IOP Conf. Series: Earth and Environmental Science **92** (2017) 012026 doi:10.1088/1755-1315/92/1/012026

On the development of a new methodology in sub-surface parameterisation on the calibration of groundwater models

D K S Y Klaas[1,2,3], M A Imteaz[1], I Sudiayem[3], E M E Klaas[3] and E C M Klaas[3]

[1]Department of Civil & Construction Engineering, Swinburne University of Technology, Melbourne, VIC, Australia.
[2] Department of Civil Engineering, Politeknik Negeri Kupang, Indonesia.
[3] Department of Health, Science and Technology, Klinik Garuda, Malang, Indonesia

E-mail: duaklaas@yahoo.com, dklaas@swin.edu.au

Abstract. In groundwater modelling, robust parameterisation of sub-surface parameters is crucial towards obtaining an agreeable model performance. Pilot point is an alternative in parameterisation step to correctly configure the distribution of parameters into a model. However, the methodology given by the current studies are considered less practical to be applied on real catchment conditions. In this study, a practical approach of using geometric features of pilot point and distribution of hydraulic gradient over the catchment area is proposed to efficiently configure pilot point distribution in the calibration step of a groundwater model. A development of new pilot point distribution, Head Zonation-based (HZB) technique, which is based on the hydraulic gradient distribution of groundwater flow, is presented. Seven models of seven zone ratios (1, 5, 10, 15, 20, 25 and 30) using HZB technique were constructed on an eogenetic karst catchment in Rote Island, Indonesia and their performances were assessed. This study also concludes some insights into the trade-off between restricting and maximising the number of pilot points and offers a new methodology for selecting pilot point properties and distribution method in the development of a physically-based groundwater model.

1. Introduction

In groundwater modelling, accurate estimation of groundwater discharge over a catchment requires a proper approach in the parameterisation step [1,2]. In the parameterisation step, parameters are conditioned until the simulated values match the observed measurements. Proper distribution of spatial variations of parameters that could represent intrinsic heterogeneity of the geologic formation, in the absence of adequate pre-measured parameter values, is a challenge for modellers [1,3]. To cope with data limitation, modellers often use numerically aided geostatistical techniques with the aid of high-speed processors. An alternative to the classical zonation method, pilot-point method (PPM) [4] is a geostatistical technique that has been widely used in different hydrogeological conditions in many parts of the world [5,6,7]. However, organising pilot points into a model to achieve a good fit is still considered subjective and less user-friendly for real case examples [8]. Thus, we introduce a practical head zonation-based (HZB) method to assign pilot points in each head guided zone of the model domain by incorporating the practical zone ratio. Therefore, the main objectives of this paper were to present a modelling-oriented analysis of groundwater flow to:

- investigate the impact of pilot-point properties (number, distance and distribution method) on the calibration of groundwater models using HZB method; and

IOP Conf. Series: Earth and Environmental Science **92** (2017) 012026 doi:10.1088/1755-1315/92/1/012026

- provide recommendations on the selection of pilot-point properties (zone ratio) to obtain a better calibration result of a groundwater model assessed by statistical measures.

2. Materials and methodology

2.1. Study area

This study exercised 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. Having a topographically bounded surface-drainage basin area of 20.11 km^2 (figure 1a), the spring is located around 3 km from Ba'a, the capital of the Rote Island.

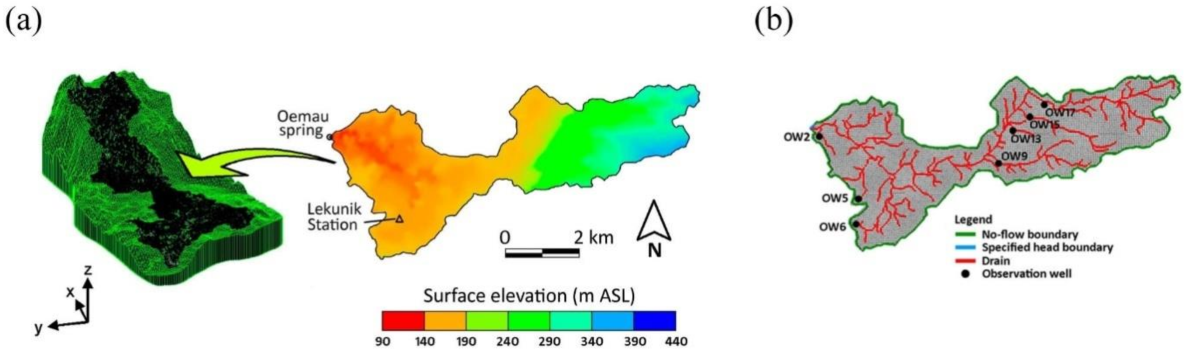

Figure 1. (a) Topography of Oemau spring catchment; (b) conceptual model of the modelled area.

Amoonsonal climate characterised by two distinct seasons: dry (May-November) and wet (December-April) dominates the study area [9]. Humidity is 75-92% and annual rainfall is between 1000 and 2300 mm. Karst landscape characterised by carbonate formations dominates the area. Typified by the absence of preferential flow paths and conduits and geomorphologicaly characterised by low karstification degree, the area is grouped as an eogenetic karst [10].

2.2. Groundwater model

Seven models were developed using HZB method and used to simulate the groundwater flow. The pilot-point distribution is based on the hydraulic-gradient distribution of groundwater flow. Several studies have demonstrated that the groundwater elevation often follows the spatial distribution of hydraulic conductivity [11,12]. It was found that the gradient of groundwater contours relatively corresponds to the hydraulic conductivity of the region. In areas with low conductivity, water travels slower implying a high hydraulic gradient of groundwater. Similarly, the hydraulic gradient would be lower when travelling through a high conductivity area. Therefore, the hydraulic gradient can be used as an initial graphical indication of hydraulic conductivity distribution. In this method, the catchment was divided into four zones following a 40-m head difference between hydraulic head contours [13,14].

The interval is considered sufficient to allow ample space for placing numerous pilot points and to spatially incorporate the subsurface heterogeneity over the model domain. The pilot points were then evenly distributed into the four zones by manual placement. Each zone contained the same number of pilot points. In this study, seven models were developed employing seven zone ratios (i.e., 1, 5, 10, 15, 20, 25 and 30; figure 2) to investigate the model performance. The simulations of groundwater flow under both steady-state and transient conditions were carried out using MODFLOW code [15], operated and visualized within the groundwater modelling system, GMS [16]. The model was discretised in the Layer Property Flow package, LPF [17], using a homogenous horizontal model of 50 m by 50 m grid cells. The catchment boundary was set as a no-flow boundary assuming no flux flowing through the boundary (figure1b). Downstream, a small stream after the spring was set as a specified head boundary using time-variant specified head, CHD [18].A constant value of 0.3 was set for the porosity to represent the carbonate formation [19]. The drain package, DRN [18] was used to model the surface drainage network of the recharge area. The streams' surface drain conductance was set between 2,700 and 8,125 m/d. To simulate recharge to the aquifer, the recharge package RCH [18] was used. The SCS-CN [20] and Penman-Monteith [21] methods were applied to calculate surface runoff and evapotranspiration respectively.

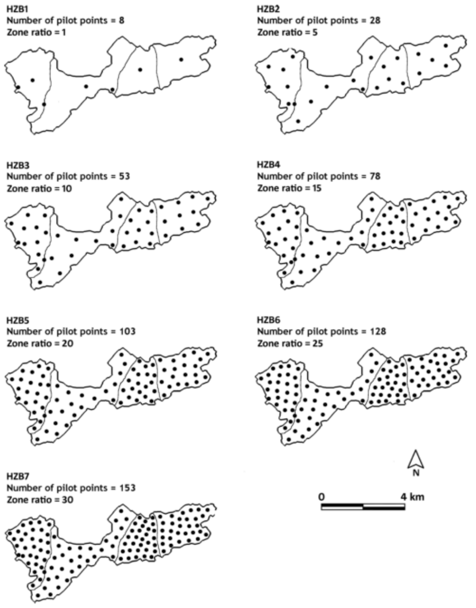

Figure 2. Spatial distributions of pilot points in seven models constructed using HZB distribution.

2.3. Model calibration

The K_h values are set to range between 0.1 and 250 m/d to represent karst limestone [22,23]. The initial K_h values then feed the transient simulation which aims to calibrate the specific yield (Sy) and K_h values. Transient simulation covers the period from January 2011 to August 2011, divided into 8 monthly stress periods, with each comprising of 10time steps. In both steady–state and transient simulations, PEST [24] was used. 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 the models' performance specified by statistical goodness-of–fit measures – the mean absolute error (MAE_h), root mean squared error of head ($RMSE_h$) and Nash-Sutcliffe coefficient (NSE_h)– as objective functions.

3. Results and discussion

3.1. Model calibration

Generally, the error statistics of all models using the two pilot points distribution methods are small in regards to $RMSE_h$ values (between 0.35 m and 0.71 m), confirming that all models are capable of reproducing hydraulic heads to a satisfactory level.The model performances in transient simulation are overall considered satisfactory in regards to $RMSE_h$ values, which vary from 0.36 m to 0.44 m.

3.2. Effect of pilot-point properties on model performance

Figure 4a show the model performances of the seven models developed using the HZB method. The model performances, represented by $RMSE_h$, increase by 13.49% when the zone ratio increases from 1 to 15, resulting in the increase of pilot-point number from 8 to 78. Conversely, the model performance drops by 20.04% for subsequent increase of pilot-point number from 78 to 153 as a result of the zone ratio increase from 15 to 30. Although assigning more pilot points in the parameterisation step helps to increase the model performances, represented by decreased $RMSE_h$, too many pilot points prevent the model from achieving better result during calibration. This condition might be attributed to improper parameterisation of pilot-point properties, which causes over-parameterisation, thus overfitting. Processing speed is principally essential when dealing with a large number of pilot points. As the complexity arises due to the added number of points, large numbers of iterations take place in the optimisation process. Figure 4b shows the processing time incurred by the HZB methods.

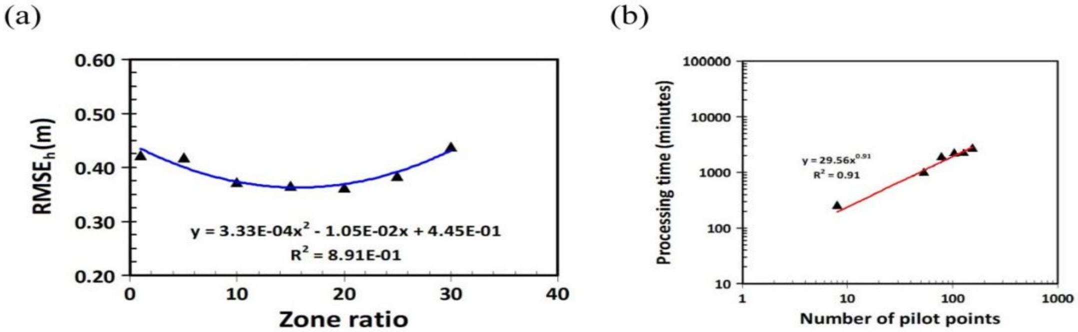

Figure 3. The result of model calibration showing: (**a**) model performance ($RMSE_h$) vs. zone ratio, which shows the impact of pilot-point density on the performances of the HZB models; and (**b**) Processing time incurred by the HZB models.

4. Conclusions

In this study, new approach of using geometric features of pilot point and distribution of hydraulic gradient over the catchment area is presented to efficiently configure pilot point distribution in the calibration step of a groundwater model. The Head Zonation-based (HZB) technique was applied on seven zone ratios (1, 5, 10, 15, 20, 25 and 30) on an eogenetic karst catchment in Rote Island, Indonesia and their performances were assessed. Overall, the observed-versus-simulated scatterplots of the seven models represented by considerably low $RMSE_h$ values in the transient simulation, indicate that a satisfactory level of model-to-observation fitting is obtained. The results show that the model performance increases by 13.49% when the zone ratio increases from 1 to 15, resulting in the increase of pilot-point number from 8 to 78. Conversely, the model performances drop by 20.04% after the increase of pilot-point number from 78 to 153 as a result of increased zone ratio from 15 to 30. It appears that although the use of many pilot points' results in significant increase of model performance, the excessive pilot-point number obviously increases the computational time, and to some extent could lead to a decrease of model performance. Therefore, choosing a reasonable pilot-point number and an appropriate distribution method using a practical guideline is important in the parameterisation step of groundwater modelling. Hence, appropriate selection of pilot-points properties is critical in developing a physically-based groundwater model. Therefore, based on the model simulations developed in this study, the recommended zone ratio is between 10 and 20 when using the HZB distribution method.

Acknowledgments

The authors wish to acknowledge the Australian governmentfor supporting the research through the Australia AwardsScholarship (AAS) and Allison Sudrajat Prize Award in the Swinburne University ofTechnology, Australia.

References

[1] Klaas D 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.* **25** 1703–1719

[2] 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**
[3] Klaas D K S Y, ImteazM A, Sudiayem I, KlaasE M E and Klaas E C M 2017 Novel approaches in sub-surface parameterisation to calibrate groundwater models *IOP Conf. Series: Earth and Environmental Science* **82** 1-8
[4] 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
[5] Carniato L, Schoups G, van de Giesen N, Seuntjens P, Bastiaens L, Sapion H 2015 Highly parameterized inversion of groundwater reactive transport for a complex field site *J. Contam. Hydrol.* **173** 38-58
[6] Klaas D K S Y and Imteaz M A 2017 Development of a groundwater model for a tropical eogenetic karst aquifer in Rote Island, Indonesia *Proc.37thHydrol. and Water Res.Symp.* 228-235
[7] Klaas D K S Y, Imteaz M A and Arulrajah A 2016 Evaluating the impact of grid cell propertiesin spatial discretization of groundwater model for a tropical karst catchment in Rote Island, Indonesia *Hydrol. Res*.
[8] Certes C and de Marsily G 1991 Application of the pilot point method to the identification ofaquifer transmissivities *Adv. Water Resour*. **14** 284-300
[9] Klaas D K S Y 2008 *Indigenous Water Management: Sustainable Water Conservation Strategies in a Karstic Dominated Area in Rote Island, NTT Province, Indonesia* (Monash University: Melbourne, Australia)
[10] Vacher H L, Mylroie J E 2002 Eogenetic karst from the perspective of an equivalent porous medium *Carbonates Evaporites* **17** 182-196
[11] Worthington S R H, Schindel G M and Alexander E C J 2001 Aquifer-scale Properties for Hydraulic Characterization of Carbonate Aquifers *Proc. Geol. Soc. of Am. Meet*. (Boston, USA)
[12] Scanlon B R, Mace R E, Barrett M E and Smith B 2003 Can we simulate regional groundwater flow in a karst system using equivalent porous media models? *J Hydrol* **276** 137–158
[13] Fetter CW 2001 *Applied hydrogeology* (Upper Saddle River: Prentice-Hall)
[14] Hudak PF 2010 *Principles of hydrogeology* (Boca Raton: CRC)
[15] Mc Donald M and Harbaugh A 1988 *A Modular Three-Dimensional Finite-Difference Groundwater Flow Model (USGS)*
[16] BYU 2014 *Groundwater Modeling System* (GMS) version 9.2.9. (Provo: Environmental Modeling Research Laboratory, Brigham Young University)
[17] 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)
[18] Harbaugh A W, Hill M C and Mc Donald 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
[19] Johnson A I 1967. *Specific Yield – Compilation of Specific Yields for Various Materials* pp 1-74
[20] Viessman W and Lewis G L 2003 *Introduction to Hydrology* (Upper Saddle River: Pearson Education)
[21] 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
[22] Davis S N 1969 *Porosity and Permeability of Natural Materials in Flow Through Porous Media* (New York: Academic Press)
[23] Freeze R A and Cherry J A 1979 *Groundwater* (Englewood Cliffs: Prentice-Hall)