A NOVEL APPROACH TO INCORPORATE HETEROGENEITY IN GROUNDWATER FLOW MODELS

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ABSTRACT

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Legitimate models simplify reality without forgoing important components or traits of the simulated systems. Using automated parameter estimation, it is possible to fabricate well-calibrated groundwater models without proper depiction of crucialgeological and hydrological features in the simulated systems. Failing to reasonablyrepresent geology and hydraulic heterogeneity may limit the usability of groundwater models and make them susceptible to technical and legal criticism.Realistic and reasonable representation of the modelled groundwater system configuration and heterogeneity has been achieved in the Lower Manawatu Catchment groundwater flow model through coupling pilot point calibration with a three-dimensional stratigraphical model.The technique proved to be practical and produced a defensible representation of the modelled system.The approach is particularly critical for stratified heterogeneous aquifer systems as it can increase modelling confidence level.

Keywords: Groundwater model, Stratigraphical model, Stratified aquifer, Heterogeneity, Pilot Points Calibration

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1 INTRODUCTION

Numerical groundwater flow models use mathematical equations, boundary and initial conditions to simulate aquifers and their responses to stresses. A legitimate model simplifies the simulated system without forgoing any of its important components or traits.Conventionally, hydraulic properties have been uniformly incorporated in groundwater flow models in discrete homogeneous zones, which is not a common happening in nature. There has been an increasing trend to try to imitate reality more closely through spatialparametrisation ofthe aquifer properties by estimating a parameter value in every cell in the model domainas an expression of heterogeneity.This is commonly achieved automatically by using pilot points that serve as surrogate parameters at which values are estimated and interpolated onto the modelling domain (Doherty et al., 2010).

Automated parameter estimation enables producing well-calibrated models, which seeminglyare better representations of the simulated systems than less well-calibrated models(Maliva, 2016).However, the technique has an history of misuse.Repeatedly, it has been used to produce well-calibratedgroundwater models that are not hydrogeologically reasonable. Hydrogeological unreasonablenessin groundwater models impliesconceptual inadequaciesand/or a need for conditioning to constrain the calibration process (Poeter & McKenna, 1998, Usman et al., 2018).Therefore, modelers are increasingly accepting greater discrepancies in the match between field observations and model results to maintain reasonable model parameters(Maliva, 2016).

In theory and in practice, groundwater model zonal andpilot point calibration methods can produce good fits between field and model data without giving muchregard to the lithostratigraphy, with the later method normally achieving better fits. However, failing to adequately incorporate the lithostratigraphy and hydraulic heterogeneity of the modelled systems could limit the usability of models in future predictions and make them susceptible to criticism in technical and legal forums regardless of the goodness of their calibration. Groundwater flow models must not only be well-calibrated, but to be defensible,they should also demonstrate being respectful of the hydrogeology.Stratigraphically sound definition of aquifer geometry is essential for having confidence in groundwater models (Barnett et al., 2012).The stratigraphical framework of the modelled groundwater system should be used to condition automated parameter estimation by constraining pilot point interpretationextent within specified zones in the model domain.Automated parameter estimation values interpolation should not be allowed to cross boundaries like contacts between aquifer strata and aquitard or impermeable material.

A steady-state groundwater flow model has been developed for the Lower Manawatu Catchment (LMC) in the North Island of New Zealand to provide an integrated analytical framework for hydrogeological assessment and groundwater resource management. Realistic representation of the modelled groundwater system configuration and heterogeneity has been achieved through coupling spatial parametrisation inverse modelling techniques with a three-dimensional (3D) lithostratigraphical model. The approach proved to be practical and produced a realistic, defensible representation of the modelled groundwater system, including its lithostratigraphy. The approach is critical for stratified heterogeneous aquifer systems as it can reduce modelling uncertainty, and increase model representativeness, solution uniqueness, and hydrogeological reasonableness.

2 METHODS AND MATERIALS

The LMC groundwater system comprises the upper part (c. 350 m) of a thick Pliocene-Quaternary sedimentary sequence that is mainly tapped in the Late Quaternary strata ≤360 ka (kilo annum, i.e. thousand years.).The system is largely controlled by topography, a manifestation of an history of tectonic activity and eustasy.It consists of alternating glacial periods represented bygravelly alluvial strata and interglacial periods comprisingsand and fine material layers deposited in marginal marine and marine settings.

Attempts to construct stratigraphical models in the LMC commenced in the 1970s, with most investigators concentrating on correlating gravel zones in well drilling cutting descriptions (e.g. Schumacher, 1999, Martley, 2001).Well depth variability, geological heterogeneity and structural and geomorphological complexitieshave made direct lithostratigraphical correlation impractical.To overcome these problems, imaginary boreholes set along transects drawn perpendicular to the general bedding strike have been utilised to interpolate the extent and configuration of various lithostratigraphical units in cross sections. A general lithostratigraphical framework has been determined based on understanding the area’s geological history that resulted in a stratigraphical sequence of alternating terrestrial and marine strata.Key lithological indicators and markers such as grain size and peat and shell content have been used to determine stratigraphical units and contacts in boreholes. Stratigraphical contacts determined at boreholes were then projecting onto the imaginary wells, enabling construction of usable representative stratigraphical cross-sections.Finally, a 3D geological model has been completed through interpolation of the surface geologydata obtained from the national geological mapping project QMAP(**Q**uarter-million**MAP**.) (Heron, 2014), stratigraphical contacts determined at real boreholes and the synthetic stratigraphicalcross sections drawn through imaginary boreholes. The model’s land surface elevation was sourced from 15 m resolution digital elevation model (DEM) (Columbus et al., 2011).

The LMC 3D geological model was transformed into a steady state finite difference cell centred numerical groundwater flow model using the GMSv. 10.3 software (Fig. 1).The flow model has beenimplemented using the Layer-Property Flow (LPF) package of MODFLOW 2000 (Harbaugh et al., 2000)and the preconditioned conjugate-gradient (PCG) solver. The model domain is defined on geological and hydrological bases. It covers the entire catchment except where basement rocks crop out. The top of the model domain is defined by the land surface and the bottom is defined at 350 mbgl or the basement rock contact, whichever is shallower. The model domain covers an area of 112x41 km (4,592 km²), divided into 224 columns and 82 rows (fixed 500x500 m cell size). Vertically, the model thickness has been divided into seven 50-metre thick layers. Model cells that fall outside the area and/or depth of interest have been inactivated.

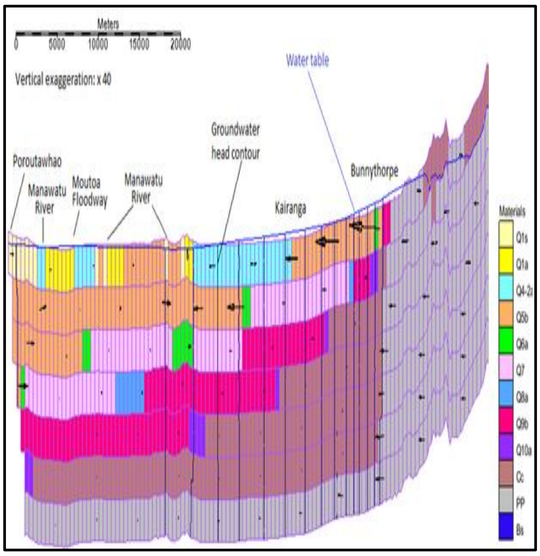

Figure 1. Transpose of lithostratigraphical units onto the groundwater model finite difference grid.

Boundary conditions at the coast have been set as specified-head in the topmost layer and no-flow in layers 2 through 7 at the groundwater-seawater interface estimated by the Ghyben-Herzberg relation described in Todd & Mays (2005). No-flow boundary conditions has been defined at the bottom of the model and along the contact between the Pliocene-Quaternary deposits and the greywacke basement rocks. The groundwater divide that is assumed to coincide with the surface water divide has also been set as no-flow boundary. The top boundary for the LMC groundwater flow model is defined by the water table, which is conceptualised as a free surface recharge boundary that is not subject to losses by evaporation and transpiration. Groundwater recharge for the model has been estimated using a soil moisture balance (SMB) model compliant with internationallyrecommended best practice (Allen et al., 1998).The SMB model is described in detail by Zarour (2017). MODFLOW 2000“RIV1” package has been used to simulate rivers and streams and the “DRN” package has been used to simulate coastal lakes. Groundwater abstraction from the c. 4,600 wells in the LMC has been estimated using the method developed by Zarour (2008). Hydraulic conductivity has been incorporated into the model using the 3D geological model material shown in Fig. 1 and the value ranges presented in Table 1. All materials have been assumed to be horizontally isotropic ($K_x/K_y = 1$) butvertically anisotropic ($Kh/Kv = 10$).

Table 1. Lithostratigraphical model units and their expected hydraulic conductivity (*K*) initial values and ranges (in m/d).The number following the letter Q in the code field correspond to the Oxygen Isotope Stage (OIS) during which the strata have been deposited and the letter suffix indicate depositional environment (s: sand dunes, a: alluvial, b: beach).

Code	Description	General lithology	*K*(m/d)	
			Initial value	Expected range
Q1s	Holocene sands	Sand	0.15	0.1 – 1
Q1a	Holocene alluvium	Gravel	100	1 – 1,000
Q4-2a	Last Glacial alluvium	Gravel, sand	10	0.1 – 50
Q5b	Last Interglacial beach deposits	Sand, silt, minor gravel	20	1 – 100
Q6a	Marton alluvium	Gravel, sand	10	0.1 – 50
Q7	Rapanui marginal marine deposits	Sand, silt	1	0.1 – 50
Q8a	Burnand alluvium	Gravel & sand	10	1 – 50
Q9b	Brunswick marginal marine deposits	Sand, silt	1	0.1 – 50
Q10a	Waituna alluvium	Gravel, sand	2	0.1 – 50
Cc	Castlecliffian strata (≥ OIS 11)	Sand, silt	2	0.1 – 50
PP	Plio-Pleistocene strata	Silt, sand, limestone, mainly consolidated	2	0.1 – 10
Bs	Basement rock	Indurated rock	–	–

It has been assumed that the SMB model estimated recharge is trustworthy and should not be changed during model calibration. So, the LMC groundwater flow model calibration entailed manipulating only horizontal hydraulic conductivity, hydraulic conductivity vertical anisotropy, and river and drain bed conductance values. The model has been calibrated for average heads and flows (exchange of groundwater with surface water), assumed to be representative of long-term average steady state conditions.

The LMC model was firstly set up using initial *K* values from Table 1, then automatically calibrated assuming homogeneous and heterogeneoushydraulic conductivities in various geological materials.

3 RESULTS AND DISCUSSIONS

Fig. 2 and Fig. 3 present the hydraulic conductivity and head distribution in layer 1 of the LMC model, respectively,assuming homogeneity (zonal calibration) and heterogeneity (pilot point calibration restricted in zones). Table 2 presents the main modelling results and basic metrics for the three modeliterations. The three models produced acceptable percent of variance explained by the model (R^2)and are hydrogeologically reasonable.The results and metrics of the three models are largely similar, giving confidence in the underlying conceptual model and the hydraulic conductivity value rangesused.However, the values obtained from all model setups are understandably different from the real hydraulic properties as each of the estimated values within a model domain is in reality a weighted average of the true hydraulic properties over the much greater volume it represents (Moore & Doherty, 2006).

It seems that pilot point calibration of hydraulic conductivities for various geological material (heterogeneous calibration) has performed better than the other two model setups in terms of head R^2, MAR and RMSR. Advantage of heterogeneous calibration is not so clear in terms of flow metrics. Flow calibration targets are less certainty than head calibration targets because they are related to surface water measurements that have larger measurement error than groundwater heads. In addition, groundwater water-surface water exchange calibration targets have a larger error margin than groundwater head calibration targets due to their strong relationship with climatic extremes that affect the mean values used for model calibration.

Similar results and metrics obtained from the three model realisations confirm that groundwater modelling solutions are inherently non-unique and numerous sets of hydraulic parameters values can produce a given set of results.Sensitivity and uncertainty analyses and analytical hydrogeological reasoning are required to decipher the outcome of model calibrations. Comparison of the three model setups also confirm that added complexity does not necessarily lead to improved performance of models and that model performance greatly depends on conceptualisation (Orth et al., 2015).

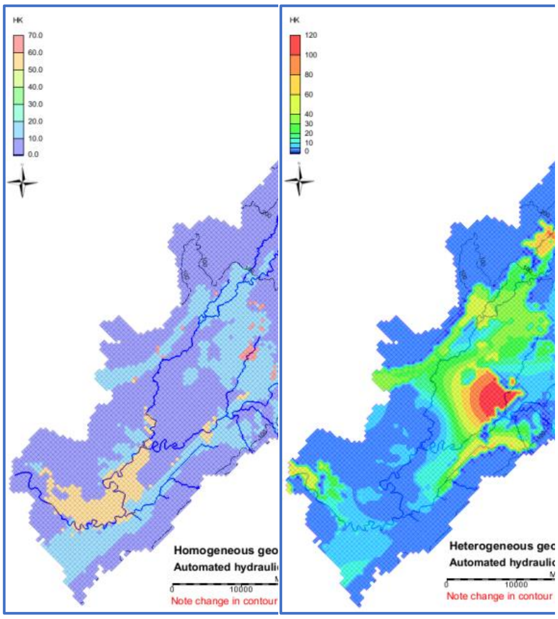

Figure 2.Hydraulic conductivity in layer 1 assuming homogeneity (left) and heterogeneity (right).

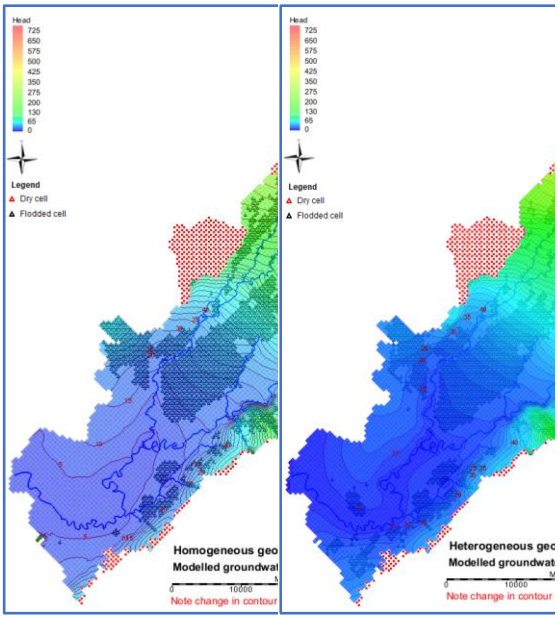

Figure 3. Head distribution in layer 1 assuming homogeneity (left) and heterogeneity (right).

Table 2. Main results and basic metrics for the LMC models set up manually, and automatically calibrated assuming homogeneous and heterogeneous geological materials.

Measure and units	**Manual**	**Homogeneous**	**Heterogeneous**
Groundwater recharge [m³/d]	1,991,586.40	1,991,083.51	1,991,083.51
Groundwater abstraction [m³/d]	-99,633.76	-99,561.93	-99,546.93
Net groundwater exchange with rivers [m³/d]	-1,876,529.93	-1,883,939.62	-1,866,841.82
Flow into the coastal lakes [m³/d]	-14,818.51	-7,974.42	-20,724.30
Flow into the ocean [m³/d]	-826.75	-1,177.01	-3,632.20
R² - Head[dimensionless]	0.92	0.92	0.94
Mean Residual(MR) - Head [m]	5.02	3.40	4.09

Mean Residual (MR) - Flow [m³/d]	176,212.18	127,676.73	136,396.22
Mean Absolute Residual (MAR) - Head [m]	8.52	7.95	6.50
Mean Absolute Residual (MAR) - Flow [m³/d]	281,428.48	230,428.04	248,031.17
Root Mean Squared Residual (RMSR) - Head [m]	10.31	10.82	8.46
Root Mean Squared Residual - (RMSR) Flow [m³/d]	518,864.51	410,214.82	433,616.31

4 CONCLUSIONS

Conditioning automated pilot point calibration in zones corresponding to stratigraphical units is a feasible method for representing the geometric configuration and hydraulic heterogeneityin stratified aquifers. It reduces model uncertainty, makes it more realistic, increases its solution uniqueness and enhances overall confidencein the produced model. The approach may not be totally warranted for site or local scale models, but it is a must for catchment and regional scale models.

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