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Research paper

Evaluation of alternative conceptual models for groundwater modelling

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A B S T R A C T

This study evaluates the alternative conceptual models for groundwater modelling. A true model was created with a synthetic alluvial fan-plain hydrogeological framework. Various alternative conceptual models were evaluated for groundwater flow simulations. The first alternative model is a single aquifer layer model; the second alternative model is a 3-layer aquifer model; and the third model is a 5-layer model consisting of 3 aquifers separated by 2 aquitards. All models could fit very well to the observations with optimized values of hydraulic conductivities. However, the single aquifer layer model can only compute water balance components with good accuracy. The 3-layer aquifer model can be used for water balance computation and groundwater head simulation with small errors. The 5-layer model is capable of simulating water budget, groundwater head distribution and travel times with high accuracy. Multi-model analysis found only the 3rd alternative model superior.

1. Introduction

Conceptual model is defined as a simplified version of real world system (Anderson and Woessner, 1991). Conceptual models are formulated by including major physical processes operating on simplified hydrogeological formations within the generalized boundary conditions. However, hydrogeological systems are complex, rendering them prone to multiple interpretation and conceptualizations (Poeter and Anderson, 2005). Uncertainties in groundwater conceptual models come from various sources (Hill and Tiedeman, 2007). For example, uncertainty in estimated parameter values, boundary conditions, assumed model structure and hydrological stresses. Recent research indicates that the largest prediction uncertainty may come from the conceptualization of hydrogeological system (Bredehoeft, 2005; Hojberg and Refsgaard, 2005; Rojas et al., 2010). Ignoring the conceptual model uncertainty may result in biased predictions and/or underestimation of predictive uncertainty.

Since the real world groundwater systems are very complex because of spatial variation of geology and involving of different types of flow process, there is a need for simplification of real world systems. Over-simplification may result in a model with lack of information and under-simplification may result in a costly model. Both generate unrealistic predictions. It is therefore important that all features relevant to the real system must be included in the conceptual model and irrelevant ones be excluded. There are usually insufficient data to completely characterize the groundwater system. It is difficult to select a single appropriate conceptual model for the system (Bredehoeft, 2005). Then, alternative conceptual models can be developed based on different set of simplified assumptions (Hojberg and Refsgaard, 2005; Poeter and Anderson, 2005) and evaluate them to select most appropriate model for the system (Poeter and Anderson, 2005).

A number of statistical criteria have been used to evaluate alternative conceptual models (Poeter and Anderson, 2005). These include Kashyap Information Criterion (KIC), Bayesian Information Criterion (BIC), Corrected Akaike Information Criterion (AICc), and the Sum of Weighted Squared Residuals criteria (SWSR). Statistical discrimination criteria are calculated based on conceptual model predictive uncertainties. Generally, more than one model provides a similar acceptable fit to the observations: thus model discrimination should be made from multiple models. Multi-model analysis method (MMA) (Poeter and Hill, 2007) is one of computer code developed for identifying alternative models for the groundwater system using KIC, BIC, AICc, SWSR criteria.

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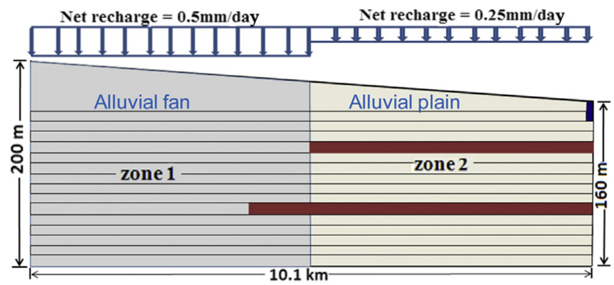

Figure 1. Cross-section of a synthetic alluvial fan-plain aquifer and model layers for the true model, red colour layers are clayey silt.

In this paper, a synthetic alluvial fan-plain aquifer system was created to test alternative conceptual models for simulating groundwater flow and travel time. Multi-model analysis method was used to identify the best alternative model. The results show that for computing water budget, a single layer model is sufficient. However, for simulating groundwater travel time, a conceptual model consisting of multiple aquifer-aquitard model layers must be used. The results provide guideline for choosing appropriate complexity of the conceptual model for different modelling purposes.

2. Generation of synthetic alternative conceptual models

Alluvial fan-plain aquifer is widely distributed and usually consists of multiple hydrogeological layers (Zhou et al., 2012). Hydrogeological layers can be conceptualized into a single aquifer up to multiple layers of aquifers separated by aquitards. Thus, alternative conceptual models are plausible. A true model and three alternative conceptual models were created for the analysis of alternative conceptual models for groundwater modelling in this study. These alternative models are differed only in the number of model layers; boundary conditions and hydrological stresses are kept the same.

The synthetic alluvial fan-pain aquifer consists of an alluvial fan of gravels and pebbles and an alluvial plain of sand layers separated by two clayey silt layers (Fig. 1). The hydraulic conductivity is specified as 100 m/d for the alluvial fan; to be 20 and 0.1 m/d for the aquifer and aquitard in the alluvial plain, respectively. Net groundwater recharge is uniformly distributed in two areas: 0.5 mm/d in the alluvial fan and 0.25 mm/d in the alluvial plain. The boundary on the west is assumed in contact with the impermeable rocks as no-flow boundary. The east boundary is a perennial river defined as a head-dependent flow boundary. Boundaries in the north and south are specified no-flow boundaries since groundwater flow is assumed parallel to these boundaries under natural flow.

The true model was constructed to generate benchmark data sets for comparing alternative conceptual models. The true model consists of 16 model layers (Fig. 1). The thickness of the model layer 1 varies from 10 m in the east to 50 m in the west. The thickness of the rest layers is 10 m. The model grid consists of 101 columns and 100 rows with a uniform cell size of 100 m. The model covers an area of 10,100 m × 10,000 m. MODFLOW-2000 (Harbaugh et al., 2000) was used to simulate the steady state groundwater head distribution. Groundwater heads computed at locations of observation wells (Fig. 2a) were used as observation values to compare model results of alternative conceptual models. All observation wells are single-layer well in the true model. There are 5 clusters of observation wells; each cluster consists of 5 observation wells. Two shallow wells are located in the layers 4 and 5 (just above the first aquitard) representing hydraulic heads in the shallow aquifer. Two middle wells are located in the layers 10 and 11 (just above the second aquitard) representing hydraulic heads in the middle aquifer. One deep well is located in the layer 16 (just above the bottom of the aquifer) representing hydraulic head in the deep aquifer. Computed hydraulic heads with the true model (16 layer

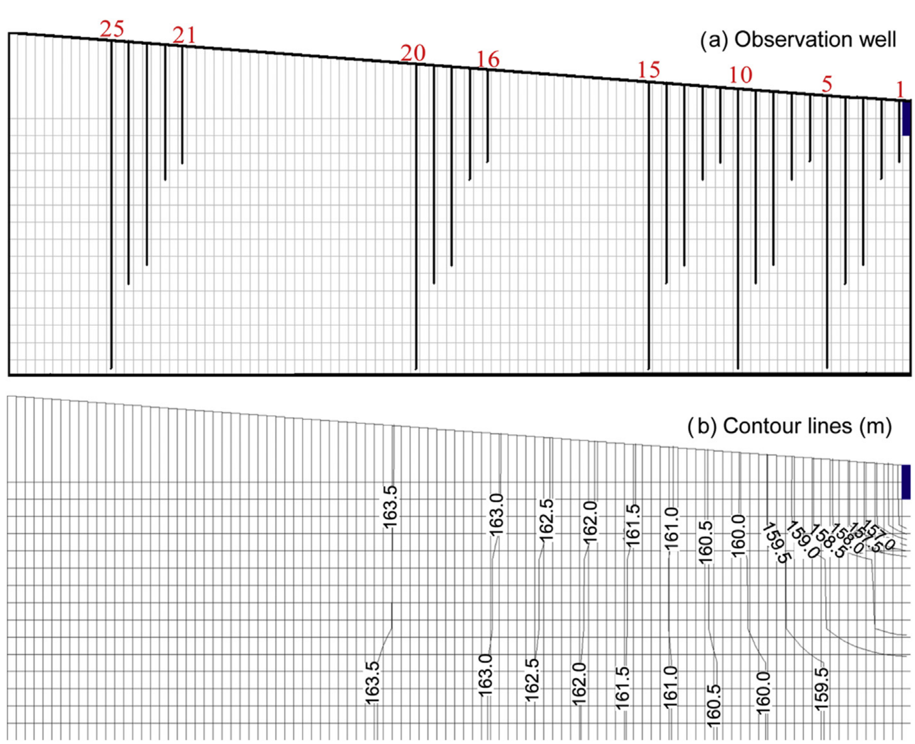

Figure 2. (a) Locations of 5 clusters of observation wells at various depths of the aquifer, observation wells are numbered in sequence from east to west; (b) Contour lines of computed hydraulic heads in the west-east profile with the true model.

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model) were read from these observation wells and considered as actual measurements. For all 3 alternative models, the same observations were used for parameter optimization and sensitivity analysis. Fig. 2b shows the contour lines of computed hydraulic heads in the west-east profile with the true model. Three-dimensional flow pattern is obvious near the river.

The alternative conceptual model-1 simplifies the alluvial fan-plain formations into a single unconfined aquifer which was simulated with a one-layer model (Fig. 3). Three hydraulic conductivity zones were delineated based on the true model. Initial values of hydraulic conductivities in 3 zones were calculated as the arithmetic mean of the hydraulic conductivities from the true model. The alternative conceptual model-2 combines the formations into 3 aquifer layers (Fig. 3). The first aquitard is included in the second aquifer layer and the second aquitard is included in the third aquifer layer. In this case, four distinct hydraulic conductivity zones are delineated. Harmonic mean was used to compute representative hydraulic conductivity values of the parameter zones. A 3-layer model was developed accordingly. The alternative conceptual model-3 represents the aquifer system with 3 aquifers separated by 2 aquitards (Fig. 3). Two aquitards are modelled explicitly. In this case, six distinct hydraulic conductivity zones are delineated. A 5-layer model was developed accordingly. All models were evaluated under the steady natural flow conditions. Abstractions were not considered.

3. Optimization and sensitivity analysis of alternative models

For three alternative models, hydraulic conductivities were optimised in order for model computed groundwater heads to match 25 observations generated by the true model. Sensitivities of parameters and observations were also analysed to identify most important parameters and observations for 3 alternative models. MODFLOW-2000 (Hill et al., 2000) and UCODE_2005 (Poeter et al., 2005) were used for parameter optimization and sensitivity analysis.

3.1. Parameter optimization and sensitivity analysis of the alternative model-1

The optimized values of hydraulic conductivity for 3 zones are: HK_1 = 100.80 m/d, HK_2 = 96.33 m/d, and HK_3 = 17.74 m/d. The scatter plot between the model computed head and the true head is show in Fig. 4. The R-square value is 0.94 indicating a good model fit. However, it is clear that the model-computed heads near the river is higher than the true heads.

The computed composite scaled sensitivities (Hill and Tiedeman, 2007) of 3 hydraulic conductivities are shown in Fig. 5a. It is clear that low hydraulic conductivity value in the parameter zone near the river is most sensitive to the model results.

The Cook's D influence statistics (Hill and Tiedeman, 2007) measures the importance of each observation values for parameter optimization. A larger value indicates that the observation is very influential. Fig. 5b shows the Cook's D statistics for the alternative model-1. It identifies observation well #20 is most influential to the model calibration. The observation well #20 is located in the transition zone from the alluvial fan to the alluvial plain.

3.2. Parameter optimization and sensitivity analysis of the alternative model-2

The optimized parameter values for horizontal and vertical hydraulic conductivities are listed in Table 1. The scatter plot shows

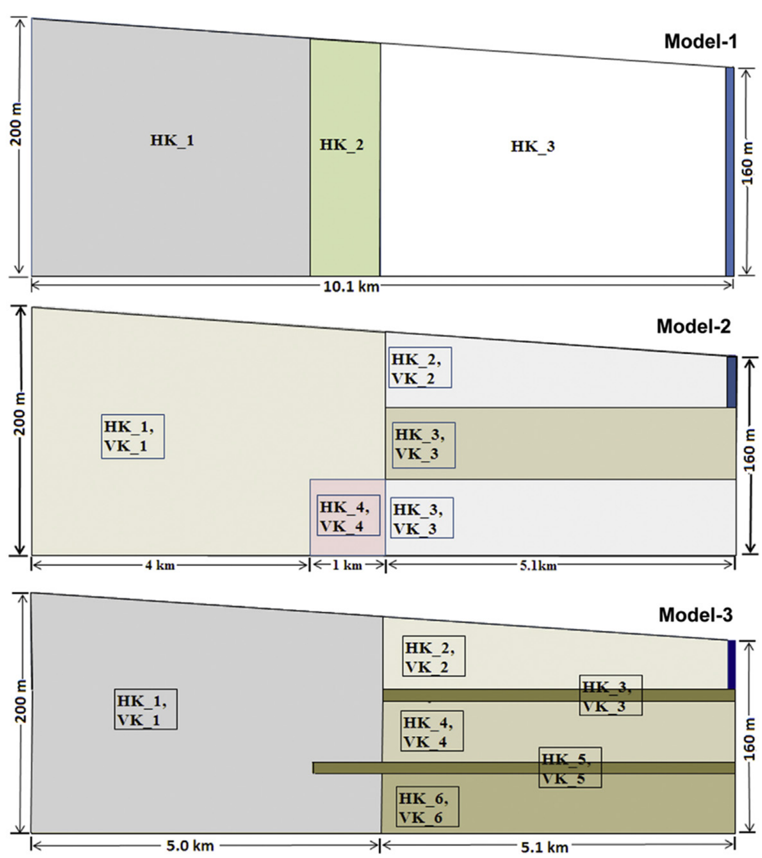

Figure 3. Cross-sections of the alternative conceptual models and hydraulic conductivity zones.

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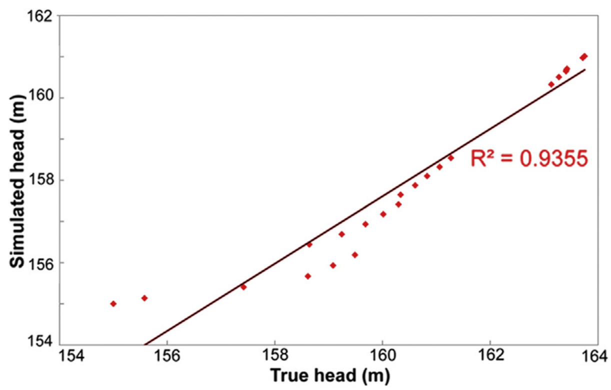

Figure 4. Scatter plot between the model-computed head and true head for the alternative model-1.

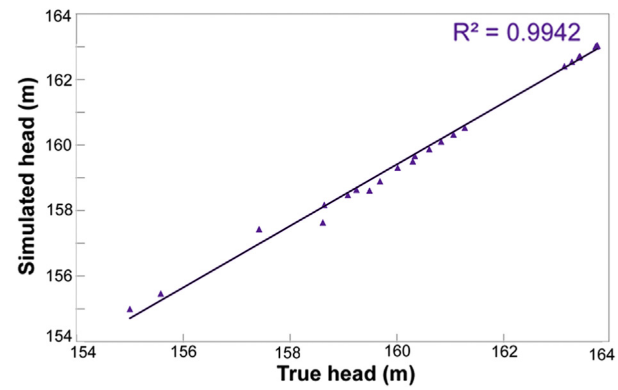

Figure 6. Scatter plot between the model-computed head and true head for the alternative model-2.

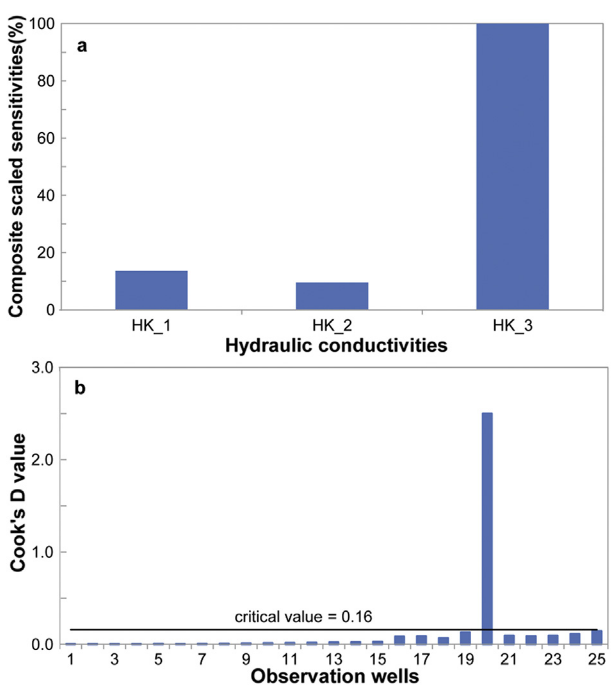

Figure 5. (a) Sensitivities of hydraulic conductivities in 3 parameter zones, and (b) Cook's D statistics of the alternative model-1.

that the model is able to reproduce all observations with high accuracy with the R-square value of 0.99 (Fig. 6). The most sensitive parameters are horizontal hydraulic conductivities in the alluvial plain (Fig. 7a). The most influential observations are from observation wells #2, 3, 16, and 21 (Fig. 7b). It is interesting to notice that observation wells 2 and 3 are located in the second model layer near the river; observation wells 16 and 21 are located in the top model layer; no observation wells in the third model layer are found influential.

Table 1
Hydraulic conductivity values estimated by UCODE_2005 for the alternative model-2.

Hydraulic conductivity	HK_1	HK_2	HK_3	HK_4	VK_1	VK_2	VK_3	VK_4
Initial values (m/d)	100.0	20.0	16.83	83.5	10.0	2.0	0.48	0.57
Optimized values (m/d)	99.84	19.83	16.39	84.6	9.97	2.01	0.48	0.56

3.3. Parameter optimization and sensitivity analysis of the alternative model-3

The optimized parameter values for horizontal and vertical hydraulic conductivities are listed in Table 2. The scatter plot shows that the model produces almost the same observations in all wells (Fig. 8). The most sensitive parameters are horizontal hydraulic conductivities in 3 aquifer layers in the alluvial plain (Fig. 9a). The vertical hydraulic conductivity of the first aquitard is more sensitive comparing to other layers. The most influential observations are from observation wells #2, 3, 4, and 18 (Fig. 9b). Observation wells 2, 3 and 4 are located in the first aquitard, the second aquifer, and the second aquitard near the river, respectively; observation well 18 is located in the second aquifer in the transition zone; no observation wells in the third aquifer are found influential.

4. Multi-model analysis

Information criteria (Poeter and Hill, 2007) are used for model discrimination. Akaike information criteria are defined as:

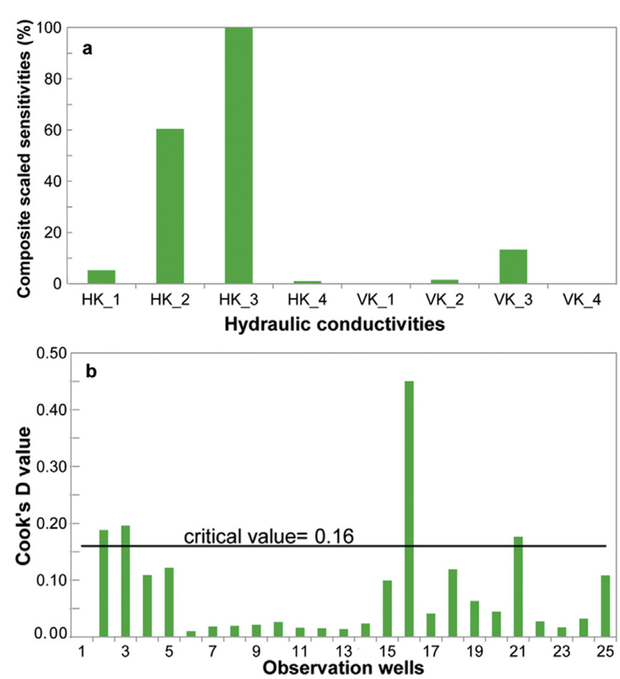

Figure 7. (a) Sensitivities of hydraulic conductivities in 4 parameter zones, and (b) Cook's D statistics of the alternative model-2.

Table 2
Hydraulic conductivity values estimated by UCODE_2005 for the alternative model-3.

Hydraulic conductivity	HK_1	HK_2	HK_3	HK_4	HK_5	HK_6	VK_1	VK_2	VK_3	VK_4	VK_5	VK_6
Initial values (m/d)	100.0	20.0	1.0	20.0	1.0	20.0	10.0	2.0	0.1	2.0	0.1	2.0
Optimized values (m/d)	99.9	18.16	0.86	20.75	0.87	20.79	9.95	3.17	0.09	2.37	0.12	1.77

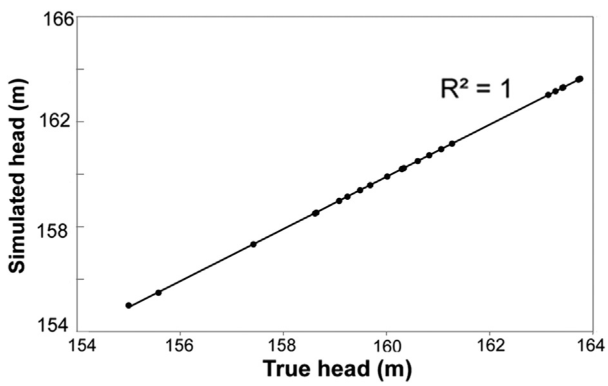

Figure 8. Scatter plot between the model-computed head and true head for the alternative model-3.

$$\text{AIC} = n\ln\left(\sigma^2\right) + 2k \tag{1}$$

$$\text{AICc} = n\ln\left(\sigma^2\right) + 2k + \frac{2k(k+1)}{n-k-1} \tag{2}$$

$$\sigma^2 = \frac{\text{SWSR}}{n} \tag{3}$$

$$\text{SWSR} = \sum_{i=1}^{n} \omega_i\left[y_i - y_i'(\underline{b})\right]^2 \tag{4}$$

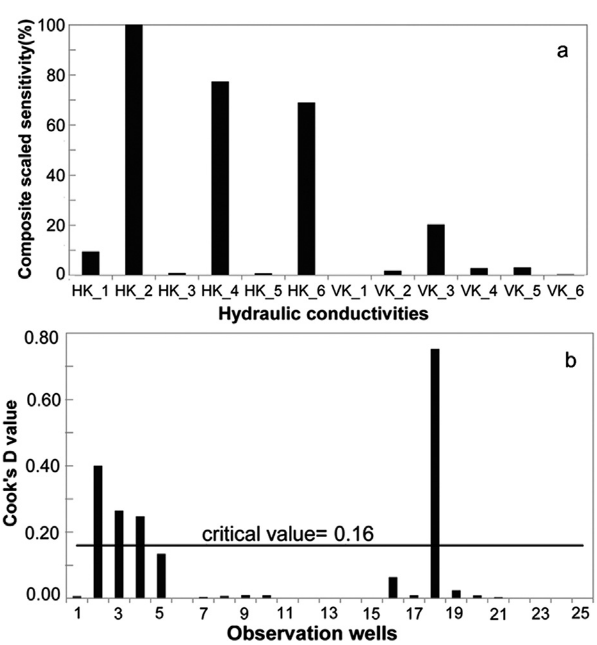

Figure 9. (a) Sensitivities of hydraulic conductivities in 6 parameter zones, and (b) Cook's D statistics of the alternative model-3.

where:

n: is the number of observations, same for all models
k: is the number of model parameters = NPE + 1
NPE: is the number of process model parameters
σ^2: is the residual variance
SWSR: is the sum of weighted squared residuals
ω_i: is the weight for the ith observation
y_i, y_i': are measured and model calculated groundwater heads, respectively.

The minimum AIC or AICc among alternative models indicates the best model. In order to compare all models, a posterior model probability (p_m) is defined as:

$$p_m = \frac{e^{-0.5\Delta_m}}{\sum_{j=1}^{M} e^{-0.5\Delta_j}} \tag{5}$$

where:

$$\Delta_m = \text{AIC}_m - \text{AIC}_{min} \tag{6}$$

where:

AIC_m: is the AIC value for model m
AIC_{min} is the minimum AIC values of all models

The larger is the probability, the better is the model. The posterior model probabilities are used as the model weighting coefficients to compute the model-averaging predictions.

Bayesian information criterion is defined as:

$$\text{BIC} = n\ln\left(\sigma^2\right) + k\ln(n) \tag{7}$$

Kashyap information criterion is defined as:

$$\text{KIC} = (n-(k-1))\ln\left(\sigma^2\right) - (k-1)\ln(2\pi) + \ln\left|X^T\omega X\right| \tag{8}$$

where X is the sensitivity matrix. The posterior model probability for Bayesian and Kashyap information criteria is also calculated with Eqs. (5) and (6).

MMA code (Poeter and Hill, 2007) was used to compute Akaike, Bayesian, Kashyap information criteria and their posterior model probabilities for 3 alternative models. The results are shown in Fig. 10. Alternative model-3 scores minimum values for all three criteria. The posterior probability for the model-3 reaches the maximum 1.0 and 0 for model-2 and model-1. All three criteria indicate that alternative model-3 is superior, model-2 and model-1 can be disregarded.

5. Comparison of alternative model simulations

Although all 3 alternative models can fit observations very well, Multi-model analysis found only alternative model-3 is superior while model-1 and model-2 were disregarded. Here, we compare if these models can compute groundwater balance, water table profile, and travel times with good accuracy.

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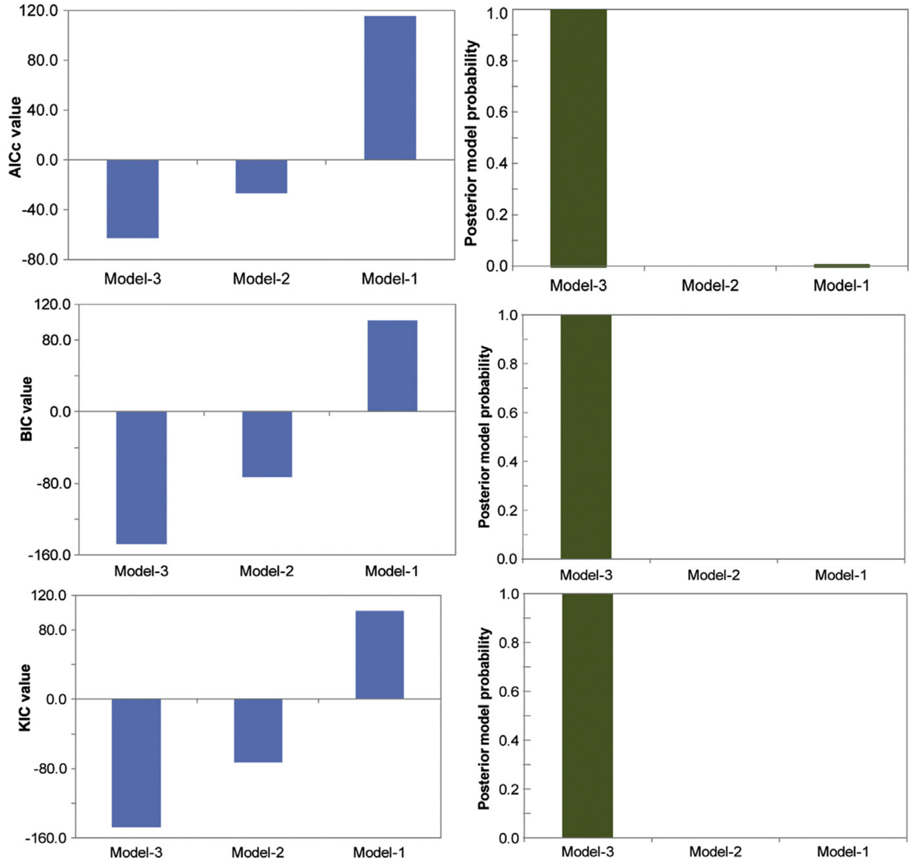

Figure 10. Akaike (AICc), Bayesian (BIC), Kashyap (KIC) information criteria and their posterior model probabilities for 3 alternative models.

The true model and 3 alternative models compute the same recharge (37,500 m^3/d) and discharge under the steady state condition. Since the recharge is the same for all models, all models are forced to compute the same discharge equal to the recharge under the steady state condition. However, the model doesn't include groundwater evapotranspiration. Since groundwater evapotranspiration depends on groundwater level depth, groundwater evapotranspiration will be most likely different in 3 alternative models; therefore, discharge to rivers will be also different.

The computed water table profiles are shown in Fig. 11. Alternative model-3 can reproduce the same water table profile as the true model, but model-1 and model-2 underestimate the water tables.

The particle tracking model MODPATH (Pollock, 1994) was used to compute a water particle placed on the water table from any distance to travel to the river. All models have the same porosity of 0.25. One hundred particles were placed at water table surface of each column cells. They were tracked forward to arrive at the river cell. In this way, travel times from the minimum to maximum are computed. The travel times are plotted as a function against the distance from the river in Fig. 12. Results show that alternative model-3 estimates approximately the same travel times as the true model, while model-1 and model-2 overestimate the travel times for shorter distances and underestimate the travel times for long distance.

6. Conclusions

This study uses the widely distributed alluvial fan-plain aquifer to create a synthetic true model, and conceptualizes the true model

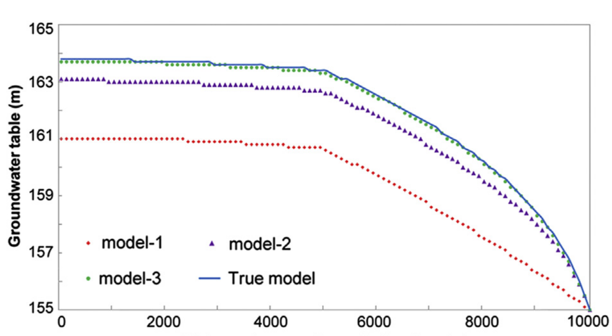

Figure 11. Simulated water table profiles with 3 alternative models in comparison with the true model.

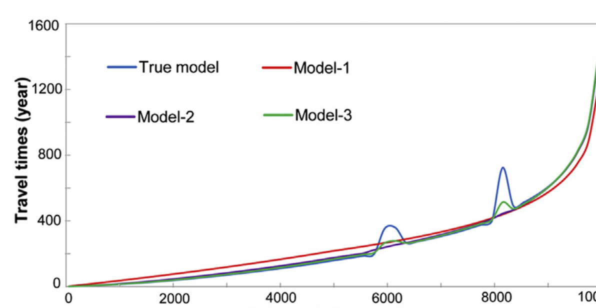

Figure 12. Computed travel times with 3 alternative models in comparison with the true model.

with 3 alternative conceptual models with the increasing complexity: a simple one-layer aquifer model, a 3-layer aquifer model, and a 5-layer model of alternating aquifers and aquitards. The true model was constructed to generate "observed" values of groundwater heads at selected 25 observation locations. The parameter zones of the conceptual models were delineated from the true model. The hydraulic conductivities of three alternative models were optimized with the parameter optimization method. Multi-model analysis based on statistical criteria was used to discriminate the alternative conceptual models. The calculated water budget, water table profile, and travel times of alternative models were compared with those of the true model.

Although all three alternative models can fit the observations very well with very high R-square values, multi-model analysis only found the 5-layer model is superior and other two models were disregarded. It implicates that the traditional model calibration using the observed heads to compare with the measured heads along is not adequate to identify the best conceptual model.

Composite scaled sensitivity from 3 alternative models all indicates that horizontal hydraulic conductivities in the alluvial plain are most sensitive to model simulations. The vertical hydraulic conductivity of the upper aquitard is more sensitive than the lower aquitard. Importance of the locations of observation wells depends on the conceptualization of the model. For the one-layer aquifer model, only one well was found influential which is located at the transition zone. For the 3-layer aquifer model, two wells in the second aquifer in the alluvial plain, and one well in the transition zone and one well in the alluvial fan in the top aquifer were found more influential. For the 5-layer aquifer model, three wells in the alluvial plain and one in the transition zone were found more influential. No observation wells in the third aquifer were found influential.

The comparison of the water budget, water table profile, and travel times calculated by 3 alternative conceptual models with the true model reveals that the model complexity is proportional to information required. To calculate the water balance only, a simple one-layer aquifer model would be sufficient. To display the spatial groundwater head distribution, a 3-layer aquifer model would be accurate enough for practical application. However, to capture travel time distribution, a 5-layer model with explicit representation of aquitards is necessary.

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