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Calibration of a transient transport model to tritium measurements in rivers and streams in the Western Lake Taupo catchment, New Zealand

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Abstract

Here we present a general approach of calibrating transient transport models to tritium concentrations in river waters developed for the MT3DMS/MODFLOW model of the Western Lake Taupo catchment, New Zealand. Tritium is a time-dependent tracer with radioactive half-life of 12.32 yr. In the transport model, the tritium input (measured in rain) passes through the groundwater system, and the modelled tritium concentrations are compared to the measured tritium concentrations in the river outlets for the Waihaha, Whanganui, Whareroa, Kuratau and Omori river catchments from 2000–2007. For the Kuratau River, tritium was also measured between 1960 and 1970, which allowed us to fine-tune the transport model. In order to incorporate all surface flows from rivers to small streams, an 80 m uniform grid cell size was selected in the steady-state MODFLOW model for the model area of 1072 km². The groundwater flow model was first calibrated to groundwater levels and stream flow observations. Then, the transport model was calibrated to the measured tritium concentrations in the river waters. The MT3DMS model results show good agreement with the measured tritium values in all five river catchments. Finally, the calibrated MT3DMS model is applied to simulate groundwater ages that are used to construct groundwater age distributions for the river catchments.

1 Introduction

There is still limited understanding of the dynamics of the groundwater component that transmits much of the water from rainfall to streams (Loague et al., 2005; Ebel et al., 2008). Tritium, a direct age-tracer linked to groundwater dynamics, can greatly improve our conceptual understanding of streamflow generation, and be used to calibrate quantitative groundwater flow and contaminant transport models. Better understanding of groundwater flow paths and travel times is essential to improve understanding of

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movement of contaminants (e.g. nitrate) through the groundwater system into surface waters such as streams and lakes.

Numerical modelling of tritium concentrations in surface water catchments is not yet available in the peer-reviewed literature. Over the past decades it has been difficult to use tritium for age-calibration due to the interference of the bomb-tritium from the atmospheric nuclear weapons testing in the early 1960s. Now, fifty years after those tests, tritium has declined back to natural low concentrations in most parts of the world, making tritium an effective tracer for calibration of groundwater flow and transport models. Because of improved accuracy of tritium measurements in the low-tritium environments (Morgenstern and Taylor, 2009), it is now possible in the Southern Hemisphere and becoming so in the Northern Hemisphere to establish with one tritium measurement the age of groundwater and stream and river water (Stewart et al., 2012). This will also enable measurement of the seasonally changing age of stream and river water (Morgenstern et al., 2010). We predict that tritium will become a routine tool for age-calibration of groundwater flow and transport models in the future.

Several studies have modelled tritium concentrations at monitoring wells using transport models. Zuber et al. (2005) modelled tritium and SF₆ concentrations in five observation wells in the 200 m deep Bogucice multi-aquifer system with a MODFLOW/MT3DMS finite-difference model in Southern Poland. The study area of 172 km² was represented by 250 m by 250 m grid cell size and five layers in the finite-difference grid using Visual MODFLOW (VMOD) graphical user interface (Zuber et al., 2005; SWS, 2010). Zoellmann et al. (2001) modelled tritium and SF₆ with MODFLOW/MT3DMS in nine monitoring wells installed in the basalt aquifer, Germany. Several studies compared groundwater residence times from tritium and CFCs to MODPATH particle tracking in the Trout Lake, Wisconsin (Pint et al., 2003; Hunt et al., 2006; Walker et al., 2007). In the Trout Lake watershed, Fielen et al. (2009) used measured stable oxygen isotopes and tritium concentrations in bores to refine groundwater pathways between the Big Muskellunge and Crystal Lakes in a cross-sectional model. Starn et al. (2010) distributed particles with assigned isotope concentration and estimated

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groundwater recharge by backwards particle tracking from the wellbore to the model surface. In addition, transport models were used to model ^{18}O and ^2H concentrations – Krabbenhoft et al. (1990) identified groundwater and lake connectivity by modelling ^{18}O transport in the four layer finite-difference model. The deuterium concentrations were modelled by particle tracking in the finite-element FEFLOW model for Lake Warden wetland system Western Australia (Marimuthu et al., 2005; Reynolds and Marimuthu, 2007). Stichler et al. (2008) estimated Lake Leis contribution to pumping wells by modelling ^{18}O and ^2H concentrations in the transient FEFLOW model.

In this work, we present a general approach of calibrating transport models to tritium concentrations in river waters developed for the MT3DMS/MODFLOW model of the Western Lake Taupo catchment (WLTC). The groundwater flow (MODFLOW) and contaminant transport (MT3DMS) models are constructed using field data of WLTC. The steady-state MODFLOW model was calibrated to groundwater levels and stream flow observations. The MT3DMS model was calibrated with the measured tritium values in rivers for the Waihaha, Whanganui, Whareroa, Kuratau and Omori River catchments and used to simulate groundwater ages for WLTC.

2 Approach

2.1 MODFLOW model setup

In the conceptual model for WLTC, the aquifer system receives recharge from rainfall and drains into Lake Taupo via streams or directly through the lake bed. In Fig. 1, Oruanui Ignimbrite, Whakamaru Ignimbrite, Pakaumanu Ignimbrite and Greywacke basement units that are listed from the most to least conductive materials were extracted from the existing 3-D geologic model for the WLTC area (White et al., 2009). The Whakamaru unit was subdivided into “a” and “b” areas that are separated by a hidden fault based on the geological map for the WLTC area. These units were represented by 16 grid layers with uniform thickness of 20 m and each grid cell was assigned the

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hydrogeological properties of one unit. The model area of 1072 km² was represented by a finite-difference grid of 500 rows and 335 columns with a uniform grid cell size of 80 m to allow small surface water features to be included in the model albeit with an exaggerated width (Haitjema et al., 2010).

The top elevation of the model grid was obtained from modified Lake Taupo bathymetry and digital terrain model (DTM) data and processed to reduce higher elevations in adjacent cells that exceed a specified vertical difference of 10 m and to have slopes of no more than 12.5%. This DTM adjustment allowed us to reduce the slope of the terrain in steep slope areas such as ridges and cliffs while maintaining a constant layer thickness in the entire model. In layer 1, the Lake Taupo water level of 357 m was incorporated as a constant head boundary and surface water features such as rivers were incorporated as drain cells with uniform conductance of 40 m² day⁻¹ (Fig. 1). The locations of the drain cells were obtained from the 1 : 50 000 topographic dataset based on vector data of the streams and the assigned drain bottom elevation was 1 m below the top elevation of layer 1. Groundwater recharge was assigned to the topmost saturated model layer (McDonald and Harbaugh, 1988; Harbaugh et al., 2000). The groundwater recharge values were obtained from the difference of average annual rainfall (Tait et al., 2006) and actual evapotranspiration data (Tait and Woods, 2006) between 1960 and 2006 and reclassified into 10 zones with a discrete recharge value from 400 to 1300 mm yr⁻¹ with 100 mm yr⁻¹ increments.

The model domain was divided into 49 unique non-overlapping zones to include 30 river gauging stations using ZONEBUDGET (ZBUD), which is a post-processing water flow and mass budget utility for MODFLOW (Harbaugh, 1990). The modelled river flows were extracted from the ZBUD output and routed from headwaters towards the Lake to obtain cumulative river flows at gauging stations. The steady-state groundwater flow model was calibrated to median values of river flows at 30 gauging stations and of groundwater levels at 18 bores, which are screened in layer 1–2 except for the deepest borehole of 58 m screened in layer 3. After the trial-and-error calibration to groundwater levels and stream flows, all input recharge values shown in Fig. 1 were

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multiplied by 0.88. The hydraulic conductivity values in the calibrated groundwater flow model are 1 m day^{-1} for the Oruanui unit, 0.2 m day^{-1} for the Whakamaru unit (W5a), 0.08 m day^{-1} for the Whakamaru (W5b) and Pakaumanu (P7) units and 0.01 m day^{-1} for the Greywacke. These calibrated values are comparable to the values measured in the field. The results of the groundwater flow model are shown in Fig. 2. Modelled groundwater elevations range from 357 m above mean sea level at the Lake Taupo lakeshore to over 1000 m in the northern part of the model domain and are influenced by the surface water network. Groundwater divides occur at elevated terrain areas below the model top layer. The depth to water table in plan and cross-sectional views indicate potential thickness of the unsaturated zone.

2.2 Tritium input and measurements

Monthly concentrations of tritium in rainfall were aggregated to annual averages and assigned as annual recharge concentrations in MT3DMS from 1950 to 2012. Tritium concentrations are reported as the tritium ratio (TR) or tritium units (TU). From 1960, the rainwater has been sampled monthly for tritium concentrations at the Kaitoke station near Wellington. The tritium concentrations between 1955 and 1960 are deduced from waters in the Hutt River (Morgenstern and Taylor, 2009) and prior to 1955 are considered as ambient tritium concentrations estimated to be 2 TR. Tritium was also measured at several rainfall stations across New Zealand to establish the scaling factor for the various regions to the Kaitoke record. Tritium analysis details are given in Morgenstern and Taylor (2009).

Tritium concentrations measured in river waters of the Waihaha, Whanganui, Whareroa, Kuratau and Omori catchments were used as calibration targets for the MT3DMS model. Tritium data from 2001 and 2002 are obtained from Vant and Smith (2002) and from 2004 to 2007 from Morgenstern (2007). In addition, tritium data from 1964, 1966 and 1970, the time of the tritium peak in rainwater due to the nuclear weapons testing in the early 1960s, are shown in Morgenstern and Taylor (2009) for

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the Kuratau River. These data allow us to resolve the bomb-peak ambiguity in age interpretation (Stewart et al., 2012), and to fine-tune the transport model.

2.3 MT3DMS model setup

In the MT3DMS model, tritium was specified as a single species with first order decay of 12.32 yr (Morgenstern and Taylor, 2009). Both single- and dual-domain transport model settings were used for tritium transport simulations in fractured ignimbrite rocks using MT3DMS version 5.2 (Neville, 2006; Zheng and Wang, 1999). In the single domain model, tritium concentrations occur in flowing groundwater. For the dual-domain model, stagnant groundwater is present with tritium concentrations that are exchanged with the mobile phase using the mass transfer coefficient in the MT3DMS model. The high and low values of the mass transfer rate makes the dual-domain model equivalent to the single-domain model with combined porosity and the single-domain model with porosity of mobile domain, respectively (Zheng and Wang, 1999). The immobile domain was assigned uniform porosity of 0.001 and the first-order mass transfer coefficient between mobile and immobile domains was estimated to be 1.54×10^{-5} based on values of the sphere shape of the fractures and the molecular diffusivity and porosity of the immobile domain (Neville, 2006; Bear and Cheng, 2010). The effective porosity was used to represent the porosity of the mobile domain in the model and was obtained from the tritium calibration to be 0.1 (–) for the Oruanui unit (O3a), 0.035 for the Whakamaru unit a (W5a), 0.006 for the Whakamaru unit b (W5b) and Pakaumanu unit (P7), and 0.001 for the Greywacke unit (B2).

The longitudinal dispersivity was selected to be 10 m and ratios of horizontal to longitudinal dispersivity and of vertical to longitudinal dispersivity are 0.1 and 0.01, respectively (Zheng and Wang, 1999). An implicit GCG solver with upstream finite-difference advection was selected and the time steps for the MT3DMS simulation were specified with a Courant number of 0.75, a step multiplier of 1.0, and a step size of 365 days (Zheng and Wang, 1999). The total MT3DMS run time was 62 years to simulate tritium concentrations from 1950 to 2012. Annual tritium concentrations were assigned as

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recharge concentrations in the MT3DMS model using a MTH recharge concentration boundary condition file for VMOD that was prepared with a custom Python code.

The tritium concentrations in river waters were obtained by extracting modelled tritium concentration values at drain cells in each of five river catchments using Python script. The python script allowed us to interrogate the binary array output fluid (BGT) and concentration (UCN) files. For each drain cell, the amount of tritium was obtained by multiplying the modelled tritium concentration at that cell by the modelled groundwater outflow. The average tritium concentration at the river catchment outflow was obtained by weighting the amount of modelled tritium for a river catchment by the total modelled river flow at that catchment.

In addition, tritium concentrations in river waters were obtained by using fluid budget ZBUD and mass budget MT3MS Transport Observation Package (TOB). The MODFLOW drain cells in each catchment were selected for the MT3DMS TOB mass flux object (Zheng, 2006). The groundwater flow MODFLOW and transport MT3DMS models were run using “translate and run” in VMOD (SWS, 2010). The translated MT3DMS model files by VMOD are used to run the MT3DMS model with mass flux output file from command prompt. This was required due to inability of VMOD to include the TOB package for MT3DMS. The mass of tritium reported by the TOB mass flux object reports is converted to tritium concentration with the use of modelled base flow for each of the five river catchments. However, the ZBUD and TOB approach is more cumbersome to set up for large catchments.

3 Results

3.1 Modelled tritium concentrations

The tritium concentrations modelled with the MT3DMS transport model are shown in Fig. 3 for the Waihaha, Whanganui, Whareroa, Kuratau and Omori river water catchments. For clarity in Fig. 3, the measured tritium concentrations in Kuratau river water

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only are shown. The measured tritium values between 1960 and 1970 were essential to fine-tune the transport mode to produce modelled tritium concentrations during the bomb-peak. Having tritium measurements taken between 1980 and 1990 would further improve tritium model calibration during the decline of tritium concentrations. The modelled tritium concentrations had the best match with measured time series data for the dual-domain model in both 1960–1970 and 2000–2008. For single domain results, the modelled tritium concentrations matched 1960–1970 measurements but were too low for 2000–2008 measurements.

For all five river catchments, the modelled tritium concentrations show similar patterns with the largest difference of modelled tritium concentrations at the bomb-peak (Fig. 3). The modelled tritium concentrations are highest for the Omori river catchment with modelled river flow of $0.5 \text{ m}^3 \text{ s}^{-1}$ from a drainage area of 27.4 km^2 and lowest for the Whareroa river catchment with modelled river flow of $1.4 \text{ m}^3 \text{ s}^{-1}$ from an area of 59.3 km^2 . The Whanganui and Kuratau catchments have similar modelled tritium concentrations although these two catchments have different hydrogeologic settings. For example, the Whanganui catchment has modelled river flow of $1.6 \text{ m}^3 \text{ s}^{-1}$ from an area of 65.3 km^2 and the Kuratau catchment has modelled river flow of $5.6 \text{ m}^3 \text{ s}^{-1}$ from an area of 199.6 km^2 . The Waihaha river catchment with modelled river flow of $3.9 \text{ m}^3 \text{ s}^{-1}$ from an area of 155.4 km^2 has modelled tritium concentrations that fall in-between modelled tritium concentrations for the Whareroa and Kuratau river catchments.

The influence of groundwater and transport model parameters on modelled tritium concentrations in rivers was investigated following Zuber et al. (2011). In all conducted comparisons, model parameters such as dispersion, aquifer porosity, hydraulic conductivity, conductance and rainfall recharge had the most influence on the modelled tritium concentration during the bomb-peak. In advective dominated aquifer systems such as WLTC, the dispersion and immobile domain porosity have very small influence on the modelled tritium concentrations in rivers. For example, an order of magnitude increase of dispersion relative to the tritium calibrated model resulted in up to 4% reduction of modelled tritium concentrations in Whareroa between 1960 and 1970. An order of

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variable input histories of chemicals (e.g. nitrate) to groundwater and to obtain nitrate concentration at any stream reach.

From the tritium calibrated MT3DMS model, the groundwater age concentration was assigned as a single mobile species with negative zero-order decay reaction that allows aging of groundwater by a day per day (Zheng, 2009). Zero age was assigned to the top of the model (as recharge concentration) and the transient MT3DMS model was run for 200 yr to reach steady-state conditions of groundwater age concentrations. The modelled groundwater age concentrations were determined in each drain cell that is included in the surface water network of the river catchment and groundwater age distribution was constructed for the stream outlets of the five river water catchments. The groundwater age distributions for the Waihaha, Whanganui, Whareroa, Kuratau and Omori river water catchments are shown in Fig. 4 with MRTs of 9.5, 6.1, 15.1, 7.1 and 3.3 yr, respectively. In Fig. 4, MRTs for the Waihaha, Whanganui, Whareroa Kuratau and Omori river catchments correspond to 55.1 %, 65.1 %, 49.7 %, 62.4 % and 56.4 % of cumulative frequency distribution (CFD), respectively. The MRT is equal to 63 % of the CFD for the exponential shape (Haitjema, 1995; Abrams, 2012). This implies that the modelled CFDs, except for that at Whareroa, are very similar to the exponential CFD. To investigate the effect of the stagnant groundwater in the dual-domain transport model, groundwater ages were simulated using the single domain transport model setting. The resulting groundwater age distributions are very similar to those of the dual-domain transport model with smaller MRT values by 0.2–0.6 yr and are not shown. In addition, the exact MRT values were obtained using the TOB package available for MT3DMS as an independent check for these river catchments.

In order to understand the age distributions in Fig. 4, the modelled groundwater ages in the mobile domain are shown in Fig. 5 for the model cross-sections along rows 129, 213, 299, 330 and 386. These reveal complex surface-groundwater flow interactions influenced by aquifer hydrogeology. In cross-section 129 for the Waihaha catchment, the youngest water (< 5 yr) occurs near the water table and groundwater becomes older with aquifer depth (up to 200 yr at the bottom of the Whakamaru unit). This is consistent

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with a groundwater age distribution described by the exponential model (Maloszewski and Zuber, 1982). It can be seen that old groundwater upwells from the bottom of the aquifer and discharges into the river network. This results in a mixture of old and young groundwaters in the river water giving an age distribution similar to that of the exponential model. In Fig. 4, CFDs for Waihaha, Whanganui, Kuratau and Omori are similar to that of the exponential model in spite of the hydrogeologic settings of these catchments being much more complex, see Figs. 1 and 2. In cross-section 213 for the Whanganui catchment, the groundwater age for Pakaumanu unit (on the left) is very young (< 5 yr) and for Whakamaru unit (on the right) is up to 20 yr old (Fig. 5). A groundwater divide is also observed to the left of the vertical formation boundary, which makes the river behave as a weak-sink that captures only part of the old groundwater arriving from the divide, while the rest passes underneath the river towards the lake (Abrams, 2012). A similar pattern is observed in cross-section 386 that shows the Whakamaru unit in the Kuratau and Omori river catchments. The groundwater age at the aquifer bottom below the Omori river water catchment is much younger than that in the Kuratau catchment. The groundwater divide occurs near the catchments' boundary and separates two catchments hydraulically. Note that these groundwater divides do not always coincide with the boundaries of the surface water watersheds.

In cross-sections 299 and 330, complex exponential and piston flow patterns are present as a result of surface-groundwater interactions and the presence of the more conductive Oruanui formation above the Whakamaru formation. For the Oruanui unit, the groundwater ages show an exponential flow pattern with young groundwater ages near the water table and ages increasing with aquifer depth. For the Whakamaru unit, a piston flow pattern occurs due to groundwater flow from the groundwater divide at the Pakaumanu unit toward Lake Taupo and is shown by vertical groundwater age contour intervals. The piston flow continues underneath the Oruanui unit and the old groundwater upwells into rivers at the surface; see the middle of cross-sections 299 and 330. In cross-section 330, groundwater with young ages underflows the river from the surrounding groundwater watersheds in the Whakamaru and Pakaumanu units. This

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results in a mixture of young and old groundwater underneath the river and indicates that rivers and streams may receive old groundwater depending on the hydrogeologic conditions in the aquifer.

4 Concluding remarks

We have presented a new approach to calibration of a transient MT3DMS transport model to measured tritium concentrations in river waters. Steady-state MODFLOW groundwater flow model and transient MT3DMS transport model were developed for the Western Lake Taupo catchment (WLTC) using a uniform 80 m model grid to include small surface water features. The results of the groundwater flow model gave groundwater elevations ranging from 357 m above mean sea level at the Lake Taupo lakeshore to over 1000 m in the northern part of the model domain. Tritium measurements for the Waihaha, Whanganui, Whareroa, Kuratau and Omori river water catchments of the WLTC were used to calibrate the tritium transport model while maintaining the groundwater flow MODFLOW model calibration to groundwater elevation and stream flow data. The Kuratau catchment had tritium results for 1960–1970 in addition to the 2000–2007 measurements, which allowed us to fine-tune the transport model at the bomb-peak. The calibrated model parameters such as aquifer porosity and hydraulic conductivity were comparable to the values measured in the field.

Tritium concentrations and groundwater ages were modelled with single- and dual-domain models. The modelled tritium concentrations matched the measured data best for the dual-domain model in both the 1960–1970 and 2000–2008 periods. For the single domain model, the modelled tritium concentrations matched 1960–1970 measurements but were too low for 2000–2008 measurements. In the single domain model, tritium concentrations occur in flowing groundwater. For the dual-domain model, stagnant groundwater is present with tritium concentrations that are exchanged with the mobile phase using the mass transfer coefficient in the MT3DMS model. High and low values of the mass transfer rate in the dual-domain model make the dual-domain model

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distributions illuminate complex surface-groundwater interactions and are essential for management of nitrate loading in the WLTC.

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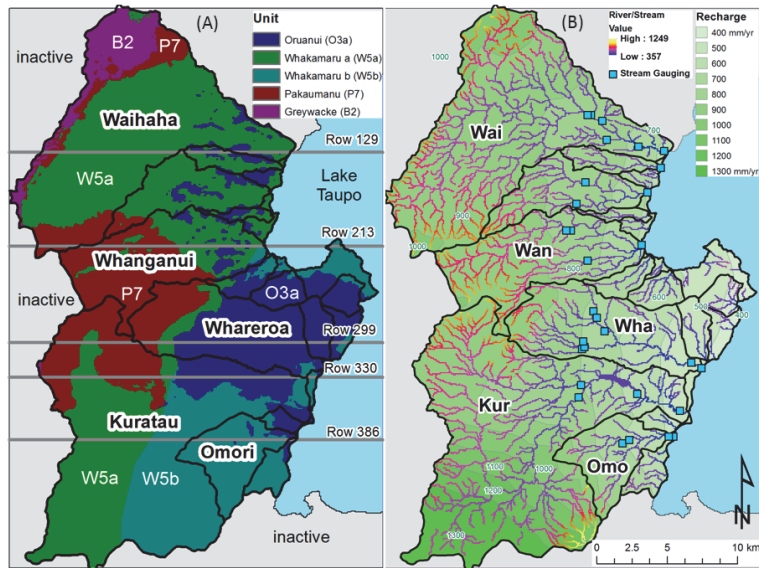


Fig. 1. Plan view of the Western Lake Taupo catchment model on hydrogeology model **(A)** and boundary conditions **(B)**. The catchments boundaries are shown by solid black lines and inactive cells are shown by the light grey color. For the hydrostratigraphy in **(A)**, the dark blue is the Oruanui unit (O3a), the dark green color is the Whakamaru unit a (W5a), the light green is the Whakamaru unit b (W5b), the dark red is the Pakaumanu unit (P7) and the pink color is the greywacke basement unit (B2). The cross-section along rows 129, 213, 299, 330 and 386 are shown in Fig. 2. The Waihaha (Wai), Whanganui (Wan), Whareroa (Wha), Kurataua (Kur) and Omori (Omo) catchments with tritium measurements are indicated with letters on the right panel **(B)**. For boundary conditions (BC) in the MODFLOW model, Lake Taupo is represented as a constant head (blue area), rivers/streams implemented as Cauchy head-dependant drain cells, and groundwater recharge is implemented in 10 zones as specified flux. The elevation of drain cells is shown in colour code from 357 m to 1249 m. For the MT3DMS model, the tritium input concentrations are assigned as recharge concentration. The stream gauging stations are shown by blue boxes.

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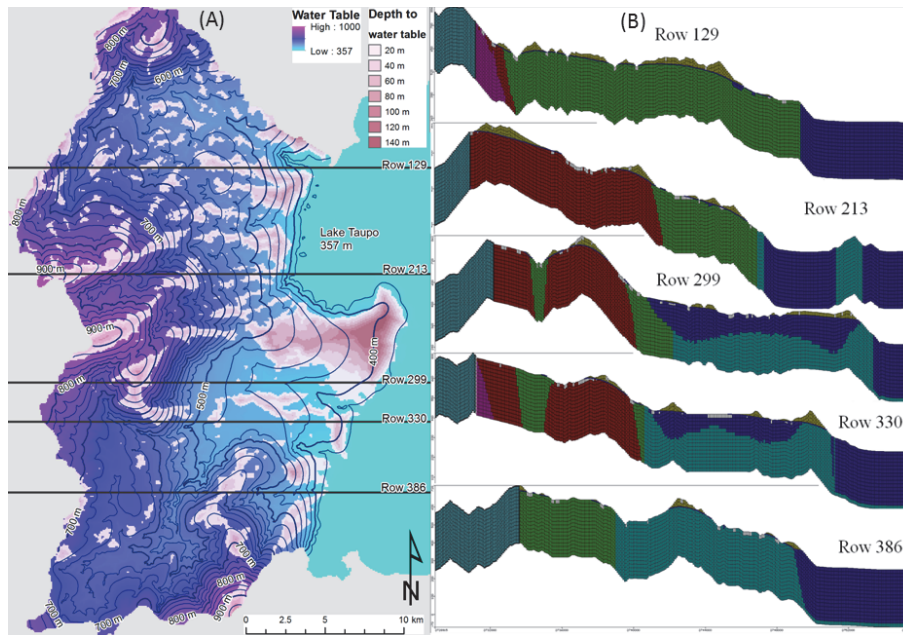


Fig. 2. Contour-fill map of modelled groundwater levels in plan view **(A)** and in cross-sections **(B)** along rows 129, 213, 299, 330 and 386. Modelled groundwater levels are shown by contour lines with 25 m contour interval and the colour code starting at 375 m (light blue at the shoreline) to 1000 m (pink at the mountain tops). Depth to groundwater is shown up to 140 m by areas of red colour. For the cross-sections, the drains are shown in light grey in layer 1. The groundwater table is shown by solid blue line and the dry cells are shown by dark yellow colour. The colour codes for the hydrogeologic units are described in Fig. 1. The cross sections are shown with 10 times vertical exaggeration.

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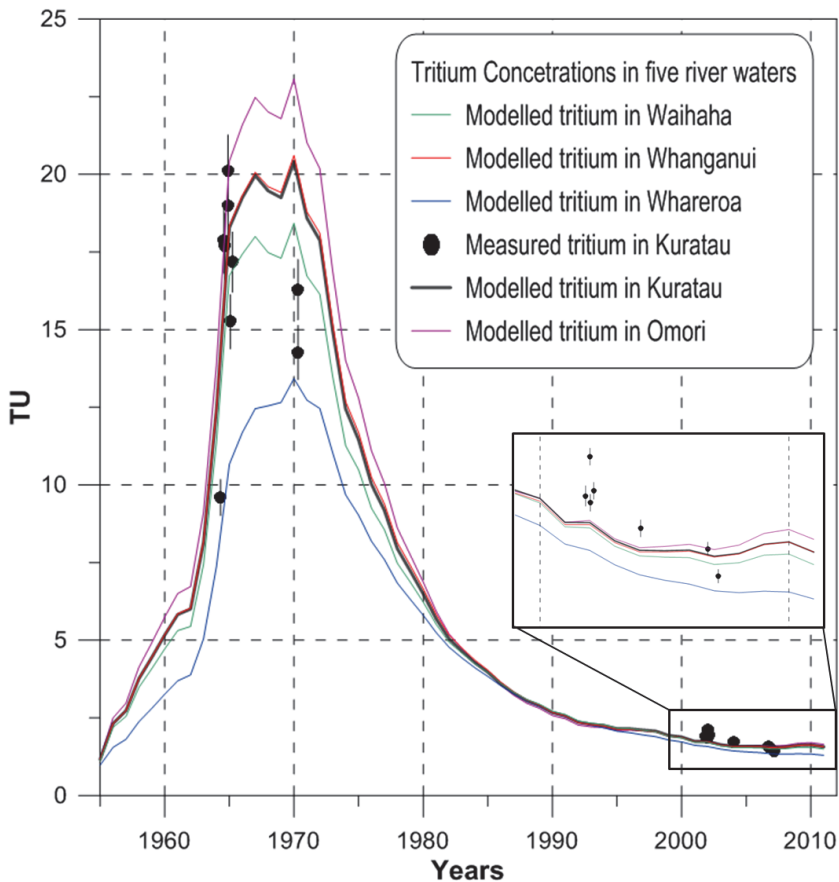


Fig. 3. Modelled tritium concentrations with the MT3DMS transport model for the Waihaha, Whanganui, Whareroa, Kuratau and Omori river catchments of the Western Lake Taupo catchment. Black dots are measured tritium concentrations in Kuratau river water and vertical lines are the one-sigma measurement errors (Morgenstern and Taylor, 2009).

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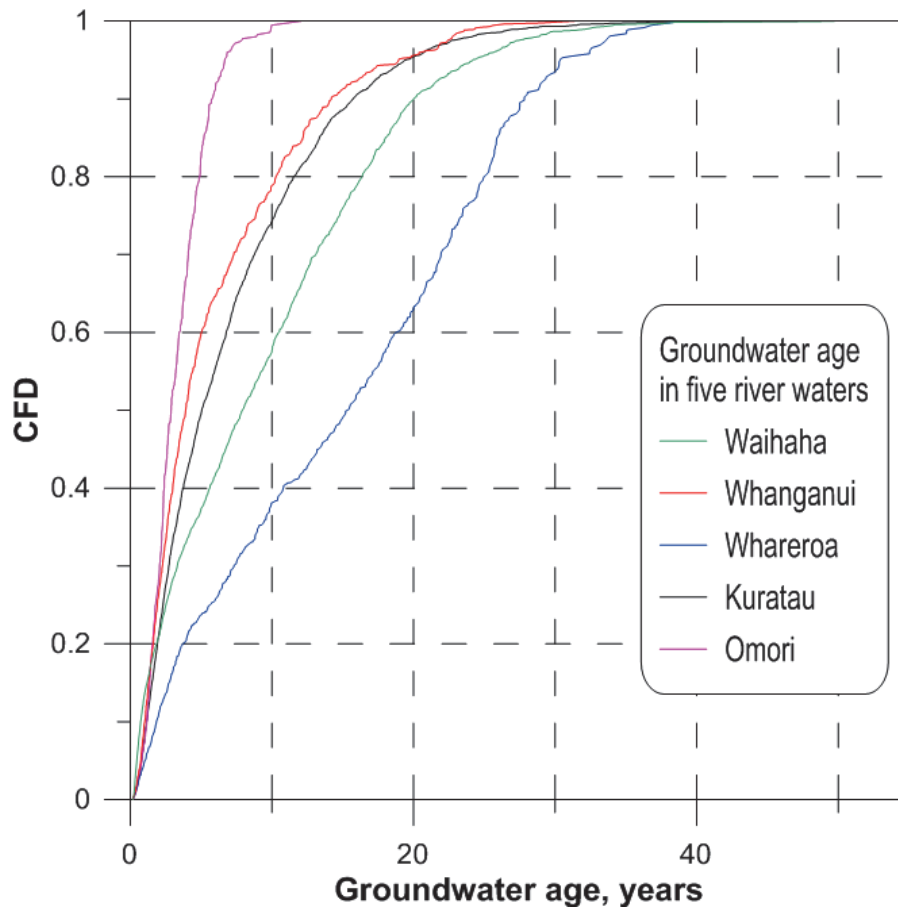


Fig. 4. Groundwater age distributions in river waters of the Waihaha, Whanganui, Whareroa, Kuratau and Omori catchments near their outflow into Lake Taupo.

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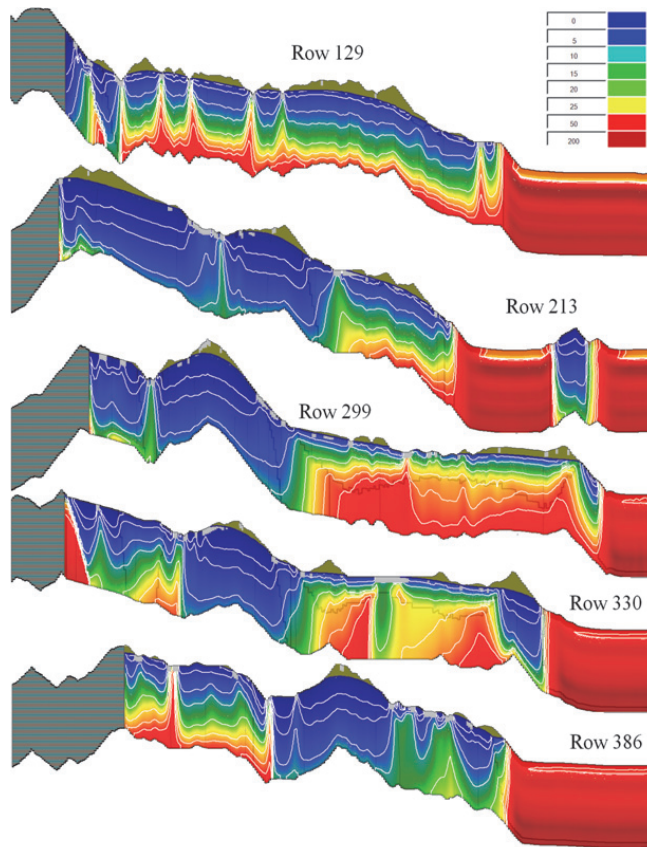


Fig. 5. Groundwater age in model cross-sections at rows 129, 213, 299, 330 and 386 obtained from the tritium-calibrated MT3DMS model. Groundwater age is indicated by 1, 2, 6, 10, 20, 30, 40 and 50 yr contour lines and by colour coding from 5 yr (dark blue) to > 50 yr (light red). The solid dark blue line indicates the boundaries of the hydrogeologic formations. On the top of the model, the light grey cells are drain cells in the layer 1 and dark yellow are dry cells.

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