Development and Verification of a Three-Dimensional Variably Saturated Flow Model for Assessment of Future Global Water Resources

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Abstract Global water resource assessment has been conducted primarily for surface water and shallow groundwater (unconfined aquifers). Groundwater is a major water resource worldwide. Nevertheless, future water resource assessment integrating surface water and groundwater has not been carried out at the global scale. Large grid sizes are used in global-scale models due to computer resource constraints.

Plain Language Summary The state of future water resources at the global scale, taking into account climate change, remains highly uncertain. To date, water resource assessments have been conducted mainly on surface water. However, groundwater is one of the most important water resources and has not been included in water resource assessments. This is largely due to the lack of a groundwater model that can be applied at the global scale. Therefore, we have developed a new groundwater model applicable at the global scale and verified its code. As a result, it was confirmed that the developed code provides a correct solution compared with experiments and other model results. In the future, we intend to use this code to conduct future water resource assessments, including assessments of groundwater. This is expected to produce outcomes that contribute to sustainable development.

1. Introduction

Global assessment of future water resources integrating surface water and groundwater is essential to identifying future water resources under conditions of climate change and population growth. Furthermore, such assessment would help guide policies for future development.

To date, global water resource assessment has been conducted mainly on surface water, represented by rivers, and on shallow groundwater (Alcamo et al., 2007; Arnell, 2004; Haddeland et al., 2014; Vörösmarty et al., 2000). As shown by Döll et al. (2012), groundwater is used for 36% of domestic purposes, 42% of agricultural purposes, and 27% of industrial purposes, making it one of the most important water resources worldwide. Surface water and groundwater are intimately interconnected through unsaturated zones and unconfined layers, with both surface-to-underground and underground-to-surface interactions. In particular, in arid and semiarid regions, groundwater is an essential water resource. Globally, unconfined and confined aquifers (containing shallow and deep groundwater, respectively) are highly utilized for human activities. Despite this importance, assessment of future water resources, including both surface water and various depths of groundwater, has not been conducted at the global scale.
Various models have been developed to assess future water resources at the global scale, including the H08 (Hanasaki et al., 2008a, 2008b), WaterGAP (Alcamo et al., 2003; Döll et al., 2003), and PCR-GLOBWB (Beek & Bierkens, 2008) models. Research to predict future water resources that accounts for climate change and human water usage has been conducted using these models. However, these models do not explicitly consider groundwater flow and provide unclear results about changes in groundwater flow due to pumping. In addition, these models cannot reveal the effects of changing groundwater flow on surface water and climate.

Fan et al. (2013) modeled groundwater flow at the global scale at high resolution using 30 arc-second (~1 km) grids. Graaf et al. (2015, 2017, 2019) coupled a groundwater flow model (MODFLOW) and a land surface model (PCR-GLOBWB) to reveal groundwater flow and effects of groundwater pumping on environmental flow. However, in these models, the unsaturated zone is not explicitly considered or is treated as a vertical dimension, and thus, they do not correctly express underground water flow, particularly in mountainous areas. Mountain areas have steep slopes, causing water in the unsaturated zone to exhibit three-dimensional flow. In addition, the thickness of the unsaturated zone may change under future climate change conditions, and extreme weather will further complicate water flow in this zone. Therefore, these models may produce significant uncertainties in future predictions. From the basin to the continental scale, some models consider variably saturated flow in three dimensions (e.g., PFLOTRAN and ParFlow). With the recent development of computer resources, variably saturated flow calculation using a spatially dense grid can be conducted at the continental scale (Maxwell & Condon, 2016).

The ultimate goal of our research is to conduct future water resource assessment that integrates surface water and groundwater and considers water usage at the global scale. Even considering the rapid growth of computational resources, performing three-dimensional calculations based on physical equations at the global scale will be costly. Therefore, we may need to perform parameterization to estimate fine-scale underground physical process, and this process requires a model based on the full physical governing equations as a reference. Furthermore, it is necessary to account for the availability of freshwater, which may be affected by factors such as water pollution and salinization, in future predictions and evaluations. Because the code could be improved in the near future and it is necessary to exchange infiltration, soil moisture, and discharge for land surface models like MATSIRO (Takata et al., 2003) and CuMa-Flood (Yamazaki et al., 2011) and to apply high-speed and scalable numerical methods (e.g., the multigrid method) for large-scale modeling, we developed new code for future water resource assessment at the global scale. As noted above, surface water and groundwater interact with each other through unsaturated zones, depending on the topographic gradient. To reproduce these phenomena in a numerical model, we developed a three-dimensional variably saturated flow model with groundwater storativity: This model, which is based on the full physical governing equation, incorporates numerous modern mathematical methods and can perform fast and robust calculations. We believe that it can be used as a part of Earth System Model and as a reference model for parameterization.

2. Equation and Numerical Solution

2.1. Governing Equation

As shown in 1, the equation used in this study can integrate the saturation/unsaturation and confined/unconfined conditions of groundwater. This equation was adapted to a variably saturated flow model based on Richards’ equation (Richards, 1931) to consider the storativity of groundwater. Underground conditions, particularly unsaturated zone thickness, show significant differences over the global scale depending on climate conditions, soil and geological structure, plants, and terrestrial elevation. Future underground conditions will also be affected by climate change. Therefore, we decided to employ the following equation, which considers unsaturated water flow and the effects of groundwater storativity:

$$\frac{\partial \theta}{\partial t} + S_s S_w(\varphi) \frac{\partial \varphi}{\partial t} = \nabla \cdot [K(\varphi) \cdot \nabla (\varphi + Z)] + Q \tag{1}$$

where $\theta$ is the volumetric water content ($-$), $\varphi$ is the pressure head (L), $S_s$ is the specific storage coefficient
\[ L^{-1} \]

\( S_p \) is the saturation, \( K(\varphi) \) represents the hydraulic conductivity tensors \((L/T)\), \( Z \) is the position head \((L)\), \( Q \) is the source/sink term \((L^3T^{-1})\), and \( \cdot \) is the inner product. As shown by Celia et al. (1990), using the pressure-form equation, the Picard method can preserve sufficient mass balance only over a short time step. Therefore, in this study, the mixed form was applied, as shown in Equation 1.

By combining the pressure head and the position head in Equation 1, Equation 2 is obtained to determine hydraulic head \((h)\). Because the numerical result we want to obtain is hydraulic head, we use Equation 2 as a governing equation. This equation is discretized spatially and temporally to reach the final solution.

Pressure head \((\varphi)\) is used to calculate the volumetric water content (saturation) and hydraulic conductivity.

\[ \frac{\partial \theta(\varphi)}{\partial t} + S_p S_w(\varphi) \frac{\partial h}{\partial t} = \nabla \cdot [K(\varphi) \cdot \nabla h] + Q \]  

(2)

To discretize Equation 2 and obtain a solution, relative permeability and volumetric water content (saturation) must be determined from the pressure head in the unsaturated zone. In this study, the van Genuchten (1980) and Mualem (1976) model, described in Equations 3 and 4, was used as the water retention curve.

\[ S_r = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left( 1 + |\alpha \varphi|^n \right)^{-m} \]  

(3)

\[ K_r = S_r^{1/2} \left[ 1 - \left( 1 - S_r^{1/m} \right)^{m/2} \right] \]  

(4)

In the above, \( S_r \) is the effective saturation \((-\)), \( \theta_s \) is saturated volumetric water content \((-\)), \( \theta_r \) is residual volumetric water content \((-\)), and \( \alpha \) are parameters that describe the shape of the curve. Using volumetric water content and effective saturation obtained from van Genuchten, relative permeability is calculated, and then hydraulic conductivity is determined through multiplication with saturated hydraulic conductivity.

2.2. Numerical Solution

2.2.1. Spatial Discretization

The governing equation shown in 2 exhibits nonlinearity for hydraulic conductivity and volumetric water content in the unsaturated zone. For this reason, computational resource requirements are assumed to be greatest for calculations in the unsaturated zone. In addition, active groundwater extraction occurs in a small portion of the overall land area. Therefore, we employed the finite volume method (FVM) for spatial discretization. Because FVM can use a flexible grid with strict conservation of mass, it appears to be an effective use of computer resources. A structured grid is used for linear solution, which consumes the greatest portion of computational time, to maintain the matrix conditions more effectively.
In the governing equation 2, the term related to space on the right side is described by Equation 5 in volume integral form using the control volume $V_p$ and grid center $p$.

$$\int_{V_p} \nabla \cdot (K \phi) \cdot \nabla h \, dV + \int_{V_p} Q \, dV$$  \hspace{1cm} (5)

In Equation 5, the first term represents the inflow and outflow from the grid adjacent to the control volume, and the second term is the source/sink term for the target grid. The source/sink term represents groundwater pumping or injection, recharge, and evapotranspiration losses.

The first term of Equation 5 can be expressed in areal integral form using Gaussian divergence theorem, as shown in 6.

$$\sum_f S \cdot (K \phi) \cdot \nabla h \big|_f$$  \hspace{1cm} (6)

Here, $S$ is an area vector composed of each grid adjacent to the target grid, and $f$ is a subscript representing a variable on the grid surface. If $S$ in Equation 6 is orthogonal, the direction and magnitude of the outward vector to the grid surface will be the same, and $\nabla h$ can be calculated from the grid distance and the difference in hydraulic head. If it is not orthogonal, correction is required. However, as McBride et al. (2006) noted, no correction was used because this extremely distorted grid is not used at the global scale. Thus, Equation 6 can be expressed as Equation 7 to consider the area $A(m^2)$, distance $d(m)$, and hydraulic head $h(m)$ between the target grid ($p$) and the adjacent grid ($n$).

$$K(p, n) \frac{h_n - h_p}{d_n + d_p}$$  \hspace{1cm} (7)

The hydraulic conductivity $K(p, n)$ at the grid surface is calculated from hydraulic conductivity values in the target grid and each adjacent grid. In the saturated zone, the harmonic average described by Equation 8 is used. This calculation in the unsaturated zone is a topic of ongoing research. Warrick (1991) proposed the Darcian mean approach, which is based on the assumption that the instantaneous value of the flux between two grids is equal to its steady-state condition. Baker (2000) showed that the Darcian mean is equal to the integrated mean for horizontal flow. Based on these findings, Szymkiewicz (2009) proposed three different approximating equations that can be used for various types of flow (infiltration in dry soil, drainage, and capillary rise). We employed the upwind method only for relative permeability and the harmonic average method for saturated hydraulic conductivity, because solution of the upwind method does not show oscillations and has lower calculation cost.

$$K_{sp,n} = \frac{d_p + d_n}{A_p / K_s + A_n / K_s}$$  \hspace{1cm} (8)

### 2.2.2. Time Discretization

For time discretization, the implicit Euler method is used based on consideration of calculation stability and mass conservation. An appropriate time step can be determined in advance, as shown by Diersch and Perrochet (1999), but their results showed that multiplying values within a certain range carried a lower calculation cost. Thus, we employed the multiplication method in this study.
When the implicit Euler method is used in a finite volume, the term on the left side of Equation 2 is discretized, as shown in Equation 9.

\[
\frac{\partial}{\partial t} \int_V \theta \phi (t) \, dV + S_{sW} \phi (t) \frac{\partial}{\partial t} \int_V \phi \, dV = \frac{V_p}{\Delta t} \left\{ \theta_p (m+1) - \theta_p (m) \right\} + S_r \left[ \theta_p (m+1) h_p (m+1) - \theta_p (m) h_p (m) \right] \quad (9)
\]

The superscript represents a time step, \(m+1\) represents the time for which a solution is being found, and \(m\) represents the time one step prior to that being solved.

### 2.2.3. Nonlinear Solution Method

Because the governing equation 2 used in this study exhibits nonlinearity as a function of pressure head in its calculation of hydraulic conductivity and volumetric water content in the unsaturated zone, a nonlinear solution is required. To date, two primary methods have been adopted for nonlinear solution of Richards’ equation: the Picard method and the Newton-Raphson method.

The Picard method, which is a fixed-point technique, and the modified Picard method proposed by Celia et al. (1990) show linear convergence when reaching a stable solution. The Newton-Raphson
method shows quadratic convergence, and this is generally considered faster than the Picard method. However, for the former to exhibit quadratic convergence, the calculated initial condition must be sufficiently similar to the solution, and numerical divergence is caused if the initial condition is wrong.

To date, each solution has shown superior performance under various conditions. Paniconi and Putti (1994) showed that a solution combining these two methods results in faster convergence. In this study, however, we aimed to prevent divergence by providing a good numerical initial condition. We adopted the Newton-Raphson method for faster convergence. Furthermore, we used the inexact Newton method, which was proposed by Eisenstat and Walker (1996). The Inexact Newton method is a technique of adaptively changing the convergence condition for linear equations. Using it, the number of iterations of the linear solution is expected to be reduced, and thus, a faster calculation speed is reached.

As noted above, we applied the Newton-Raphson method. This method may fall into a local convergence solution. Therefore, we used a global method to relax the Newton-Raphson method to improve convergence and robustness. The global method is composed of a line search method and a trust region method. We also used backtracking (Brown & Saad, 1990), a type of line search method, because of its simplicity and ease of application to the Newton-Raphson method. This technique can use the convergence process of the Newton-Raphson method and the step length determined from the descent direction, thereby further improving convergence.

Figure 6. Diagram of Test Problem 3 (3-D well pumping).

Figure 5. Diagram of Test Problem 3 (3-D well pumping).
2.2.4. Linear Solution Method

The linear equation created using the Newton-Raphson method becomes an asymmetric positive definite matrix, for which we adopted the preconditioned bi-conjugate gradient stabilized method (Bi-CGSTAB) (van der Vorst, 1992). In preconditioning, ILU (0), which does not consider fill-in for incomplete lower-upper (ILU) decomposition, was used.

Because this model uses a three-dimensional structured grid, it generates a sparse matrix with 7-point differences. To reduce the computational storage capacity, the matrix employs a commonly used Compressed Row Storage (CRS) format.

2.2.5. Convergence Criteria

In this study, iterative methods are used for both linear and nonlinear solution. Because we used the inexact Newton method, a convergence criterion is needed only for nonlinear solution. As a convergence condition, the absolute hydraulic head $L_{\infty}$-norm, stated in 10, is used for the nonlinear solution:

$$\max_p \left| h_p^{m+1,k+1} - h_p^m + 1,k \right| \leq \varepsilon_h$$  \hspace{1cm} (10)

where $k+1$ is the current nonlinear iteration, $k$ is one step prior to the nonlinear iteration, and $\varepsilon_h$ is the convergence criterion of the nonlinear solution.

2.2.6. Boundary Conditions

Boundary conditions can be broadly classified into Dirichlet and Neumann conditions. In this study, boundary conditions were handled in the variably saturated flow model under the following four conditions.

Figure 7. Comparison of results for three-dimensional well pumping problem with the Thiem solution (confined conditions).

Figure 8. Comparison of results for three-dimensional well pumping problem with Thiem solution (unconfined conditions).
1. Recharge centered on precipitation from the surface (Neumann condition).
2. Evapotranspiration from underground (Neumann condition).
3. Water-level boundary such as sea, river, or lake (Dirichlet condition).
4. Groundwater pumping or underground water injection (Neumann condition).

Moreover, this model can designate grids where the calculation is not conducted and flux from the outside of the calculation range becomes zero. Similarly, flux from the bottom of the lowest grid is zero. To express fluxes to or from the surface, this model switches to Dirichlet conditions (surface elevation) when outflow occurs and to Neumann conditions (zero flux) when it does not.

3. Code Verification Results

Verification results for the developed code are provided below. As boundary conditions are particularly important to water resource assessment at the global scale, we verified considering the problems of infiltration from precipitation, subsequent runoff, and behavior of groundwater pumping, taking into account the future use of this model. We also confirmed the water balance, which is important when conducting water resource assessment. All test problems shown below used the numerical solution criterion with values of $1.0 \times 10^{-6}$ in a nonlinear solution and used the parameters in each test shown in Table 1.

![Figure 9. Diagram of Test Problem 4 (2-D seepage).](image)

![Figure 10. Relationship between pressure head and hydraulic conductivity in Test Problem 4 (2-D seepage).](image)
3.1. Test Problem 1: One-Dimensional Infiltration

To confirm the infiltration of precipitation into the unsaturated zone, the problem conducted by Paniconi et al. (1991) was used. Paniconi et al. (1991) assumed a vertical column of 10 m height and used flux, which changes with time, from the top of the column as a boundary condition. The bottom layer is set to a pressure head of zero (see Figure 1). The results of this model are shown in Figure 2 and are consistent with the results obtained by Paniconi et al. (1991).

Note that this model uses a staggered grid and the unknown value, hydraulic head, has a value at the center of the grid. For this reason, because the graph is plotted at the center of the grid, the referenced solution does not correspond to the position. The same pattern applies to subsequent calculations.

3.2. Test Problem 2: Two-Dimensional Variably Saturated Water Table Recharge

A two-dimensional test problem was used, assuming that recharge arises from a river. This problem is based on an experiment conducted by Vauclin et al. (1979) (Figure 3). Clement et al. (1994) estimated van Genuchten’s parameters from the results of Vauclin et al. (1979). We used their parameter values. The results of applying this problem to the model are shown in Figure 4. The model results appear consistent with those of the experiment conducted by Vauclin et al. (1979).

3.3. Test Problem 3: Three-Dimensional Well Pumping

When water is taken from the saturated zone through a well, the hydraulic head drops around the well (Figure 5). To reproduce this phenomenon, we compared our calculation results with the Thiem solution. Because the Thiem solution is based on steady-state radial flow, we performed this problem using a
calculation range of 60° (Figure 6) and no time step, which means that the time discretization term is excluded from the governing equation 2. This change sometimes leads to divergent results. Therefore, we used different groundwater pumping rates under confined and unconfined conditions. For this problem, we determined the solution with different hydraulic conductivity values, and arbitrary values were used for the residual saturation and van Genuchten parameters under the assumption that these values do not affect the solution.

### 3.3.1. Confined Condition

The Thiem solution in confined conditions is expressed by Equation 11. 

\[
h = H - \frac{Q}{2\pi m K_s} \ln \frac{R}{r}
\]

Here, \( h \) represents the hydraulic head at a location radius \( r \) from the well; \( H \) is the hydraulic head as a boundary condition at a distance of radius \( R \) from the well, which is considered unaffected by groundwater pumping; \( Q \) is the amount of groundwater pumped; \( m \) is the thickness of the aquifer; and \( K_s \) represents the saturated hydraulic conductivity of the aquifer. The boundary condition \( H \) at radius \( R \) was set to 8 m, and groundwater pumping was set to 30 m\(^3\)/s for the Thiem solution and to 5 m\(^3\)/s for model input based on the model grid. The results of a comparison between the model calculation and the Thiem solution are shown in Figure 7. The calculation results from this model are consistent with the Thiem solution under confined conditions.

### 3.3.2. Unconfined Condition

We also conducted a comparison with the Thiem solution under unconfined conditions. The Thiem solution under unconfined conditions is expressed by Equation 12. Each symbol represents the same parameter as that under confined conditions. In unconfined conditions, the boundary condition \( H \) at radius \( R \) was set to 0 m and groundwater pumping to 18 m\(^3\)/s for the Thiem solution and to 3 m\(^3\)/s for model input based on the model grid. With groundwater pumping set to 30 m\(^3\)/s, we could not obtain a solution through model calculation. The results of comparing the model output with the Thiem solution are shown in Figure 8. The calculation results of this model are consistent with the Thiem solution under unconfined conditions.

\[
h = \sqrt{H^2 - \frac{Q}{\pi m K_s} \ln \frac{R}{r}}
\]

### 3.4. Test Problem 4: Two-Dimensional Seepage in a Hillslope

This model is ultimately targeted at the global scale. Therefore, we confirmed the mechanism of ground-to-surface seepage, which is particularly prominent in mountainous areas of humid regions.
based on an experiment conducted by Fredlund and Rahardjo (1993). The problem is diagrammed in Figure 9.

In this problem, van Genuchten’s parameters were unknown. As shown in Figure 10, we estimated the parameters that describe the relationship between hydraulic conductivity and pressure head. Of the volumetric water contents used in this problem, that for fine sand was 0.456 based on Rulon et al. (1985), and that for medium sand was 0.431, which is the average value of data for medium sand in Rulon’s doctoral dissertation (1984). The specific storage coefficient set by Fredlund and Rahardjo (1993) is in units of kPa⁻¹, so the density of water (977 kg/m³) and gravitational acceleration (9.8 m/s²) are used with this model. The specific storage coefficient in this model is 0.01954 m⁻¹. Moreover, because seepage is determined only through the surface, we used the grid shown in Figure 11.

The comparison results are shown in Figure 12. The calculated hydraulic heads after 4.6, 31, and 208 s are indicated by the red line in Figure 9. The model results showed little difference from the calculation results of Fredlund and Rahardjo (1993). This difference results from the soil parameters and grids used (they used a flexible grid with a finite element method). Nevertheless, the model results are in accordance with the results of Fredlund and Rahardjo (1993), and we judged that the model achieved reliable results for seepage.

3.5. Confirmation of Water Balance

For future use of this model, it is necessary to confirm its performance not only for the hydraulic head but also for the water balance at a given place and time. Using the vertical one-dimensional infiltration problem described by Celia et al. (1990), we confirmed water balance performance. Hydraulic head is set as a boundary condition, which differs from the pressure head determination performed by Celia et al. (1990). Therefore, the value was converted into hydraulic head and input to the top grid as a boundary condition.

The calculation results of this model and the results obtained by Celia et al. (1990) are shown in Figure 13. Our results differ compared to those of Celia et al. (1990), likely because the upwind method is used for relative permeability when calculating the hydraulic conductivity. To confirm this cause, we used the arithmetic mean of hydraulic conductivity in the same way as Celia et al. (1990), as shown in Figure 13. Based on these results, this model is consistent with the results of Celia et al. (1990).

In this model, water balance determination considers inflow or loss from the ground surface, inflow or loss through wells, flux among grids, and changes in storage volume. In this problem, because there is no inflow or loss from the ground surface and no inflow or loss from wells, the water balance was confirmed using Equation 13. The water balance result is exactly 1, indicating that no calculation errors occurred. Thus, this model is considered to appropriately determine the water balance through numerical calculation.

\[
\text{Water balance} = \frac{\text{Outflow volume from whole area}}{\text{Storage Change}}
\]  (13)

4. Summary and Conclusions

For application at the global scale, we constructed a three-dimensional variably saturated flow model with various numerical methods. For spatial discretization, we use a FVM that satisfies the law of mass conservation and can consider the flexibility of the grid. For temporal discretization, the implicit Euler method was used, which considers the stability of the numerical method. The Newton-Raphson method was also used so that the calculation could quickly attain convergence. To reduce calculation cost and computational storage, the Bi-CGSTAB method with ILU(0) preconditioning and the CRS matrix format were used as a linear solution. The newly developed code was subjected to verification. Considering the future application of this model, we confirmed it based on vertical one- and two-dimensional infiltration problems, a three-dimensional groundwater pumping problem, seepage problem, and water balance.

Our code appeared to give an accurate solution to each problem. Therefore, we believe that models based on this code can reproduce various underground water flows. Because this model's target area, the region beneath the surface, has not been explicitly in Earth System Model, the model should achieve more realistic results through coupling it with a land surface model. That is, this model can be used as a part of Earth System Model. Furthermore, as this model is based on a physical equation, it can be used as a reference
model for parameterized models, allowing for efficient validation of parameterized models. In the near future, we will make a comparison with observed hydraulic head data and couple this model with a land surface model and report the results. Ultimately, we will conduct future water resource assessments integrating surface water and groundwater to clarify the best direction for future development policies.

Appendix A: Discretized Equations

In this study, an iterative method was used for a linear solution, as described in section 2.2.4. Discretization of the governing equation is shown based on the iterative Newton-Raphson method.

The Taylor expansion, ignoring the higher-order terms related to \( h \), was applied to \( \partial(\varphi)^{m+1} \) in the temporal variation term of volumetric water content, which is the first term on the right side of Equation 9. Thus, Equation A.1 is obtained. If this equation is substituted into Equation 9, the right side of Equation 9 becomes Equation A.2.

\[
\begin{align*}
\partial(\varphi)^{m+1, k+1} & \approx \partial(\varphi)^{m+1, k} + \left[ \frac{\partial \partial(\varphi)}{\partial h} \right]^{m+1, k} \left[ h^{m+1, k+1} - h^{m+1, k} \right] \\
& \quad \quad \quad \quad \quad \quad \quad + \frac{V_p}{\Delta t} \left[ \partial(\varphi)^{m+1, k} - \partial(\varphi)^{m} \right] + \frac{\partial \partial(\varphi)}{\partial h} \left[ h^{m+1, k+1} - h^{m+1, k} \right] + S_i \left( \partial_u(\varphi)^{m+1, k} h^{m+1, k+1} - \partial_u(\varphi)^{m, k} h^{m, k} \right)
\end{align*}
\]

(A.1)

The Newton-Raphson method is expressed as the determinant shown in Equation A.3 based on the iterative method, and hydraulic head, which is the unknown value in this study.

\[
J^k(h^{k+1} - h^k) = -R^k
\]

(A.2)

where \( J^k \) is the Jacobian matrix one step prior to the nonlinear iteration, \( R^k \) is the residual vector one step prior to the nonlinear iteration, and \( h^{k+1} \) and \( h^k \) are hydraulic head vectors for the nonlinear iteration. Residual \( R_p \) in the target grid is expressed as inflow/outflow from the adjacent grid, source/sink designation, and storage amount changes, as shown in A.4.

\[
R_p = \sum_{n \in \Gamma_p} K(\varphi)_{p,n} \frac{A_{p,n}}{d_{p,n}} \Delta h + Q_p - \frac{V_p}{\Delta t} \left[ \partial(\varphi)^{m+1, k} - \partial(\varphi)^{m} \right] + S_i \left( \partial_u(\varphi)^{m+1, k} h^{m+1, k+1} - \partial_u(\varphi)^{m, k} h^{m, k} \right)
\]

(A.4)

The Jacobian matrix \( J_{i,j} \) in each grid is expressed as A.5 using the residual \( R \) and the unknown value, hydraulic head. Here, \( i \) and \( j \) indicate rows and columns in the Jacobian matrix, respectively.

\[
J_{i,j} = \frac{\partial R_i}{\partial h_j}
\]

(A.5)

If the discretization equation of space is considered, the discretization equation for the target grid becomes A.6.

\[
\begin{align*}
\frac{V_p}{\Delta t} \left[ \partial(\varphi)^{m+1, k} - \partial(\varphi)^{m} \right] + \frac{\partial \partial(\varphi)}{\partial h} \left[ h^{m+1, k+1} - h^{m+1, k} \right] + S_i \left( \partial_u(\varphi)^{m+1, k} h^{m+1, k+1} - \partial_u(\varphi)^{m, k} h^{m, k} \right) + Q_p^{m+1}
\end{align*}
\]

(A.6)

Although it is possible to obtain the Jacobian matrix analytically, because it was complicated to do so in this study, we opted to use the perturbation method A.7.
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Data Availability Statement
The data we used in this paper, that is, model source code and input file, are available online (through http://doi.org/10.15083/00079364).

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