexico, USA

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Abstract

The self-calibrated approach is applied to the stochastic analysis of groundwater flow and advective mass transport in the WIPP site. Multiple equally likely realizations of logtransmissivity fields are generated, followed by the solution of variable density groundwater flow and particle tracking. Five different cases have been analyzed. The first one regards the modeling of variable-density groundwater flow and the remaining four regard the generation of the logtransmissivity fields. Results show that (i) it is important to model variable-density flow as accurately as possible, (ii) conditioning to piezometric head data helps in reducing the uncertainty in flow and transport predictions, (iii) accounting for uncertainty in boundary conditions helps improving the match to measured heads, and (iv) the interpreted value at location P-18 is not consistent with the model of spatial variability inferred from the data. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

1.1. Description of the WIPP site

The Waste Isolation Pilot Plant (WIPP) is a US Department of Energy facility that has been chosen as a potential location to host a repository for the disposal of radioactive waste. It has been used for research and development aimed to demonstrate the safe underground disposal of transuranic waste from defense related activities. It consists of an underground repository mined from a thick-bedded salt unit and the associated facilities at land surface. It is located near Carlsbad, southeastern New Mexico, in an evaporite-bearing sedimentary basin known as the Delaware basin (Fig. 1(a)). If approval is granted, the repository will be used for the permanent disposal of approximately 170,000 cubic meters of transuranic waste. The approval relies on performance assessment analyses to show compliance with the US Environmental Protection Agency regulations. A key component in the assessment of the long term performance of the facility is evaluating the potential

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for radionuclide transport from the underground repository to the accessible environment, as defined in US DOE (1996), by groundwater. In 1983, independent technical reviews by the National Academy of Sciences and by New Mexico’s Environmental Evaluation Group recommended further study to clarify uncertainties about the groundwater flow in the rock units that overlay the evaporite section above the repository. Our research team got involved in the WIPP site through the INTRAVAL project. INTRAVAL was an international project that lasted 8 years funded by nuclear waste management agencies from several countries with the purpose of comparing different codes and approaches for the modeling of flow and transport in formations related to underground nuclear waste disposal (Andersson et al., 1996). WIPP was chosen as one of the examples to be used for this comparison.

The WIPP repository is located approximately 650 m below the land surface in the lower part of the predominantly halite Permian Salado Formation (Fig. 1(b)). Among the upper seven formations in the vicinity of the WIPP site there is the Rustler Formation, composed of interbedded halite, anhydrite, fine-grained clastics, and two dolomite members. Three laterally persistent water bearing units have been identified above the Salado rock units: the Magenta Dolomite and the Culebra Dolomite Members of the Rustler Formation, and the rocks of the contact zone between the Rustler and Salado Formations. Of these three zones, the Culebra Dolomite Member is the most transmissive zone and is considered to be the principal pathway for transport of radionuclides due to inadvertent human intrusion by drilling through the repository.

Based upon observations, the Culebra Dolomite has been characterized at the site as a fractured medium where secondary processes, such as halite dissolution, subsidence, and calcium sulfate hydration have produced important changes in the formation permeability and variations in fluid density ranging from fresh water to saturated brine. These density values range from 1000 to 1030 kg m\(^{-3}\) west of the WIPP site and can reach values as high as 1040–1150 kg m\(^{-3}\) east of this region. The Culebra center elevations were determined from borehole and shaft data. The observed elevation data are higher in the northwest area (969 m above mean sea level), and lower elevations are in the southeast and northeast (679–705 m above mean sea level). Generally, the Culebra dips gently to the southwest, on the order of 2 deg. The thickness of the Culebra Dolomite at the WIPP site region ranges from 5.5 to 11.3 m, with a mean thickness of 7.7 m. (See Cauffman et al. (1990) for further details on the data.)

The transmissivity values for the Culebra Dolomite have been obtained from drill stem tests, slug tests and pumping tests, some of them of long duration. Transmissivity values interpreted from these tests extend over a range of seven orders of magnitude. Each measurement was reported with an error estimate.
According to Davies (1989), the formation fluid density in the Culebra has an important impact on the groundwater flow direction. In the sequel, we show the impact that explicitly accounting for spatially variable fluid density has in the pressure distribution within the aquifer and in the flow model parameter identification process. Geochemical investigations suggest that the chemical constituents within the Culebra represent the remnants of a paleohydrologic flow system and that these constituents may not be at steady state with the present flow field. However, for modeling purposes we will assume that the system was at steady state prior to the sinking of the shafts. We will also assume, for modeling purposes, that the fluid density is at steady state throughout the simulation period. While this is an unrealistic assumption for very long simulation periods, properly accounting for density variations in time requires the coupling of a mass transport model which is beyond the scope of this paper. Because of the spatial variability in the fluid density, equivalent fresh water heads are used throughout. Hereafter any reference to piezometric heads is understood as equivalent to fresh water heads.

There exist some controversial opinions on the nature of Rustler recharge. Rock units of the Rustler Formation are considered to be relatively isolated vertically, and there may be some recharge coming from an area somewhere in the north. We have not accounted for any recharge in the present study.

1.2. Purpose of the analysis

The purpose of this paper is to show the possibilities offered by the self-calibrated algorithm to characterize uncertainty on flow and mass transport model results, thus complementing, with the application to a real case, the first two papers of the series (Gómez-Hernández et al., 1998; Capilla et al., 1998). We chose the WIPP site because it is a very well known and documented area in which probabilistic assessment is especially relevant. In addition, it contains transmissivity data spanning several orders of magnitude, which poses additional problems for the stochastic analysis. The paper focuses on the stochastic analysis of single-phase single-porosity saturated variable-density flow and advective transport in the Culebra Formation. This dolomite formation would be the fastest path for radionuclides to reach the accessible environment transported by groundwater under a human intrusion scenario by an abandoned borehole through the repository. It is not our purpose to question the existing conclusions and evaluations about the WIPP site. In fact, the conceptual model for mass transport has been strongly simplified with respect to the double porosity approach used in the performance assessment by SANDIA.

Due to the specific characteristics of the WIPP site, the self-calibrated method had to be adapted to the simulation of variable-density flow. The self-calibrated method was then applied to the generation of equally likely realizations of transmissivity fields conditional to transmissivity and steady-state head data. These realizations serve as input to a Monte-Carlo analysis of flow and transport.

The method has also been used to analyze the uncertainty in the boundary conditions.

2. Conceptual model of the aquifer and mathematical approach

2.1. Conceptual model. Physical and hydrodynamic parameters

The area of study is a 21,500 m x 30,500 m rectangle of Culebra Dolomite, approximately centered above the potential repository. It corresponds to the same area for which LaVenue et al. (1990) calibrated a deterministic model for steady and transient conditions, using the pilot point methodology (de Marsily et al., 1984) and for which, later, LaVenue et al. (1995) and Ramachandran et al. (1995) performed a stochastic analysis.

The flow in the Culebra Formation within the area of study can be considered as confined. As already mentioned, it is not clear whether vertical flows from adjacent layers occur so this possibility has not been considered in this paper. The flow in the formation is very slow because of the small values of hydraulic conductivity. Similarly to previous exercises by LaVenue et al. (1990) we will consider that the data provided prior to the excavation of the shafts correspond to steady-state conditions.

The modeling area includes 37 transmissivity measurements and 33 piezometric measurements. The water density has been sampled at 31 different
locations. The thickness of the formation is known at 64 locations and the elevation of its midpoint at 75.

The structural analysis of transmissivities, as well as the stochastic simulations are carried out in log-space. The variogram of the 37 logtransmissivity measurements is anisotropic (Fig. 2) composed of three nested structures displaying a strong zonal anisotropy. The logtransmissivity variance (as indicated by the sill of the variogram) in the north–south direction is much smaller than the variance in the east–west direction. Well P-18, towards the east–central part of the study area (Fig. 3(a)), was not included in the structural analysis due to its extremely low value. We will return to the specific problems posed by the transmissivity value interpreted at this well location.

The strong zonal anisotropy displayed by the data can also be modeled using a random function model with an explicit trend in the local mean of the attribute. This type of model has not been used. Whether to use zonal anisotropy or a spatial trend is a model choice that must be taken by the modeler on the basis

![Fig. 2. Logtransmissivity model variograms: (a) east–west; (b) north–south.](image)

![Fig. 3. Ordinary kriging estimates from measured data: (a) logtransmissivity; (b) piezometric head. The piezometric head estimate uses, for the purpose of interpolation, the boundary values as data. White dots show measurement locations.](image)
of information not contained in the data set; for instance, a logtransmissivity spatial trend could be related to the existence of a dissolution front in the formation. We decided to keep the zonal anisotropy model. It was not the purpose of this paper to analyze the impact of using different random function models in a given data set, but to show the capabilities of the self-calibrated approach to incorporate piezometric information within a stochastic simulation context. The issue, however, was of our concern and the reader interested in the impact of random function model choice is referred to the paper by Hendricks Franssen and Gómez-Hernández (1997), in which it is shown that, for the WIPP case, with a significant amount of conditioning data, the use of either model has little transcedence.

Prescribed head boundary conditions are assumed along the entire boundary. Fig. 4 shows the prescribed values starting at the northwest corner and moving clockwise along the boundary. These values are taken from LaVenue et al. (1990) who calculated them based on a regional flow model with geologically-based boundary conditions positioned further away from the WIPP limits.

In order to have a first idea of the overall spatial trends in both transmissivity and piezometric heads, the measured values were interpolated by ordinary kriging. For the piezometric head map, a crude variogram was estimated from the data values and, for the purpose of interpolation, the prescribed boundary conditions of Fig. 4 were considered as data. Fig. 3 shows the resulting interpolated maps on a grid with 61 by 43 square blocks of 500 m side (this grid is the same grid that will later be used for the stochastic analysis).

The effective porosity used to derive flow velocities from specific discharges has been set constant and equal to 0.13. Neither spatial variability nor uncertainty in porosity are considered in this paper. For the purposes established at the beginning of the paper, these assumptions are not important.

Recent field experiments (Beauheim, 1995) have shown important differences, from a hydraulic point of view, in local vertical cross sections of the Culebra Formation. It seems that the upper third part is much less pervious than the lower two thirds. If this fact is further evidenced for the whole area, it would be necessary to consider that the transmissivity measurements correspond to a smaller thickness, with the net effect of larger flow velocities.

2.2. Flow and transport models

Confined steady-state groundwater flow has been numerically simulated using finite differences over a 61 by 43 mesh of square blocks of 500 m by 500 m. The standard five-point block-centered approach is used with two exceptions: the interblock transmissivity is approximated by the geometric mean of adjacent blocks, according to the first paper of the series (Gómez-Hernández et al., 1998), and the effect of fluid density spatial variation is taken into account according to Capilla et al. (1995) and summarized in Appendix A.

Adective mass transport is simulated using particle tracking. Velocities are continuously defined
within each block by bi-linear interpolation of their two components from the estimates at the center points of block sides.

2.3. Monte-Carlo analysis

A Monte-Carlo analysis of steady-state confined groundwater flow and advective transport is carried out using the self-calibrated approach described in the previous two papers of the series (Gómez-Hernández et al., 1998; Capilla et al., 1998). This method was earlier delineated by Sahuquillo et al. (1992). In order to account for the spatially variable fluid density, the method had to be modified as explained in Appendix A. Multiple equally likely realizations of transmissivity fields conditioned to measured transmissivities and equivalent fresh water heads are generated. Then flow and transport are simulated in each conditional realization.

Several hypotheses are formulated and different sets
Table 1  
Different characteristics of the hypotheses studied

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<th>H-II</th>
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<td>SC(^b)</td>
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\(^a\) Sequential simulation.
\(^b\) Self-calibrated method.

of 300 realizations generated. Comparing Fig. 3(a) and Fig. 5(a.1) it can be concluded that 300 simulations are enough to represent the mean behavior of \(
\log T
\). A comparison of the variance field in Fig. 5(a.2) and the kriging variance map (not shown) also indicates that 300 realizations are sufficient to represent the local variance of the random function model adopted. The different hypotheses explore (i) the impact of neglecting the formation elevation gradient term for the calculation of the specific discharge (second term of Eq. (A1) in Appendix A), (ii) the impact of incorporating piezometric head information to the transmissivity spatial variability characterization, (iii) the impact of considering uncertainty of boundary conditions and (iv) the impact of including P-18, a well with a suspiciously low transmissivity measurement. Table 1 shows a summary of the characteristics of the different hypotheses studied.

The self-calibrated approach proceeds sequentially by first generating a transmissivity field, conditioned only to transmissivity data and referred to as the seed transmissivity field. This seed field is later updated to produce a transmissivity field also conditional to piezometric head measurements. In all hypotheses, except H-IV, the same 300 seed transmissivity fields, generated by sequential multi-Gaussian simulation, are used. Their ensemble mean and variance are shown in Fig. 5(a.1) and (a.2)—given how the seed fields are generated, their ensemble mean and variance coincide with the kriging estimate and the kriging variance maps. The variograms of all 300 seed fields are shown in Fig. 5(b.1) and (b.2) together with the average variogram and the model variogram. The departure of the average variogram from the model variogram is partially explained by the inclusion of extreme values, such as the transmissivity at well P-18, as conditioning values in the simulation process. For H-IV a different set of seed transmissivity fields was used without conditioning to the measurement at P-18.

The conclusions of the study are based on the analysis of ensemble mean and variance fields of log-transmissivity and piezometric head, and on histograms of travel times and pathlines of particles released from the repository area to the south boundary of the area of study.

3. Hypotheses analyzed

3.1. Treatment of variable fluid density

A preliminary study of the alternative approximations to model variable density flow in the Culebra Dolomite was carried out by Davies (1989) who compared the ratio of the magnitude of the two components of the velocity vector in Eq. (A1). He concluded that this ratio could be large therefore density effects should be explicitly addressed in a rigorous manner.

We show that the combined effect of the spatial variations of fluid density, aquifer elevation and transmissivity warrant a better approximation of the effect of variable density than the use of equivalent fresh water heads. Hypothesis 0 (H-0) and hypothesis I (H-1), referred to in Table 1, have been considered to analyze the above effect. In the first one, the flow and transport problems for the 300 seed fields are solved using equivalent fresh water heads and neglecting the second term of Eq. (A1) in Appendix A to compute specific discharges. In the second one, both problems are solved using the more accurate representation of the impact of variable fluid density...
Fig. 6. Density and formation elevation maps obtained by ordinary kriging interpolation of the data values. White dots show measurement locations.

as described in Appendix A. None of these two hypotheses requires the application of the self-calibrated method since piezometric data are not included as conditioning data in these simulations.

The maps of elevation and density in the model domain were obtained by kriging interpolation using the measured data provided in Cauffman et al. (1990). (See Fig. 6.)

The difference in resulting equivalent fresh water heads can be as high as 8 m in individual realizations.

Fig. 7. Comparison of equivalent fresh water heads computed with and without accounting for the impact of variable density: (a) H-0; (b) H-I.
The ensemble average piezometric head fields for H-0 and H-I are shown in Fig. 7. Their discrepancy is large in those areas in which the density gradient is high, particularly towards the east and southeast of the site.

Fig. 8 shows the histograms of arrival times and the paths of a single particle released from well H-2a in all 300 realizations for both H-0 and H-I. The paths are longer and show larger curvature for hypothesis H-I (Fig. 8(b)) than for hypothesis H-0 (Fig. 8(a)). In some realizations the particle path travels through a more impervious area in the east yielding higher travel times. The histogram of travel time for H-I shifts its mean and first quartile to lower values than those for H-0, and also displays a longer tail.

Hereafter, all remaining hypotheses are analyzed using the more accurate description of density effects used in H-I.

3.2. Conditioning to piezometric head data

Hypothesis II, H-II, shows the impact of conditioning to piezometric head data by means of the self-calibrated algorithm. The 300 seed fields are modified by adding to them a smooth perturbation field which has been parametrized as a function of the perturbations at a set of master points. The set of master points is composed of the transmissivity measurement locations plus 70 additional locations that change from one realization to another. Each of the latter 70 locations is selected at random from each of the equal-sized subareas resulting from a partitioning of the area of study by a mesh of 10 rows and 7 columns.

The objective function used in the minimization for the calculation of the perturbation field, weights the measured piezometric heads by a factor proportional to the inverse of the error amplitude of head reported by LaVenue et al. (1990). At measurement locations, the perturbation of logtransmissivity is constrained to plus or minus twice the measurement error of transmissivity given by LaVenue et al. (1990). At the remaining 70 master points, the perturbation is such that the resulting logtransmissivity values at master locations must be...
within two kriging standard deviations of the kriged value in Fig. 3.

The performance index \( \eta \) measures the degree of conditioning to piezometric heads

\[
\eta = \sqrt{\frac{\sum_{i \in \{m_i\}} \omega_i (h_i - h_i^m)^2}{m_i}}
\]

where \( m_i \) is the number of measurement locations (37 in this case), \( i \) the location index, \( h_i \) represents the calculated piezometric head, \( h_i^m \) the measured piezometric head, and \( \omega_i \) a weight. The weights are normalized so that they add up to one.

The index \( \eta \) obtained in the 300 seed fields, before conditioning to head, ranges from 2.4 to 7.7 m, with an average of 4.4 m and a standard deviation of 2.4 m.

After conditioning to head measurements, the updated fields yield \( \eta \) ranging from 0.2 to 1.7 m, with a mean of 0.5 m and a standard deviation of 0.2 m. Considering that the average measurement error is about 1 m, the fields can be considered as conditional to piezometric head measurements.

Fig. 9 shows ensemble averages of logtransmissivity and heads for H-II. Comparison of Fig. 9(a), which is conditional to both transmissivity and head measurements, to Fig. 5(a), which is only conditional to transmissivity measurements, reveals a larger variability of the logtransmissivity field in the north–south direction after conditioning to heads. The ensemble variance field of logtransmissivity conditional to both transmissivity and head measurements

![Fig. 9. Results for H-II. Ensemble averages of: (a) logtransmissivity; (b) piezometric head. White dots show measurement locations.](image)

![Fig. 10. Results for H-II. Variograms for the 300 logtransmissivity fields (faint lines) together with the ensemble mean variogram (dashed line) and the input model variograms (solid line).](image)
is not shown but it is found to be smaller everywhere than the variance of the fields conditioned only to transmissivity data. The directional variograms of the 300 logtransmissivity fields corresponding to H-II are shown in Fig. 10, together with their mean and the model variogram. The cloud of variograms has smaller spread than in Fig. 5(b) indicating the reduction of variability across the ensemble imposed by conditioning to head data.

Comparison of Fig. 9(b) with Fig. 7(b) shows the impact of including the piezometric head data as conditioning information, in the resulting piezometric head fields. Notice also that, in these two hypotheses, the boundary values are prescribed to be the same.

Fig. 11 shows the ensemble variances of piezometric head conditional to only transmissivity and to both transmissivity and head data. While incorporating piezometric head data is important since it reduces the uncertainty in the estimates of both logtransmissivity and piezometric head, it is even more important given its impact in travel times and particle paths as discussed next. Comparison of Fig. 8(b) with Fig. 12 shows that travel times are considerably reduced and that travel paths are less spread when piezometric head data are considered. The expected travel time from well H-2a to the south boundary goes down from 234 to 113 Kyr, and its standard deviation decreases from 258 to 75 Kyr. The paths taken by a single particle released from well H-2a in all 300 logtransmissivity fields conditional to both logtransmissivity and head data appear to "channel" through a well defined zone of high transmissivity located towards the southeast of the WIPP boundary, which is noticeable in the ensemble average field and appears consistently in all realizations. This channel was also noticed by LaVenue et al. (1990, 1995) in

![Graph showing travel time histogram]

Fig. 12. Results for H-II. Particle paths and travel time histogram corresponding to a single particle released at location H-2a in all 300 realizations.
both their deterministic and stochastic analyses of the WIPP site when conditioning to piezometric head data was considered, especially to transient head data.

A more detailed analysis attempting to quantify the impact of conditioning to piezometric data in a synthetic case study was carried out by Wen et al. (1996).

3.3. Accounting for uncertainty of boundary conditions

The prescribed heads at the boundaries used in the previous hypotheses have been assumed as perfectly known. They were taken from LaVenue et al. (1990) who obtained them from a regional model based on more hydrogeologically-sound boundary conditions. It is clear that there is uncertainty on the prescribed heads used until now. We decided to explore the impact of considering uncertain boundary conditions taking advantage of the self-calibrated algorithm that allows perturbation of the boundary conditions at the same time that the perturbation of the logtransmissivity field is computed.

In hypothesis III, H-III, a perturbation of the boundary conditions is parametrized as a function of the perturbations at 52 master locations regularly spaced along the perimeter of the area of study. In between master locations, perturbations are linearly interpolated. The seed prescribed heads are the same in all cases and equal to the ones taken as perfectly known in the previous hypotheses. The perturbations of boundary heads at master locations are constrained to be within ±3 m.

In H-III, each of the 300 realizations consists of a logtransmissivity field and a set of prescribed heads at the boundaries. Allowing the boundary conditions to be perturbed at the same time as the logtransmissivities are, provides a better reproduction of the
measured heads, resulting in a smaller value of the performance index η than for H-II.

Fig. 13 shows, for H-III, the ensemble average prescribed heads clockwise along the boundary, starting from the northwest corner, together with the deterministic heads used previously. The most important characteristic of the results from H-III is the increase of the "channeling" effect already noticed in H-II due to a decrease of the boundary heads in the center of the south border. Its consequence is a reduction in travel times as can be observed in Fig. 14. Logtransmissivity fields and accompanying piezometric head fields are not very different between H-II and H-III except for the values close to the edges.

3.4. Influence of P-18

In the set of transmissivity measurements, there is an extremely low value the reliability of which has been questioned: logtransmissivity at well P-18 (at the east of the WIPP area) is −10.12 (log_{10} m^2 s^{-1}). The question that arises is whether this value is an interpretation error or an outlier. We thought important to carry out a new analysis removing well P-18 from the conditioning data set (well P-18 was considered in all previous hypotheses).

Hypothesis IV, H-IV, corresponds to H-II without considering P-18 as datum. The resulting ensemble average logtransmissivity field is shown in Fig. 15.

Fig. 16. Results for H-IV. Particle paths and travel time histogram corresponding to a single particle released at location H-2a in all 300 realizations.
When P-18 is removed from the conditioning data set, a new "channel" develops in the eastern part of the study area (compare Fig. 12 with Fig. 16). This new feature allows an alternative escape path in some realizations for the particle released from well H-2a, as evidenced in Fig. 16.

To assess the likelihood of the value of P-18 reported in LaVenue et al. (1990), the histogram of logtransmissivity at location P-18 conditional to the rest of logtransmissivity and piezometric head measurements is shown in Fig. 17. The minimum of the 300 simulated values at P-18 is −8.19, therefore leaving a very small likelihood to the interpreted value of −10.12. The measured value at P-18 is not consistent with the model of spatial variability used in this analysis, whether to include it or not in the analysis has an important effect on the predicted travel times.

4. Conclusions

The self-calibrated approach has been applied to a real formation: the Culebra Dolomite in the WIPP site. The algorithm described in the previous two papers of the series has been extended to spatially variable fluid density, and its capabilities to account for uncertain boundary conditions have been demonstrated.

The analyses carried out raise the following general conclusions:

- The spatial variability of transmissivity, fluid density, and formation elevation may warrant the formulation of Darcy's law in terms of the fresh water head gradient and the formation elevation gradient in order to account for salinity effects.
- Conditioning to piezometric head data, in addition to transmissivity data, helps in reducing the uncertainty in transmissivity, piezometric head and travel times as was also shown by LaVenue et al. (1995).
- Re-adjusting the boundary conditions during the calibration phase of the self-calibrated algorithm helps in improving the conditioning to the piezometric head measurements. This re-adjustment is only justifiable when the boundary conditions are uncertain.

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Appendix A. Modeling fluid flow accounting for spatially variable fluid density

Spatially variable fluid density can be accounted for by introducing an additional component in the Darcian velocity that depends on its deviations, \( \Delta \rho \), from a reference density value, \( \rho_f \) (fresh water), on
the variations of the formation elevation, $z$, and on the hydraulic conductivity value, $K$.

Following Davies (1989), the specific discharge $v$ can be written as

$$ v = -K \left[ \nabla h_t + \frac{\Delta \rho}{\rho_t} \nabla z \right] \quad (A1) $$

where $K$ is the hydraulic conductivity for fresh water, and $h_t$ refers to the equivalent fresh water head given by

$$ h_t = \frac{p}{\rho_t g} + z \quad (A2) $$

with $p$ the fluid pressure and $g$ the magnitude of gravitational acceleration.

Assuming confined flow in a bidimensional domain, Eq. (A1) can be integrated in the vertical dimension, resulting in the expression for horizontal flow per cross-sectional unit area $q$

$$ q = -T \left[ \nabla h_t + \frac{\Delta \rho}{\rho_t} \nabla z \right] \quad (A3) $$

with $T = Kb$ the transmissivity and $b$ the formation thickness.

If both fluid and solid are incompressible and the change in fluid volume due to variations of solute concentration can be neglected, then Eq. (3) for volume conservation given by Gómez-Hernández et al. (1998) becomes

$$ -\nabla (T \nabla h_t) - \nabla \left( \frac{T \Delta \rho}{\rho_t} \nabla z \right) = Q. \quad (A4) $$

The second term on the left-hand side does not depend on the unknown $h_t$ so it can be grouped with terms included in $Q$.

Discretization of the above equation by finite differences results in a set of linear equations as shown in Gómez-Hernández et al. (1998), Eq. (4), with an additional term in the vector of stresses

$$ \{Q\} = \{Q^0\} + \{Q^v\} + \{Q^p\} \quad (A5) $$

where $\{Q^p\}$ is the term due to the variable density effect with components

$$ Q^p_i = \frac{1}{\rho_t} \sum_{j \in N,S,E,W} T_{ij} \Delta \rho_{ij} (z_i - z_j) \quad (A6) $$

with $\Delta \rho_{ij}$ the deviation of density from the reference $\rho_t$ in the area between blocks $i$ and $j$, and $z_i$ the elevation of block $i$. The summation extends to the four adjacent blocks.

The derivative of vector $\{Q\}$ needed by the self-calibrated algorithm (Eq. (15) in Gómez-Hernández et al. (1998)) contains an extra term related to $\{Q^p\}$ given by

$$ \frac{\partial Q^p_i}{\partial \Delta Y_k} = \frac{1}{\rho_t} \sum_{j \in N,S,E,W} T_{ij} \frac{1}{\lambda_i + \lambda_j} \Delta \rho_{ij} (z_i - z_j) \quad (A7) $$

in which we have used the geometric mean $T_{ij} = \sqrt{T_i T_j}$, for the interblock transmissivity. Hereafter the methodology described in the first part of this series of papers remains exactly the same except that Eqs. (A5) to (A7) have to be incorporated.

References


