3D Heat Transport Modelling the Wairau Aquifer, New Zealand

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Abstract

Using heat as a tracer is one of the economic methods for groundwater study. The hydraulic head alone is not sufficient for groundwater model calibration. Thus, 3D heat transport modelling of Wairau aquifer is used to study the characteristic of thermal parameters and the behavior of heat traverse through the aquifer. The aims of the research are to define the worth of temperature data for reducing the parametric and predictive uncertainty of the Wairau groundwater flow model. The 3D model was set up into 3 layers, 98 columns, 36 rows, and gird size 200m by 200m (width) base on the geological and hydrological condition. The methods that were used to implement in this research are particles tracking and heat transport model in order to compare with measurement data. The thermal flow path length, heat distribution catchment, and mean travel time are determined by the backward particle tracking MODPATH with the aiding of Matlab computer code. A finite difference numerical code MT3D-USGS is used for transport model employed with the existing 3D MODFLOW-NWT groundwater flow model for heat transfer solution. Thermal parameters including longitudinal dispersion, diffusion, and sorption are estimated by PEST. Sensitivity analysis of each parameter is conducted to see their roles the in transport model. The heat transport model is an advection dominant, which is highly dependent on hydraulic conductivity. The available advection solver is the explicit standard infinite different which is not a perfect match for advection dominant transport model. Even though, it is the only advection solver that is possible to converge the model with high velocity. On the hand, the numerical error of heat transport and groundwater flow model has been found during the model calibration. There is an unexpected heat lost from the model especially near dry cells. The fluctuation of net groundwater recharge reveals a negative correlation to the heat lost during the investigation of model error analysis. Due to the limitation of solver choices and model error, it causes the modelled heat data could not reach the measurement data. This impact leads to a high uncertainty of thermal parameters estimation.

Keywords: groundwater-modeling, heat transport, dispersion, diffusion, finite difference, retardation, sorption, transmissivity

Software: MODFLOW, MODPATH, MT3D-USGS, Matlab, PEST

Introduction

Fundamentals of using heat as a tracer for surface-groundwater interaction were published in the 1960s. During that time, there were many misconceptions regarding temperature in the groundwater variation until Humboldt and Arago published their work about geothermal gradient in 1844. However, his work did not solve the problem the way of the total heat flow until the discovery of radioactivity in 1909. (Davis, 1999) These breakthrough theories contributed greatly to the hydrological research of the modern day. It has been used by many scientists in different proposes by using analytical and numerical from laboratory scale to basin scales. Anderson (2005) mentioned that hydraulic head alone was not sufficient for the study of groundwater flow system. He described heat could be used to examine the submarine groundwater discharge and depth, salt, and fresh water interface delineate flows in hyporheic zone and parameters calibration for heat flow model in groundwater. Vandenbohede et al., (2009) conducted the comparison of different characteristic of heat and solute transport in the same aquifer by the push-pull test. Santilano et al., (2016) implement the 3D numerical model to assess the geothermal heat exchange potential in Sicily, Italy. Rühaak et al., (2008) discussed on the non-orthogonal structure grids 3D finite modelling of heat transport in groundwater model. Kaiser et al., (2013) researched on the sensitive mechanisms of 3D heat transport coupled with fluid modelling in the Northeast German Basin. Giambastiani et al., (2013) describes the limitation of using heat as a tracer in alluvial sediment to determine the aquifer properties including diffusion and longitudinal dispersivity. Heat is considered as one the most economical methods for scientists conducting their study of natural tracers comparing to deuterium, tritium, and radon gas and so on. Moreover, it is quite convenient to collect the temperature data in the field. Due to this reason, and including the existing Wairau River temperature data since 2010 and other 15 temperature data in observation boreholes in Wairau aquifer, researchers decide to use heat for further study.

This research is an extended study of heat transport in one dimension modelling (Higgins and Tum, 2017) and three dimension groundwater flow model (Wöhling et al., 2017). The main purpose of this study is to analyze and implement the available river temperature data for numerical modelling by coupling with 3D groundwater flow model. Heat is considered as a solute for the numerical model, thus MT3D-USGS, which is a finite different numerical code, is selected to employ with MODFLOW-NWT. The overall research questions are to define whether the temperature data measurements in the Wairau Plain are worth for reducing the parametric and predictive uncertainty. Responding to this question, there are some tasks need to be done particularly. Likewise, emphasising the uncertainty of the conceptual model assumptions and their corresponding to the boundary condition, and defining the sensitive and uncertain parameters.

Study Area

The Wairau Aquifer has around 26,000 hectares and includes confined, semi-confined, and unconfined areas (Davidson and Wilson, 2011). The Wairau Plain formations hosting the Wairau Aquifer are the Speargrass Formation and the Rapaura Formation (Wilson and Wöhling, 2015). The Speargrass Formation was deposited during the last glaciation (Otira). It consists of poorly sorted fluvial sediments such as gravel, sand, and clay, with a matrix of silt and clay (Brown, 1981). The surface of the Speargrass Formation forms the effective base of the Wairau Aquifer (Wilson 2016).

The Rapaura Formation consists of postglacial fluvial sediments transported by the Wairau River and its tributaries to Wairau plain. The parent rock of these sediments (gravel, sand, silt, and clay) was greywacke and schist pebbles (Brown, 1981). The Rapura Formation has two main layers. The Upper Facies forms a shallow, high permeability aquifer close to the Wairau River (the Rapura Facies). Outside of this area, the Upper Facies is highly stratified and conductivity varies significantly. Preferential flow is expected to occur through the gravels of the old Opawa River channel. The upper facies is separated from the lower member by a low permeability clay layer of three to six metres thick. This formation lets the lower member Wairau aquifer formation forming confined aquifer overlies the Speargrass Formation. Transmissivity values typically exceed 2000 m^2/day in the Rapura Formation and are highest in the Upper Facies (Wilson, 2016).

Regional flow in the Wairau Aquifer is from the west to the coast in the east, however, the geological structure and the land surface slope also affect groundwater flow. The Wairau River is a braided river with a highly-eroded bank. It is predominantly losing and the major source of recharge to the Wairau Aquifer. The gauging data recorded the recharge from the Wairau river to the Wairau aquifer from Rock Ferry to Wratts Road approximately 7.5 m^3/s to less than 20 m3/s. The depositional formations in the Wairau Plain contribute to anisotropy in the aquifer, and subsurface flow is rapidly drained in the horizontal direction rather than vertically. This can be the result of the river becoming perched over the aquifer (Wilson and Wöhling 2015).

Material and Method

In groundwater, only two mechanisms are taken into account for the basic heat transport; conduction and convection. Conductive transport is the movement heat from high to low temperature in solid or liquid phase.

The three dimension heat transport equation reviewed by (Domenico and Schwartz, 1998) conductive-convective equation is described below (Anderson, 2005):

$$\frac{k_e}{\rho}\nabla^2 T - \frac{\rho_w c_w}{\rho c}\nabla.(Tq) = \frac{\partial T}{\partial t}$$

Equation 1

Heat transport in groundwater is an analogy to solute transport in groundwater modelling. The formula of advection-dispersion for a solute is replaced by convection-conduction of heat transport.

$$\frac{\partial C}{\partial t} = -\frac{1}{R_f}\nabla(Cv) + \frac{D}{R_f}\nabla^2 C + \frac{CS_s}{R_f}\frac{\partial S}{\partial t}$$

Equation 2

The right hand side of the Equation 2 is the term of advection term sum with dispersion, and storage change term respectively. The concentration of solute in Equation 2 replaced by temperature in which written as Equation 3. The right hand side represents convection term sum with conduction, and storage change term respectively. (Hinkle et al., 2009)

$$\frac{\partial T}{\partial t} = -\frac{\rho_w c_w n_e}{\rho c}\nabla(Tv) + \frac{k_e}{\rho c}\nabla^2 T + TS_s\frac{\partial S}{\partial t}$$

Equation 3

3D Groundwater Flow Model

Wairau groundwater flow model, conducted by Wöhling et al., (2017), was set up as a transient surface and groundwater flow by using MODFLOW-NWT (Niswonger et al., 2011). ModelMuse, a user interface (GUI) were installed to set up a model domain and boundary conditions. The total area of the model 84.8 Km^2, consist of 3 layer base on geology condition, grid width 200m by 200m forming by 36 rows and 98 columns. The first layer represents the upper facies, 2nd layer is the lower permeability (a mixing of clay and silt), and the 3rd layer is the lower member. The domain starts from the west at Rock Ferry, the north is the Wairau River, and the south is the regional groundwater level contour line. The eastern part is a natural boundary which the groundwater in Rapaura formation forced up through Dillions Point confining layer at SH1 Bridge.

Particle Tracking

Null space Monte Carlo of 100 realizations with given parameters values was run in the 3D simulation. The 100 (5, 5, 4) particles were set at the location of the observation wells as the internal placement. They were tracking backward for 1225 time steps. Nine observation wells were selected for the particle tacking.

The computer code Matlab was used to separate the coordinates of the particles in each well and calculate the path lengths. There are 100 particles in each well for one simulation. The mean values of the path length from the simulations were used calculate the uncertainty of particle path length by using PDF method. Particles path lines through each grid from 100 NSMC simulation were plotted in the model domain to delineate the particle distribution in the aquifer. Gilmore et al., (2016) method was taken from the travel time step of particles in the simulation. As the groundwater flow model is transient simulation. The recharge volume and velocity to the aquifer are different depend on time. Thus, to simplify the calculation, it is necessary to assume that:

- The flow field doesn’t change between the time steps
- The velocity of particles equal to the mean velocity in cells of origin from the recharge
- The mean transit times are equal to particles traverse through the aquifer

The mean transit time of each simulation of the observation wells was used to define 50% mean value from the CDF plot.

Temperature analyses

Temperature data in 15 observation boreholes from 2 formations of the Wairau aquifer are measured daily, but the starting points recorded differently. Due to statistical analyse, including to the consistency, homogeneity, data gaps, outliers, and plausibility, only 12 observation wells are selected for model calibrations. The average temperature of the river is 13.67°C with the median value is 13.92°C and maximum and minimum temperature is in between 21.82°C to 6.05°C respectively. For temperature in observation wells variation range from 14.63°C (well 10608) to 0.54°C (4724). The temperature in each borehole has no significant difference since the mean value or variance less than 0.05 according to mean Chi square test and ANOVA test. However, there are some suspicious on temperature data sets of well 0903, 1685, 1696, 10426, and 10608, which are in the upper formation of Wairau aquifer, The temperature in data were used to do correlogram analysis. The residaul results from the autoregression models are in the upper and lower limit. There are some data slightly out of the boundary, which indicates temperature data was unexpected increasing during the measurement, it might be the impact of external sources during that periods. However, it is not much serious impact to the data.

The average temperature soil data is 14.52°C with range different 10.94. The maximum temperature 20.18°C and the minimum value is 9.24°C with median value is 14.27°C. This data is then used to constrain the thermal boundary condition for the first layer of the heat transport modelling.

Heat Transport Model

The MT3D-USGS is the updated version MT3DMS package, which is more flexible for solute transport solution since the previous version (MT3DMS) has the limit capacity to work with some MODFLOW packages. The decision of choosing this package is due to its capability to route the solute through the dry cells of Newton Raphson formula in MODFLOW-NWT. The mathematical equation in MT3D-USGS remains the same. It used a finite different method developed by Zheng and Wang (1999).

Packages for heat transport modelling are advection solvers choice is in ADV package. Dispersion and diffusion are in the DPS package. The value of this parameters will be calibrated by PEST numerical code. Recorded temperature from the river is used for the input data in SSM package in river cells grids. It is assumed that the river temperature is uniform all along the river. Soil temperature data is used to constrain the top layer of the model in SSM package as the thermal boundary condition. The bulk density and sorption are in RCT input file. The sorption parameter will be later on calibrate by PEST. GCG is the input file for conjugating gradient solvers converges with ADV package.

Thermal Boundary Condition

For 3D Wairau groundwater flow model, all the four boundary conditions types were applied in the model (FHB, SFR, DRN, RCH, and WEL). For thermal boundary condition, the specified boundary is applied for the top model layer by using soil temperature data. The top layer is the water table layer and also the recharge from precipitation. In groundwater flow model, precipitation recharges to the aquifer at some time steps. This recharge is much less than the recharge from the river to the aquifer. The water table boundary condition is the conduction of heat while the precipitation recharge is the advection heat transport. The specified heat and advection are used for recharge from the Wairau River. It is considered as convection and conduction heat transport as the temperature traverse through to the aquifer via Darcy velocity and conducted through the matrix of the aquifer. The bottom layer and the east boundary are considered as no heat flux boundary condition.

Result and Discussion

Particles Tracking

Flow Path

Normal distribution of the mean value of the each path length for 100 simulations were used to analyse the probability density function (PDF). The 25%, 50%, and 75% uncertainty results are listed in Table 1.

Mean Transit Time

The mean transit time for the upper member can be a good comparison to the cross correlation that was conducted in the study project and ERF (Table 2). They have a small different with two days gaps for well 0938 from the study project and 34 days from ERF. Well 10426 and well 1696 are a little bit longer than the previous studies, but it is still less than the maximum range in study project. Unlike the upper member, the lower member observation wells have twice larger value than the cross correlation and ERF while the groundwater age of Wairau aquifer is less than one year. (Wöhling et al., 2017).

Table 1. Flow path length compare to direct distance study project

Well	25% (m)	Mean (50%) (m)	75% (m)	Std/Mean	Direct distance (m)	Study project
			Lower member (3rd Layer)			
w10485	677	**1355.63**	2033	**1.02**	40	627
w10608	410	**820.47**	1230	**1.89**	20	41.5
w3821	1076	2152.28	3228	0.61	1700	1694
w4722	1175	2351.94	3527	0.67	2300	2345
w4724	1669	2226.01	3339	0.66	2000	2131.5
			Upper member (1st Layer)			
w1696	231	462	693	0.13	300	402.5
w10426	1242	2485.73	3728	0.06	2500	2701
w0398	643	1286	1930	0.28	1700	2686.2
w1685	546	1092.65	1638	0.10	1000	1193.5

Table 2. MTT result

	W10426	*W1696*	*W0938*	*W1685*	*W4724*	*W4722*	*W3821*	*Unit*
Particles tracking	171	50	75	88	**556**	**537**	**416**	Days
Cross correlation	111	12	77	51	220	240	145	Days
ERF	108	19	109	50	257	236	145	Days

Capture Zone

The central part of the catchment has a higher probability of particles traversing through the aquifer. As expected, the catchment of well 0398 has small distribution responding to the low standard deviation for the path length of PDF calculation (Figure 1)

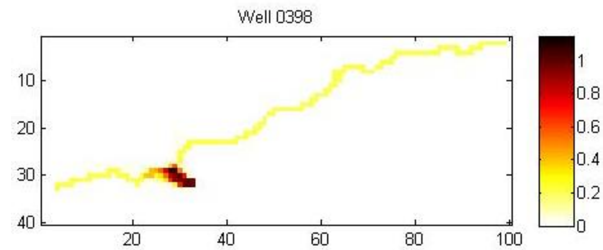

Figure 1. Catchment delineation

Heat Transport Result

Heat transport parameters model that was estimated from the study project (Higgins and Tum, 2017) are used for the input for 3D heat transport model. Though, the high value of longitudinal dispersivity in study project is not a suitable for the 3D model (RMSE is in Table 3). Well1696, and well 1685 have high RMSE in a range of 3 ^{o}C to 4 ^{o}C, while some of the wells have less RMSE around 1 ^{o}C to 2 ^{o}C (w10426, 10608, 0938). These parameters seem to have a good fit for wells likewise well 4724, 4722, and well 3821. Nevertheless, the wells which have low RMSE, do not mean the temperature oscillations match are acceptable.

Model parameters, later on, was estimated by joint calibrated between the measurement data and modelled data (Table 3). Firstly, the model calibration separated into two groups according to the location. Firs group is located near upstream included well 0938, 3821, 4722, and 4724. The second group is situated in the midstream near SH6 likewise; well 10426, 1685, 10608, and 1696. The correlation of individual groups (GC) provided a better fit for observation wells (Table 3). Yet, the SH6 group has the goodness fit coefficient only 0.82. This small correlation coefficient might get the influence from the well 10608. This well is situated in the transition zone between discharge and recharge area. There might be some influence from the instability of transient groundwater flow during the modelling. The alteration of conduction heat transport occurred the most at recharge and discharge area while less in the lateral flow. (Domenico and Schwartz, 1998) The term of macro-dispersion can be applied in modelling due to the heterogeneity of hydraulic conductivities and aquifer.

Table 3 Root mean square error model calibration (^{o}C)

	W10426	*W1696*	*W1685*	*W10608*	*W4724*	*W4722*	*W3821*	*W0938*
GC	1.672	1.633	1.782	3.456	1.293	1.161	1.051	1.184
JC	2.061	2.539	2.049	4.460	1.783	1.655	2.119	1.591
%	23.27	55.48	14.98	29.05	37.90	42.55	101.62	34.38
3D	1.906	2.891	3.386	1.429	0.697	0.697	0.592	1.357
1D	0.651	1.167	1.052	-	0.527	0.195	0.565	0.926

The upstream group parameters determined by PEST given an unreliable result. The modelled data are not fit to the measurement temperature. For this reason, the parameters listed Table 3 were calibrated manually. The joint calibration of all the observation wells by PEST provide correlation coefficient is 0.89, though the temperature fluctuation is not fit the upstream group and RMSE is much higher compared to the individual group calibration. Well 3821 RMSE increase more than 100% with the thermal parameters decrease to a smaller value. The measurement data and modelled data has large gaps. The phi value and sensitive parameters from PEST calibration show the uninfluenced of the thermal parameters to the objectives function except for diffusivity coefficient.

Longitudinal dispersivities variation reflects the heterogeneity of aquifer in different sites. It is inappropriate to demonstrate the uniform longitudinal dispersivity in a single universe line. (Gelhar et al., 1992) Increasing thermal parameters given a better fit to the upstream group while turning the SH6 group away from the data fit. Both groups have a negative correlation during the thermal parameter calibration. Consequently, it is impossible to get a satisfactory result from the join calibration.

In 3D model, the longitudinal dispersion has 2 order of magnitudes lower than in the study project, while diffusivity is one order of magnitude lower but the upstream result is in the same order. The distribution coefficients are slightly different from the previous study.

Longitudinal dispersion is the range 0.01 to 5 m which is the same range of solute transport (0.1-10m). Gelhar et al., (1992) describe that the longitudinal dispersivities of solute were in between 10^{-2} to 10^{4} m of the scale from 10^{-1} to 10^{5} m after his experiments in 59 different field sites. The largest scale that is the most reliable was 250m. Though, the argument is not literally true for thermal dispersion coefficient. Vandenbohede et al., (2009) stated that thermal dispersivity and diffusivity coefficient did not depend on scale. He also mentioned the different behaviour of thermal parameters between solute and heat in the same aquifer, but it was no significant result that could define their differences. Heat dispersivity term is expected relatively smaller than solute. The thermal diffusivity in literature review is in between 10^{-6} to 10^{-7} m^2/s. (Anderson, 2005; Domenico and Schwartz, 1998) Though, the thermal diffusivity from the calibration of the downstream group is out of this range. The high transient velocity of groundwater flow, which is account for the convection heat transport, probably is the reason behind the low dispersion term value.

Table 4. Model parameters

	D* m^2/day	***K_d*** ($m^3/^oC$)	***Retardation factor***	***α_L*** (m)	***Diffusivity*** m^2/s
Upstream	0.011	0.0035	9.194	4.92	1.34E-7
SH6	0.00425	0.001	9.631	0.01	4.91E-08
Rapaura	0.001	0.001	-	0.01	1.16E-8
Study project	0.02	0.00121	-	550.72	2.31E-07

The Peclet number is the dimensionless parameter to determine mechanism dominant of heat or solutes transport in the aquifer. It is the ratios of transport by convection over conduction. If the Pe is equal to 1, the convection and conduction are at the same rate or represents the absent of fluid motion. If the Peclet number is large than 4, the convective mechanism dominant the heat transport. (Zheng and Wang, 1999) In this model, it is impossible to define an exact number of the Peclet number due to the transient seepage velocity. However, the average net recharge flux (7.5m^3/s) to the aquifer, the low dispersion coefficient from the model, and grid width (200m) give an indication of high Peclet number. The approximate calculation Pe in the model is the larger than 100. Hence, the heat transport in Wairau aquifer is convection dominant, hence the small dispersion term value is acceptable.

However, there are some cases that should be taken into consideration regarding the small value, whether it is reliable. In heterogeneity aquifer for regional scale, thermal dispersivity term cannot be neglected even if it has a small value. (Constantz et al., 2003; Vandenbohede et al., 2009) Nevertheless, a remark of uncertainty heterogeneity aquifer should be noticed as it is very important for heat transport by conduction. Heat is not only traversed through water in the porous media but also with the matrix in the aquifer. The Wairau aquifer is highly heterogeneity with the open framework gravels outwash formation and clay stratified in some part also. The macro-dispersion is also expected in the model. These detail was not able to include in the numerical model properly. The model assumptions have simplified the reality to less complex model. For an example; each layer has uniform porosity and the hydraulic conductivities are different according to river sections. This assumption might be slightly effected to real value.

The 3D heat transport model retardation factor is expected in the range of 3 to 5 (Higgins and Tum, 2017), yet the calibration value is between 9 to 10. The value is a bit higher, but it is still lower than the previous calibration result in study project. Thus, the non-thermal equilibrium assumption is study project remain true in this modelling, as the observation well that located further from the river gave an indication the effect of retardation factor

Sensitivity Analyses

Well 1696 and 1685 are not sensitive to thermal parameters. Their RMSE remain constant even if their thermal parameter p_k is multiplied and divided by 10 times. Well 10608, is not sensitive to the molecules diffusion coefficient and distribution coefficient, but slightly sensitive to longitudinal dispersion. Wells in the upstream group is not sensitive to distribution coefficient but slightly sensitive to molecules diffusion and longitudinal coefficient. Only well 10426 that is sensitive to all thermal parameters. Its longitudinal dispersion sensitivity coefficient dominant the other thermal parameters during increasing the multiplier parameter. On the one hand, the distribution coefficient dominant during the multiplier parameter decreasing. Hydraulic conductivity is the most sensitive parameter to all the observation wells of heat transport modelling. (All result listed in Table 5)

According to the global sensitivity variations in the model, hydraulic conductivity performance an important role in the sensitivity analyses. Both increasing and reducing the hydraulic conductivity, it highly effects to the temperature fluctuation and the heat distribution in the aquifers. Each observation wells has various respond to the hydraulic conductivity. Well 3821 river has very large sensitive coefficient while well 10608 the closest one to the river has the smallest sensitivity when the hydraulic conductivity is increasing. An interesting remark, the upstream group has higher sensitivity coefficient responds to hydraulic conductivity than the downstream group.

Heat initial concentration less impact than the other parameters. Only well 3821 highly sensitive during the temperature increasing and decreasing. While initial temperature rising to 15.67^{o}C the RMSE decreases 32.79%. During temperature was reduced to 11.67^{o}C the RMSE increase 16.07%. The rest of the observation wells RMSE slightly change in less than 1.5%.

Model Limitation and Error analyses

The standard infinite different is the only that can be used, but it is not recommended for convection dominant transport model as it would deliver high numerical dispersion for the cause grid discretization. The limitation solver selection and the error from numerical modelling, let to unsuitable results from the parameter estimation form the modelling. In the joint calibration with groundwater flow parameters was also limited since it is time constrains and the instability of groundwater flow, the simulation crushed at for several time steps after running the transport model, therefore the groundwater model parameter has to be constant.

As mentioned above the observation well in the first layer was moved to the second layers, due to this reason there will be some numerical error since the second layer has lower permeability than the first layer even if it is considered as high velocity compares to other aquifers. The root means square error increases 1.67^{o}C for well 0938 and well 3821 (same grid different layer). The heterogeneity of different layers plays an important role for thermal parameters. Sommer et al., (2013) concluded that the thermal distribution got the influence from the heterogeneity of hydraulic conductivity, thus the thermal energy and thermal balance would give the less precise result from that effect. The various Wairau aquifer characteristics in both layers literally would provide different results. Hence, the model layers should be increased.

The observation wells are put in the same location of the measurement data to record the constant modelled data. Surprisingly, the result is out of the expectation. There are some wells provide the temperature fluctuation although, it was expected to be constant. The observation wells that highly impact from the numerical error are well 0938, well 3821, well 4722 and well 4724. The root means square error for the wells are 0.376, 0.146, 0.029, and 0.008 respectively. These are the wells in the upstream group and they are located near the dry cell grids. The wells located further from the dry cells (SH6 group) such as; well 1696 get slightly effect from the heat lost (RMSE=1.7E-6). There are 3 wells (10608, 1685, and 10426) remain constant at 13^{o}C which show no indication of heat lost from this well.

Conclusion and Recommendation

The backward particles tracking simulation in the first layer of the aquifer is more reliable than the 3rd layer. The flow path length, catchment delineation, and the mean transit in the first layer gave an excellent result in comparison to the past researches. Conversely, the bottom model layer provided a good agreement of flow path length and heat distribution area but product distrustful results for MTT.

For 3D heat transport modelling, it provides a very high uncertainty and inaccurate result. It is not easy to give a good conclusion for the 3D heat transport model of the Wairau aquifer. Even if, the SH6 observation group does not have significantly impact from the model, but the result is less likely reliable. On the other hand, if the thermal parameters of the SH6 group do not get any impact from the numerical error, so the result is a positive sing for reducing the parametric and predictive uncertainty of the Wairau groundwater flow model due to the thermal parameter is much less sensitive than hydraulic conductivity.

Giambastiani et al., (2013) mentioned the heat has the limitation to define the aquifer properties in the conduction dominant transport, but it could product a good result with convection dominant with fine sand and well-known boundary condition. In contrast to his conclusion, heat might not be a suitable tracer method for highly convection dominant like the Wairau aquifer. However, the 3D heat transport of this model is still able to obtain a better parameters estimation result, if the groundwater flow model is simpler and less complexity.

After the discussion in the previous section, there are plenty of numerical uncertainty and error from both particle tracking and heat transport model. Therefore, before using the result from this study for further research, there are some tasks need to be clarified. The suggestions that be implemented are:

For particle tracking MODPATH

The calculation of MTT in the lower member is less reliable. It is necessary to re- calculate by focusing on the boundary condition in the bottom layer and the velocity flow into the 3rd layer.

Determination of macro-dispersion coefficient in function of distance of Wairau aquifer should be included.

The uncertainty of the 3rd layer is higher than the first layer, thus 2D particles tracking for the individual layer is recommended for model comparison.

For heat transport MT3D-USGS

Defining the external recharge sources to the model which are the cause of initial temperature reduction and the impact of the dry cells of MODFLOW-NWT to MT3D-USGS package.

Determining the relationship of transient velocity and the heat transport model. Modellers normally assume velocity is constant so that it is more convenient to reduce the macro dispersion in the model.

Wairau aquifer has a very complex formation with high velocity. Not many numerical codes are suitable to model this aquifer better than MODFLOW-NWT. By the way, in order to have a better heat transport result, it is important to simplify the groundwater flow model. Thus, simplify model might explain better for the thermal properties and make a comparison with the current model.

Model layers should be re-discretising with a uniform grid length due to the thermal boundary conditions.

Basal heat flux boundary condition should be taking account for the future heat transport model since the geological boundary in the heterogeneity aquifer largely impacts on the modelled data.

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Appendix

Table 5. Sensitivity analysis

	W10426	W1696	W1685	W10608	W4724	W4722	W3821	W0938	Unit
				Longitudinal α_L					
Base	1.672	1.633	1.782	3.456	1.293	1.161	1.051	1.184	ºC
0.1	2.965	1.633	1.782	4.549	1.293	1.161	1.058	1.205	ºC
10	2.77	1.633	1.782	3.456	1.287	1.157	0.969	1.061	ºC
				Molecules diffusivity coefficient D*					
0.1	1.672	1.633	1.782	3.456	1.284	1.155	1.058	1.204	ºC
10	1.504	1.633	1.782	3.456	1.369	1.225	0.969	1.061	ºC
				K_d					
0.1	2.965	1.633	1.782	3.456	1.293	1.161	1.051	1.184	ºC
10	1.672	1.633	1.782	3.456	1.293	1.161	1.058	1.184	ºC
				Hydraulic conductivity					
Base	1.516	2.066	2.759	4.572	1.417	1.347	0.736	1.338	ºC
0.1	1.671	3.906	14.96	14.56	1.503	1.380	1.422	2.108	ºC
10	11.191	14.667	3.148	4.222	10.352	10.401	11.56	13.069	ºC
				Initial Temperature (13.67)					
Base	2.454	1.431	3.413	4.632	2.854	3.046	1.037	1.304	ºC
15.67	2.448	1.439	3.387	4.634	2.851	3.046	0.697	1.294	ºC
-22%	-0.24	0.56	-0.76	0.04	-0.11	0.00	-32.79	-0.77	%
11.67	2.449	1.439	3.363	4.631	2.851	3.051	1.149	1.318	ºC
+22%	-0.20	0.56	-1.48	-0.02	-0.11	0.16	16.07	1.08	%