Novel approaches in sub-surface parameterisation to calibrate groundwater models

D K S Y Klaas¹,², M A Imteaz¹, I Sudiayem³, E M E Klaas³ and E C M Klaas³

¹Department of Civil & Construction Engineering, Swinburne University of Technology, Melbourne, VIC, Australia
²Department of Civil Engineering, Politeknik Negeri Kupang, Indonesia
³Department of Health, Science and Technology, Klinik Garuda, Malang, Indonesia
E-mail: dklaas@swin.edu.au; duaklaas@yahoo.com

Abstract. Advancement towards improved configuration of pilot point into a model in parameterisation step of groundwater modeling is required to accurately obtain a satisfactory model performance. Nevertheless, the recommendations provided by the majority of current studies on this geostatistical technique are considered too empirical than practical to be applied on real catchment conditions. In this study for the first time a practical approach of using geometric features of pilot point and catchment area is proposed to efficiently configure pilot point distribution in the calibration step of a groundwater model. Three user-friendly ratios, i.e. distance-area (d/A), distance-x grid length (d/Xgrid), and distance-y grid length (d/Ygrid) are introduced in Grid-based (GB) distribution technique. Eight models of eight different pilot point distances (250 m, 500 m, 750 m, 1000 m, 1250 m, 1500 m, 1750 m and 2000 m) were developed using GB technique were constructed on an eogenic karst catchment in Rote Island, Indonesia and their performances were evaluated. Modelers can use the three practical ratios when calibrating groundwater models given the same sub-surface characteristics. This study also provides some insights into the trade-off between maximising and restricting the number of pilot points and offers a relative basis for selecting pilot point properties and distribution method in the development of a physically-based groundwater model.

1. Introduction
Using an accurate spatial conditioning in parameterisation step implies a rigorous effort both numerically and computationally. Nowadays, geostatistical techniques have become important tools in performing a robust model simulation effectively. Among geostatistical techniques, Pilot Points Method (PPM), which has been widely used in different hydrogeological conditions in many parts of the world, is an alternative to the classical zonation method which is conditional upon the number of available field observations and prior knowledge of geological information, such as geological map and stratigraphy [1]. Compared to the zonation method, PPM offers critical advantages when dealing with heterogeneity. Therefore, a number of works have been carried out to enrich the method by introducing stochastic regularization to increase numerical stability when dealing with numerous parameters [2], plausibility term for refining the heterogeneity [3] and singular value decomposition (SVD) to assist a proper selection of pilot points number, hence their locations [4].

In spite of the development on pilot point method, configuring pilot points into a model in parameterisation step is still somehow challenging. Certes and de Marsily have raised a concern on...
difficulties to properly and practically organise pilot points into a model during parameterisation step to achieve a good fit [5]. They underlined the subjectivity introduced when the number and location of pilot points are self-judged and organised by modellers, and thus brought up a fundamental necessity to develop heuristic recommendations. Some authors then proposed several recommendations to appropriately characterise the pilot point distribution by adjusting the distance between points using correlation length as its relative property [3, 6]. Nevertheless, this theoretical property is considered less practical for real case examples. Motivated by this, in this study we propose a practical approach of using pilot points’ properties (i.e. number, distance and distribution method) during calibration step of a groundwater model. For the first time, we introduce the relative distance area ratio \((d/A)\), which refers to distance between points and catchment size.

Thus using a real karst catchment in Rote Island, Indonesia as a study case, the main objectives are to carry out a modelling-oriented analysis of groundwater flow to:

- investigate the impact of pilot points’ properties (number, distance and distribution method) on calibration of groundwater models;
- provide recommendation on selection of pilot points’ properties \((d/A, d/x_{grid}, d/y_{grid}, \text{and zone ratio})\) to obtain a better calibration result of a groundwater model assessed by statistical measures.

2. Materials and methodology

2.1. Study area

The experimental area is the catchment of Oemau spring located in Rote island, Indonesia, geographically located between latitudes 10°46’42.17”S ~ 10°43’36.91”S and longitudes 123°3’14.84”E ~ 123°9’17.64”E. The catchment is a topographically bounded surface drainage basin area of 20.11 km², located around 3 km from Ba’a, the capital of the Rote Island (figure 1).

![Figure 1. Location of study area and topographical situation of Oemau spring catchment.](image)

The study area has a monsoonal climate characterised by two distinct seasons: dry (May-November) and wet (December-April). Annual rainfall is between 1000 and 2300 mm and humidity is 75-92%. In general, the land surface of the catchment is geologically covered by carbonate formations featured as karst landscape. Hydraulic head and spring discharge data from seven observation wells located within the catchment boundary provide the basis for interpreting the flow system that dictate the subsurface flux. Using modified Boussinesq approach of recession curve, a diffuse flow characterised by low hydraulic conductivity, high storage capacity and laminar flow [7].

2.2. Groundwater model

Eight models were constructed using two pilot point distribution methods (GB). The models are
principally differentiated by the distance between points and number of points in each hydraulic gradient zone. A complete explanation is provided in Section 2.4.

The simulations of groundwater flow under both steady-state and transient conditions were carried out using the modular three-dimensional numerical model MODFLOW [8] operated and visualized in the groundwater modeling system, GMS [9] user interface. The conceptual model was constructed on the basis of one horizontal layer which assumes the continuum representation of unconfined carbonate aquifer in the study area. This assumption is considered agreeable to the dominant eogenetic carbonate aquifer in the geologic stratum. The one-layer finite-difference grid is comprised of 106 rows and 210 columns resulting in 8061 active cells (figure 2(a)). The model was discretised in Layer Property Flow, LPF [10] package using a homogenous horizontal model of 50 m by 50 m grid cells. The catchment boundary is set as no-flow boundary assuming no flux flowing through the boundary (figure 2(a)). At downstream, a small stream after the spring was set as specified head boundary using Time-Variant Specified-Head, CHD [11].

![Figure 2](image)

**Figure 2.** Conceptual model of the model and land use as input for recharge coverage.

The model simulations used prior information of hydraulic conductivity and specific yield values calculated using Boulton method [12] on pumping test data at 3 locations within the catchment. A constant value of 0.3 was set for the porosity to represent the carbonate formation (Johnson 1967). Drain package, DRN (Harbaugh et al. 2000) was used to model the surface drainage network of the recharge area (see figure 2(b) for the drainage network). The streams’ surface drain conductance was set between 2,700 and 8,125 m/d correlated with the drain dimension and K values which were derived from local pumping test analysis. To simulate recharge to the aquifer the recharge package, RCH (Harbaugh et al. 2000) was used. The recharge mainly characterised by atmospheric stresses (i.e. precipitation and potential evapotranspiration) and surface (i.e. land use type) was quantified using the water balance method [13]. In this process, SCS-CN [14] and Penman-Monteith [15] methods were applied to calculate surface runoff and evapotranspiration respectively. In the conceptual model, the recharge values are assigned into each land use zonation, illustrated in figure 2(b).

### 2.3. Model calibration

The steady-state calibration was carried to assist a smooth convergence of the model for the transient simulation. Steady-state calibration aimed to determine the distribution of horizontal hydraulic conductivity ($K_h$) across the model domain during the highest recharge. The $K_h$ values are set to range between 0.1 and 250 m/d to represent karst limestone [16, 17]. Vertical anisotropy was set to 0.2. In steady-state simulation, the maximal rainfall rate of 86.5 mm/day on 19 April 2011 was chosen. The initial $K_h$ values then feed the transient simulation which aims to calibrate the specific yield ($S_y$) and $K_v$ values. Transient simulation covers the period from January 2011 to August 2011 divided into 8 monthly stress periods with each comprising of 10 time steps. In each step, an iterative matrix solver, Preconditioned Conjugate Gradient 2, PCG2 was used to increase the model’s capability to converge. In both steady–state and transient simulations PEST was used. In this automated optimisation code, the pilot points technique [18] was applied for all models by distributing pilot points according to the two distribution methods explained in Section 2.4. In the simulation, Singular Value Decomposition,
SVD (Doherty 2004) and Tikhonov regularisation (Doherty 2003) were used to stabilise the mathematical approximation. Computationally, all models were run on a desktop computer Intel® Core™ 2 Quad CPU Q6600, clock speed of 2x2.40 GHz using 4 GB RAM.

A calibration criterion for both the steady-state and transient simulations was employed to match simulated heads with observed heads. Daily data collected from 7 observation wells in the catchment for the duration of January, 2011 ~ April, 2012 were used as observed heads. The model calibration was accomplished by analysing models’ performance specified by statistical goodness-of-fit measures: Mean Absolute Error ($\text{MAE}_h$), Root Mean Squared Error of head ($\text{RMSE}_h$), and Nash-Sutcliffe coefficient ($\text{NSE}_h$) as objective functions.

2.4. Distribution of pilot points

GB distribution method is commonly used to deploy pilot points into model domain and is widely used in groundwater modelling [19-21]. The model domain was firstly divided into rectangular uniformity grids. Using orthogonality principle, the pilot points were uniformly distributed with respect to the predefined distinct homogenous distance between points [22]. The grid was rotated perpendicularly to assumed groundwater flow direction (BYU 2014), which is 178.6°. Figure 3 illustrates an example of pilot point assignment using the GB method for our model GB4.

![Figure 3](image-url)

**Figure 3.** GB spatial distribution of pilot points of model GB4, also showing the incorporation of preferred values into the model domain. $X_{grid}$ refers to the total length of the horizontal grid and $Y_{grid}$ is the total length of the vertical grid.

| Model | $d$ (m) | Number of pilot points |
|-------|---------|------------------------|
| GB1   | 2000    | 9                      |
| GB2   | 1750    | 12                     |
| GB3   | 1500    | 13                     |
| GB4   | 1250    | 15                     |
| GB5   | 1000    | 26                     |
| GB6   | 750     | 41                     |
| GB7   | 500     | 88                     |
| GB8   | 250     | 322                    |
In this distribution method, eight models of eight different predefined distances were developed (see Table 1).

3. Results and discussions

3.1. Model calibration
The complete results of the steady state simulations for the eight models are summarised in Table 1. Generally, the error statistics of all models using the two pilot points distribution methods are small in regards to RMSEh values (vary between 0.25 m and 0.81 m), confirming that all models are capable of reproducing hydraulic heads to a satisfactory level. The direction of groundwater flow also confirms the pre-set flow direction, suggesting a well calibrated model (Domenico and Schwartz 1998).

Table 2 summarise the results of the transient simulations for the eight models using GB. The model performances in transient simulation are overall considered satisfactory in regards to RMSEh values, which vary from 0.29 m to 0.44 m for all the fifteen models. A considerably high NSEh value (0.81-0.92) is categorised as very good according to the model criteria (Moriasi et al. 2007), which indicate a good simulation achievement.

| Model | NSEh  | RMSEh (m) | d/A (km–1) | d/Xgrid (-) | d/Ygrid (-) |
|-------|-------|-----------|------------|-------------|-------------|
| GB1   | 0.84  | 0.42      | 0.10       | 0.20        | 0.40        |
| GB2   | 0.86  | 0.38      | 0.09       | 0.18        | 0.35        |
| GB3   | 0.86  | 0.35      | 0.07       | 0.15        | 0.30        |
| GB4   | 0.87  | 0.32      | 0.06       | 0.13        | 0.25        |
| GB5   | 0.92  | 0.29      | 0.05       | 0.10        | 0.20        |
| GB6   | 0.92  | 0.32      | 0.04       | 0.08        | 0.15        |
| GB7   | 0.89  | 0.36      | 0.02       | 0.05        | 0.10        |
| GB8   | 0.87  | 0.35      | 0.01       | 0.03        | 0.05        |

3.2. Effect of pilot points properties on model performance
Figure 4 shows the model performance in regards to RMSEh for the eight models as a result of increased distance between pilot points. For the first time, d/A ratio was introduced as a practical pilot points property to efficiently classify a grid-guided model. When d/A is reduced from 0.10 to 0.05 km–1 the model performance increases by 43.18%. The ratio reduction implies that the distances between points become shortened (from 2000 to 1000 m) causing increased pilot point number. In opposition, the model performance drops by 18.27% when d/A is reduced from 0.05 to 0.01 km–1, giving a distance shortening from 1000 to 250 m. The figure shows that the maximum model performance is achieved at the value of d/A = 0.050. Table 3 shows the comparison of model performances associated with pilot point properties. It shows that the model with the highest performance is GB5 having the values of d/A, d/Xgrid and d/Ygrid as 0.05, 0.10 and 0.20 respectively. This study demonstrates that although pilot points are capable of representing subsurface heterogeneity hence helps to improve model performance, however their capability is influenced by the number of points and the distance between points relative to catchment size. Therefore, an optimal model performance can be reached by appropriate input arrangement of pilot points, which in this study is represented by d/A ratio.
The fitting graph demonstrates that adding up the number of pilot points into the models corresponds to the increase in model performance. However, from the figure it is clear that beyond a certain limit adding extra number of pilot points is not recommended, as it results in a drop of model performance. In this study, the reduced model performances after reaching the lowest error values at the “tipping point” might correspond to ‘model overfitting’, a condition when inaccurate model conditioning including inappropriately assigning location and density of pilot points results is used to force the model output to match the observed values [3]. In our case, the adverse effect of adding more pilot points, which narrows distance between pilot points, beyond a suggested number on model performance may introduce not only redundant measurements [23] but also a possible effect of over-smoothing between points. Therefore, although error values decrease by narrowing distance between pilot points due to increased pilot points number, after the tipping point the pilot points number is considered excessive and results in less-optimal optimisation due to over-parameterisation.

4. Conclusions
Choosing a reasonable pilot point number and appropriate distribution method using a practical guideline is important in the parameterisation step of a groundwater modelling. In this study using the GB method, for the first time distance-area ratio ($d/A$) was introduced. This ratio was found to be a practical tool to represent pilot point property in order to assess the model performance. This study demonstrated that when the distance-area ratio is decreased from 0.10 to 0.05 km$^{-1}$, implying that the number of pilot points increased due to distance shortening from 2000 m to 1000 m, the model performance increased by 43.18%. On the contrary, when the distance between pilot points was reduced from 1000 m to 250 m, the model performance decreased by 18.27%. The study shows that the maximum model performance is achieved at the value of $d/A = 0.050$.

This study is able to show an alternative practical approach in properly selecting pilot point properties (i.e. distribution method, number and distance). Based on the model simulations developed in this study, the following recommendations are proposed for using GB distribution method:

- The recommended distance-area ratio ($d/A$) is 0.05;
- The recommended distance-x grid length ratio ($d/X_{grid}$) is 0.10; and
- The recommended distance-y grid length ratio ($d/Y_{grid}$) is 0.20.

The outcomes of this study are considered applicable for any modelling analysis with similar soil characteristics, i.e. carbonate dominated aquifer, dominant diffuse flow system and hydro-climate regime, i.e. monsoonal climate. However, although the initial results presented here are promising, it is noteworthy to test the robustness of the result by conducting complementary modeling using the
same methodology for other case studies diversified by different and broader model properties, such as catchment size, geological features and climatic setting is required.

References

[1] Klaas D K S Y, Imteaz M A and Arulrajah A 2016 Evaluating the impact of grid cell properties in spatial discretization of groundwater model for a tropical karst catchment in Rote Island, Indonesia Hydrol. Res. doi: 10.2166/nh.2016.250
[2] Doherty J 2004 PEST: Model-Independent Parameter Estimation User Manual 5th ed (Brisbane, Australia: Watermark Numerical Computing)
[3] Alcolea A, Carrera J and Medina A 2006 Pilot points method incorporating prior information for solving the groundwater inverse problem Adv. Water Resour. 29 1678-89
[4] Christensen S and Doherty J 2008 Predictive error dependencies when using pilot points and singular value decomposition in groundwater model calibration Adv. Water Resour. 31 674-700
[5] Ceretes C and de Marsily G 1991 Application of the pilot point method to the identification of aquifer transmissivities Adv. Water Resour. 14 284-300
[6] Gómez-Hernández J J, Sahuquillo A and Capilla J 1997 Stochastic simulation of transmissivity fields conditional to both transmissivity and piezometric data—I. Theory J. Hydrol. 203 162-74
[7] Shuster E T and White W B 1971 Seasonal fluctuations in the chemistry of lime-stone springs: A possible means for characterizing carbonate aquifers J. Hydrol. 14 93-128
[8] McDonald M and Harbaugh A 1988 A Modular Three-Dimensional Finite-Difference Groundwater Flow Model (USGS) book 6, Chap A1
[9] BYU 2014 Groundwater Modeling System (GMS) version 9.2.9. (Provo, USA: Environmental Modeling Research Laboratory, Brigham Young University)
[10] Harbaugh A W 2005 MODFLOW-2005, the U.S. Geological Survey Modular Ground-Water Model, the Ground-Water Flow Process (USGS Techniques and Methods 6-A16, USGS)
[11] Harbaugh A W, Hill M C and McDonald M G 2000 MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model: User Guide to Modularization Concepts and the Ground-Water Flow Process (USGS Open-File Rep 00-92, USGS)
[12] Boulton N S 1963 Analysis of data from non-equilibrium pumping tests allowing for delayed yield from storage Proc. Inst. Civil Eng. (London, Great Britain) 26 469-82
[13] Bras R L 1990 Hydrology: An Introduction to Hydrologic Science (Massachusetts, USA: Addison-Wesley, Reading)
[14] Viessman W and Lewis G L 2003 Introduction to Hydrology 5th ed (Upper Saddle River, NJ, USA: Pearson Education)
[15] Allen R G, Pereira L S, Raes D and Smith M 1998 Crop evapotranspiration—Guidelines for computing crop water requirements FAO Irrigation and Drainage Paper 56
[16] Davis S N 1969 Porosity and Permeability of Natural Materials in Flow Through Porous Media (New York, USA: Academic Press)
[17] Freeze R A and Cherry J A 1979 Groundwater (Englewood Cliffs, New Jersey, USA: Prentice-Hall)
[18] de Marsily G 1984 Spatial Variability of Properties in Porous Media: A Stochastic Approach ed J Bear and M Y Corapcioglu (Boston, USA: NATO ASI Series E) 719-69
[19] Klaas D K S Y, Imteaz M A and Arulrajah A 2016 Development of a groundwater model for a tropical eogenetic karst aquifer in Rote Island, Indonesia Proc. Aust. Hydrol. Water Res. Symp. (Queenstown New Zealand) 228-35
[20] Klaas D K S Y, Imteaz M A and Arulrajah A 2017 Development of groundwater vulnerability zones in a data-scarce eogenetic karst area using Head-Guided Zonation and particle-tracking simulation methods Water Res. 122 17-26
[21] Klaas D K S Y, Imteaz M A and Arulrajah A 2017 Development of groundwater vulnerability
zones in a data-scarce catchment *Proc. 10th World Congress Water Res. Env.* (Athens, Greece)

[22] Doherty J E, Fienen M N and Hunt R J 2010 *Approaches to highly parameterized inversion: Pilot-point theory guidelines, and research directions* USGS Scientific Investigations Report 2010-5168 (USGS)

[23] Klaas Dua K S Y and Imteaz M A 2017 Investigating the impact of the properties of pilot points on calibration of groundwater models: case study of a karst catchment in Rote Island, Indonesia *Hydrogeol. J.* 1-17 doi: DOI 10.1007/s10040-017-1590-4