
Deuterium composition and flow path analysis as additional calibration targets to calibrate groundwater flow simulation in a coastal wetlands system

D. A. Reynolds • S. Marimuthu

Abstract A conceptual model of the Lake Warden coastal wetlands system, Western Australia, was developed using hydraulic, chemical and stable isotopic data, and formed the basis for a groundwater flow model using the finite element numerical code (FEFLOW). The system to be modeled is complex. The surface water and groundwater within the wetlands system show varying salinity and isotopic composition over short distances and time frames. As a first step, the flow model was calibrated to observed groundwater levels measured since 2001 for both steady state and transient stresses. Particle tracking analysis was conducted to test the source areas of water discharging to the lakes within the wetlands system. The analysis was able to delineate the connectivity between the lakes in the wetland and the flow path. Enrichment of isotopic concentration is evident along a NE–SW transect and the data set provides a means for calibrating a detailed transport model. The study incorporates the varying deuterium composition of the water bodies directly into a transport model and a good match between observed and simulated temporal variations along the transect indicates that the model closely simulated the dynamics of water exchange between the lakes and groundwater within the system.

Résumé Un modèle conceptuel du système Lac Warden, marécage côtier situé dans l'Ouest de l'Australie, a été réalisé à partir de données hydrauliques et chimiques dont les isotopes stables. Il a été utilisé comme base pour un modèle d'écoulement souterrain, réalisé avec un code

numérique aux éléments finis (FEFLOW). Le système à modéliser est complexe. Dans le marécage, la salinité et la composition isotopique de l'eau de surface et de l'eau souterraine varient sur des distances et des pas de temps courts. Le modèle hydrogéologique a tout d'abord été calibré en régimes permanent et transitoire à partir des niveaux piézométriques mesurés depuis 2001. Un suivi de trajectoire de particules, réalisé pour vérifier les zones de décharge des eaux souterraines dans les lacs du système marécageux, a permis d'identifier les connexions entre les lacs et de tracer les trajectoires d'écoulement. Une augmentation de la concentration isotopique le long d'une coupe transversale NE–SW est évidente et les données constituent un support pour la calibration d'un modèle de transport détaillé. La variation de la composition en deutérium dans les hydrosystèmes est prise en compte dans l'étude et directement intégrée dans le modèle de transport. Une bonne adéquation entre les variations temporelles simulées et observées le long de la coupe transversale indique que la dynamique des échanges d'eau entre les lacs et l'eau souterraine dans ce système a été assez bien simulée par le modèle.

Resumen Se ha desarrollado un modelo conceptual del sistema de humedales costero del Lago Warden en el Occidente de Australia usando datos hidráulicos, químicos, y de isótopos estables el cual sirvió de base para un modelo de flujo de agua subterránea que usa el código numérico de elemento finito (FEFLOW). El sistema para el cual se elabora el modelo es complejo. El agua subterránea y superficial dentro del sistema de humedales muestra salinidad y composición isotópica variable en distancias y marcos de tiempo cortos. Como primer paso se calibró el modelo de flujo con niveles de agua subterránea medidos desde el año 2001 para regímenes permanentes y transitorios. Se llevó a cabo un análisis de búsqueda de partículas para evaluar las áreas fuente del agua que descarga a los lagos dentro del sistema de humedales. El análisis permitió delimitar la conectividad entre los lagos en el humedal y la trayectoria de flujo. El enriquecimiento de la concentración isotópica es evidente a lo largo de un levantamiento NE–SW y el grupo de datos aporta medios para calibrar un modelo detallado de transporte. El estudio incorpora la variación en composición de deuterio de los cuerpos de agua directamente en un modelo de transporte y una buena consistencia entre

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variaciones temporales, simuladas y observadas, a lo largo del levantamiento indican que el modelo simuló bastante bien la dinámica de intercambio de agua entre los lagos y el agua subterránea dentro del sistema.

Keywords Conceptual model · Groundwater flow · Coastal wetlands system · FEFLOW · Deuterium composition

Introduction

The dynamics of water exchange between surface water and groundwater within coastal wetlands is of central importance for the management of such systems. In general, most such systems are unique, and complex in their interactions. As an example, the individual water bodies within the Lake Warden coastal wetlands system in Esperance, Western Australia were measured for the chemical and isotopic composition for an annual cycle and show significantly varying salinity and isotopic composition (Table 1) over short distances (800 m) and time frames (150 h; Marimuthu et al. 2005).

A conceptual model of the Lake Warden coastal wetlands system was developed using hydraulic, chemical and stable isotopic data (Marimuthu et al. 2005), which was used as the basis for a groundwater flow model using the finite element numerical code (FEFLOW; Diersch 2002). The flow model was developed to identify the role of groundwater within the system, and to assist in the mitigation of the effects of non-seasonal floods which occur in the region. Additionally, the process of developing this model has allowed for the exploration of different calibration methods with an aim towards improving the calibration process.

As a general practice, flow models depend on interpolated hydraulic parameters, because data are normally limited by the availability of borehole data, which in turn are usually point measurements in time. For this reason, model calibration and prediction are usually associated with uncertainty in the measured and interpolated data. When models are complex and parameters are uncertain, the resulting model can be difficult or impossible to validate and the modeling process becomes an elaborate curve fitting exercise with little ability to shed light on dominant processes in the subsurface (Keating

Table 1 Chemical and isotopic composition of the water samples in Lake Warden wetlands system (Spring 2002) and monthly precipitation samples taken at the Bureau of Meteorology station, Esperance

	Cl (g/L)	$\delta^2\text{H}$ VSMOW	$\delta^{18}\text{O}$ ‰	Surface water samples	Cl (g/L)	$\delta^2\text{H}$ VSMOW	$\delta^{18}\text{O}$ ‰
Groundwater				Creeks			
4/93	0.3	-24	-5.3	Coramup downstream	2.2	-18	-3.7
25/97	0.2	-26	-5.7	Bandy downstream	3.64	-21	-4.3
E02	0.5	-22	-6	Bandy upstream	18.23	-7	-2
E14	0.5	-24	-5.1	Coramup upstream	3.36	-18	-3.9
E16	0.6	-25	-5.2	Bandy Creek harbour	8.3	10	0.6
E17	0.3	-28	-5.9	Lakes			
E19	1.4	-30	-6.2	Wheatfield	3.99	6	-0.6
E22	0.2	-28	-5.9	Station	12.73	29	3.4
E32	0.1	-26	-3.7	Mullet	15	28	3.3
E34	0.1	-25	-5	Ewans	7.57	11	0.9
E35b	83.6	-6	-2.5	Woody	4.2	16	1.5
E35c	82.0	-6	-2.5	Windabout	8.08	30	3.2
E36	0.3	-30	-5.8	Pink	242	25	2.7
E38a	0.2	-22	-4.7	Warden	41.22	33	1.8
E38b	5.2	-26	-5.1	Rainfall			
E40a	28.4	-17	-3.9	April 2002	0.01	-3	-6.7
E41	0.3	-25	-5.2	May	0.00	-4	-14.7
E42	0.5	-28	-5.6	June	0.03	-4	-13.7
E43	0.4	-27	-5.9	July	0.02	-6	-19.6
E44	0.2	-27	-5.9	August	0.02	-7	-27.1
E45a	6.0	-24	-5.7	September	0.02	-6	-23.8
E45b	15.8	-22	-5.3	October	0.01	-6	-19.2
E48	1.9	-22	-5.7	November	0.02	-5	-17.8
E49b	157.7	13	-2.3	December	0.01	-3	-1.8
E49c	91.5	2	-2.2	January 2003	0.02	-3	-1.3
E50	62.9	1	-2.5	February	0.02	-4	-9.4
E51	0.5	-23	-5.9	March	0.02	-4	-14.2
E52a	3.1	-23	-5.8	April	0.01	-6	-17.3
E53	16.8	-23	-5.6	May	0.01	-6	-28.7
E54b	13.4	17	0	June	0.01	-5	-19.3
E54c	51.3	-6	-3.4	July	0.01	-6	-16.7
E55	20.4	-10	-3.3	September	0.01	-6	-20.2
E56	25.8	5	-1.9	October	0.01	-4	-12.5
E57	20.0	1	-2.5	November	0.02	-4	-11.4
E58	0.1	-21	-6				

and Bahr 1998). The situation is exacerbated if model calibration targets such as head measurements are sparse.

A number of researchers have noted some improvement in groundwater model calibration by introducing environmental tracer and chemical data as a calibration target set in addition to hydraulic head. For example, ^{14}C has been utilized to improve groundwater flow model calibration in the Middle Rio Grande Basin (Sanford et al. 2004), a regional groundwater aquifer in semiarid-arid northeastern Arizona, USA (Zhu 2000) and in a compartmental model, to constrain a finite-difference regional groundwater flow model of the Otway Basin in South Australia (Harrington et al. 1999). Similarly, Portniaguine and Solomon (1998) utilized tritium and head data to parameterize an unconfined aquifer at Cape Cod Massachusetts (USA), Reilly et al. (1994) used chlorofluorocarbons (CFCs) and tritium in conjunction with flow and transport modelling for the analysis of a shallow groundwater system in Locust Grove, Maryland (USA), and Krabbenhoft et al. (1990) utilized stable isotopes to calibrate a three-dimensional solute transport model to constrain the groundwater-lake interaction in northern Wisconsin (USA). There are numerous examples of the utilization of major ion concentrations in model calibration (Anderman et al. 1996; Keating and Bahr 1998; Keidser and Rosbjerg 1991).

The majority of these studies either have been restricted to regional flow systems or very small-scale studies (Kim et al. 1999). In addition, the application of environmental tracers in numerical modeling has also been focused mainly on radioisotopes (Harrington et al. 1999; Reilly et al. 1994; Sanford et al. 2004) with limited studies using stable isotope methods. In one of the few published studies utilizing stable isotope methods, Krabbenhoft et al. (1990) considered only steady-state conditions in a single lake for the flow field, and modeled only a constant source strength (isotope concentration).

The field site considered in this study, Esperance, is transient in nature, with climatic variations causing the water levels and isotope concentrations to vary over the yearly cycle. The study differs from those previous studies because no applications of stable isotope methods as presented in this paper have been applied in a coastal wetlands environment of the complexity inherent in the Lake Warden system.

The spatial and temporal resolution of the data from the study site (Table 1) allows for a systematic study of the utility of stable isotopes as a supplementary calibration target (Marimuthu et al. 2005). The approach adopted in this study was to calibrate the numerical model through the utilization of traditional hydraulic data only (hydraulic head distributions), and then utilize the seasonal and weekly isotope data (deuterium) collected from the study area to discern what further improvements in calibration could be obtained. The isotopic concentration data were not used to estimate flow rates, but rather to infer quantities of a concentration front passing an observation location which can then be used to test the flow model. A good match between simulated and measured relative

concentrations of deuterium within the flow system would indicate a good match between the simulated and actual flow field. Using an iterative approach, both the flow and transport model will be calibrated until an accepted agreement between observed and simulated isotope concentration is reached.

Temporal and spatial variations of chemical and isotopic composition of a number of water bodies in Lake Warden wetlands system were investigated by seasonal sampling (April 2002–November 2003). A total of 32 groundwater samples from regional, wetland and coastal plain, as well as lake and creek sources were collected seasonally (Table 1 and Fig. 1). Rain samples were also collected during rainstorm events, and were cumulated on a weekly/monthly basis. In addition, lake samples were collected on a weekly basis between May 2002 and November 2003.

The objectives of this study have been to (1) calibrate the groundwater flow model of the system to the observed groundwater levels since 2001 for both steady state and transient stresses; (2) delineate the connectivity between the lakes and the flow path, by utilizing a particle tracking analysis to test the source areas of water discharging to the lakes within the wetlands system; (3) assess variations in stable isotopic concentrations (deuterium) and evaluate their utility as a calibration target in a complex environment by using the above transient flow model as basis for a transient solute transport model; (4) assess the impact of the utilization of stable isotopic methods on the predictive ability of the model.

Site description

The Lake Warden wetlands system is located approximately 600 km south east of Perth and near the coastal town of Esperance on the south coast of Western Australia. It comprises Pink Lake, Lake Warden, Windabout Lake, Woody Lake and Wheatfield Lake as well as Station Lake, Mullet Lake and Ewans Lake in the Bandy Creek watercourse (Fig. 1). The average annual rainfall is 623 mm, and mainly occurs during winter with some periodic high-density summer rainfall events as a result of thunderstorm or cyclonic derived activity (Bureau of Meteorology, Esperance, unpublished data, January 2004). The average annual potential evaporation is 1,600 mm, which is greatest during the summer months of January and February and lowest during the winter months of June and July.

The study area is mainly underlain by Proterozoic (basement) rocks of the highly deformed Albany-Fraser Orogen, which comprises granite, gneiss, quartzite and mafic rock, Werillup Formation, Pallinup Siltstone and Quaternary deposits (Morgan and Peers 1973; Myers 1995). The drill records from the bore installations within the Lake Warden wetlands showed that the depth to basement rock varies from 18 m at Pink Lake to 90 m to the east of Lake Ewans (Figs. 1 and 2). The upper portion of the basement rocks has been weathered to a variable thickness (4–10 m) of dense kaolinitic clay. Two bore-

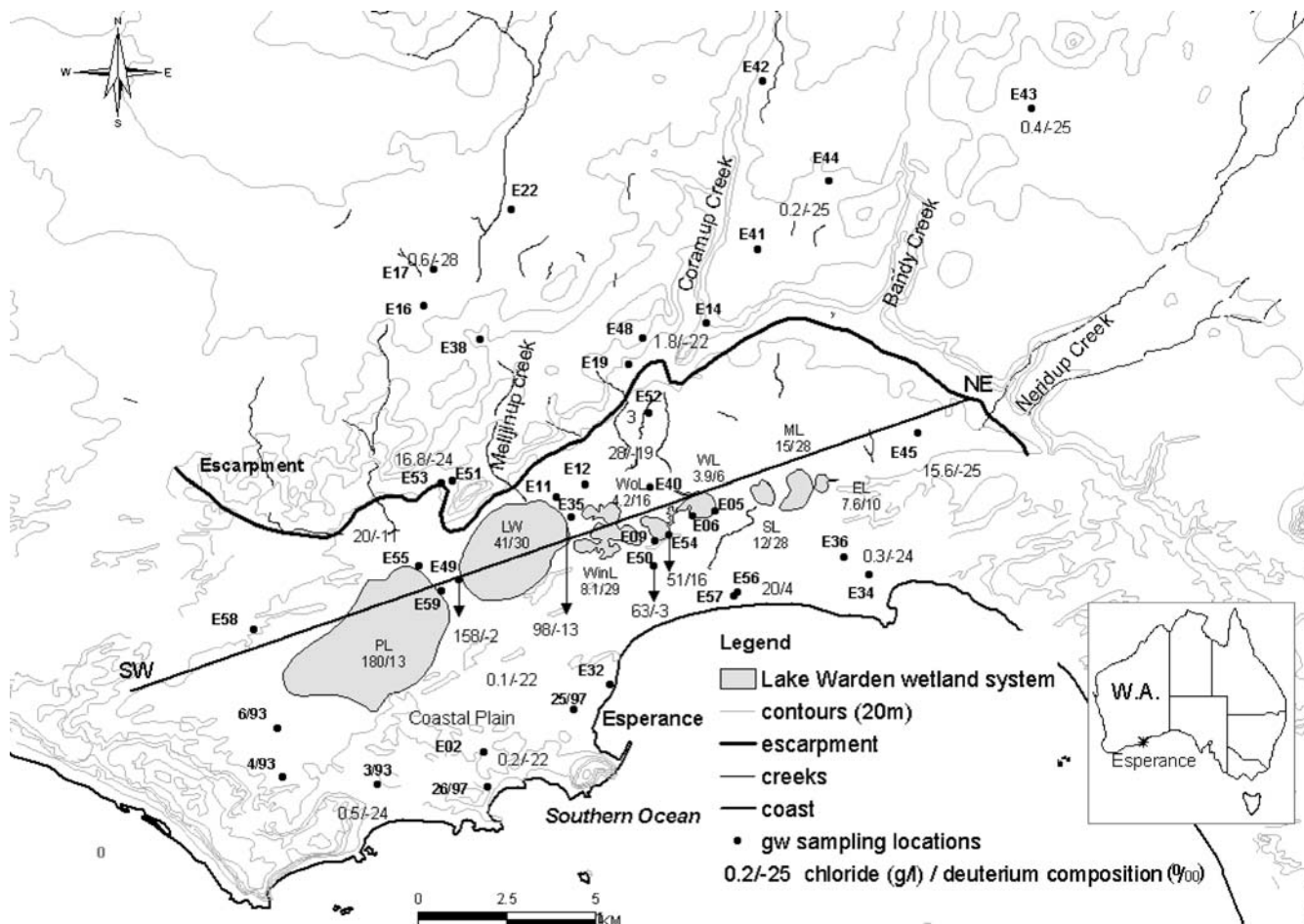


Fig. 1 Location map of Lake Warden wetlands system near Esperance, Western Australia (WA). PL Pink Lake; LW Lake Warden; WinL Windabout Lake; WoL Woody Lake; WL Wheatfield Lake; SL Station Lake; ML Mullet Lake; EL Ewans Lake. Multiple samples were collected at E35, E38, E45, E49 and E54. The chloride and deuterium composition of all the water bodies represents Spring 2002 sampling. The transect SW–NE is also located (see Fig. 2)

holes (E19 and E53) which intersected the weathered basement rock in the escarpment region are under sub-artesian pressure. The escarpment, up to 40 m above Australian Height Datum (aHD), marks the inland extent of the coastal plain where it merges with the inland sandplain.

The Werillup Formation consists of predominantly fluvial and lacustrine sediments with fine to coarse grained quartz sand overlain by clay and lignite deposited as a basal unit and thick layers of this unit were found underlying Woody, Wheatfield, Station, Mullet and Ewans lakes with the thickness generally decreasing towards Windabout Lake (Fig. 2). Borehole E45b (drilled in the Werillup Formation, 3 km NE of Ewans Lake) was under artesian pressure (wellhead 6.7 m with respect to Australian Height Datum). Measured hydraulic conductivities for the Werillup Formation fell in a narrow range from 6 to 10 m day⁻¹.

The Pallinup Siltstone (a transitional silty sandstone layer) is an extensive unit overlying either basement rock or the Werillup Formation. It was deposited in a shallow-marine environment during a major marine transgression in the late Eocene. The unit consists of multicoloured

siltstone to fine-grained clayey sandstone with minor glauconite, spongolite and various marine fossils. A fossiliferous unit within the Pallinup Siltstone comprising coral, bivalves and siliceous spicule limestone was intersected by bores E54 and E45 in the study area (Figs. 1 and 2), and is known as the “spongolite facies” (Myers 1985). Results from the drilling program indicated that the siltstone facies of the Pallinup Siltstone exists predominantly beneath Lake Warden and Pink Lake, and is characterized by low permeability due to its fine-grained lithology and cementation. The measured hydraulic conductivity ranged from 0.1 to 0.5 m day⁻¹. The highly permeable shoreline and spongolite facies of the Pallinup Siltstone were found to be laterally extensive to the east of Lake Warden (Windabout to Ewans lakes) and tended to overlay a carbaceous clay aquitard, which acts as a confining layer on the underlying sands of the Werillup Formation. These facies are characterized by medium permeability fine grained quartz sand and fossiliferous units, with measured hydraulic conductivities ranging from 1 to 5 m day⁻¹.

Quaternary coastal sediments form a cover over the basement and Tertiary rocks. The thickest of these sedi-

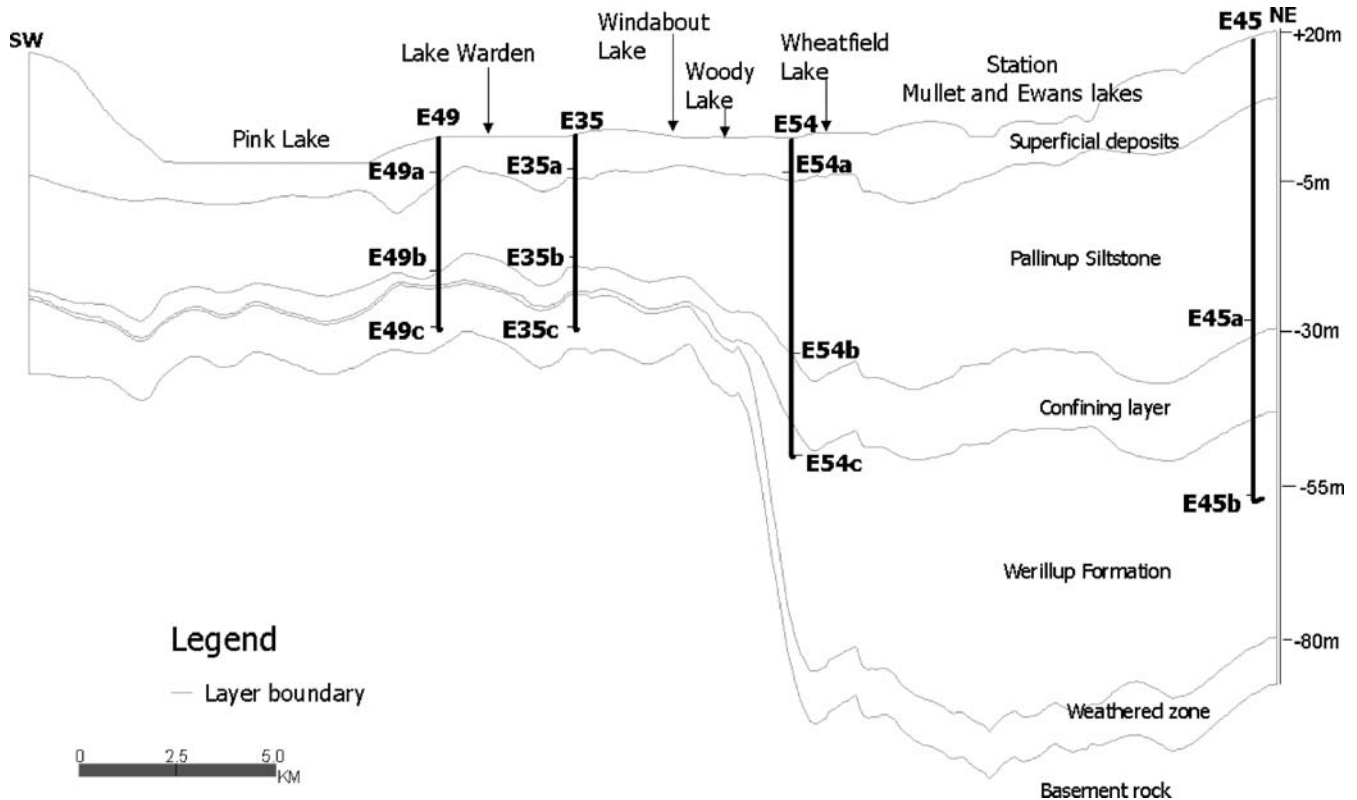


Fig. 2 Cross section of lithostratigraphic units along NE–SW transect of the Lake Warden wetlands system. Note: The confining layer is part of the Werillup Formation. Elevation in m AHD. Refer to Fig. 1 for the transect location

ments are found on the coastal plain, which form prominent sand dunes to the south of the lake system. The coastal plain is comprised of large ridges of dune sand and interbeds of thin sandy limestone and siltstone. The thickness of the Quaternary sediments is generally 20–30 m, but is more than 50 m thick in some locations (Baddock 1997).

Groundwater flow model

The numerical representation of the system was undertaken using the three-dimensional finite element modelling package, FEFLOW (Diersch 2002), which uses a Galerkin-based finite element method to solve the partial differential equations. The background map of the Lake Warden wetlands system (Fig. 1) was used as the template for the mesh creation process. The mesh was constructed using triangular planar elements with angles satisfying the Delauney criteria, which assists numerical stability by

attempting to reduce the number of obtuse triangles within the mesh. The model incorporates all the known significant features that are thought to be able to affect groundwater flow to and from the source area such as creeks, lakes, a 40-m-high spatially continuous escarpment and the coastal boundaries. The eastern side of the mesh extends along Neridup Creek, and the western side of the mesh extends far enough from Pink Lake such that the boundary does not affect the simulation results. The northern side of the mesh was chosen based on stable hydrologic boundaries. The northern boundary is intended to extend to the escarpment, but since the escarpment is quite close to the lakes system, the mesh was extended further north mirroring the shape of the escarpment (i.e. far enough from the escarpment such that the conditions imposed on this boundary do not significantly alter simulation results). The southern side of the mesh is represented along the coastline. The model mesh consisted of 203,205 nodes and 123,516 elements, composed of six ‘slices’ and five layers (layers 1–5, see Table 2). Slices are

Table 2 Summary of three-dimensional model setup

Layer	Aquifer/unit	Maximum thickness (m)	Minimum thickness (m)	Hydraulic conductivity (m/sec)
1	Superficial	45	2.0	$(0.23\text{--}2.31)\times 10^{-4}$
2	Pallinup Siltstone	38.5	1.0	$(0.09\text{--}1.15)\times 10^{-4}$
3	Confining layer	9.5	0.3	$(0.0005)\times 10^{-4}$
4	Werillup Formation	33	0.1	$(0.92\text{--}1.34)\times 10^{-4}$
5	Weathered zone	10	4	$(0.05\text{--}0.5)\times 10^{-4}$

regarded as the top or bottom planes of the (geological) layers. The five layers represent the lithostratigraphy of the study area and the depth and thickness of each layer were derived from the drilling logs and an electromagnetic survey (Street and Abbott 2004), and contoured using Ordinary Kriging.

Boundary conditions imposed along the borders of the model vary between a specified head condition and a “no-flow” condition (Fig. 3), given that the groundwater level contour map (Fig. 4a) shows that the regional flow is principally north-south and the localized flow is NE–SW (within the lake system; Fig. 4b). Specified head conditions were thus imposed along the northern and southern borders of the mesh while no-flow conditions were imposed along the eastern and western borders. The distribution of specified heads along the northern border was estimated based on topography and groundwater level measurements collected during the seasonal sampling. The coastal-discharge boundary corresponds to the annual mean tidal data at Esperance (Department of Planning and Infrastructure; DPI 2004). The outflow to the coastal-discharge boundary was constrained to the layers 1 and 2 by imposing on layers 3, 4 and 5 a no-flow boundary condition.

Lakes within the model domain are mainly flow-through lakes with the exception of Pink Lake. They were

Fig. 4 **a** Observed hydraulic head of Lake Warden wetlands system. The groundwater level contour map is derived using limited data, and is relative to Australian Height Datum. Contour intervals vary between 0.5, 2 and 10 m. Arrows denote groundwater flow and other symbols are the same as described in Fig. 1. **b** SW–NE transect of hydraulic head elevations in the Lake Warden wetlands system (density corrected). AHD Australian Height Datum. Refer to Fig. 1 for transect location and symbols

simulated through the use of a transfer boundary condition (Cauchy boundary, see Fig. 3), which is based on a reference hydraulic head outside the model domain (Diersch 2002):

$$q_{nh}(x_i, t) = -\phi_h(h_2^R - h) \quad (1)$$

Where q_{nh} represents normal Darcy flux of fluid ($L T^{-1}$; length per time), ϕ_h a transfer coefficient (dual directional; T^{-1}), h_2^R is the reference hydraulic head (L) and h is the hydraulic head (L) at the node adjacent to the boundary portion. The minimum lake level for the period of 2002 and 2003 has been assigned as the reference head for initial steady-state simulations.

Creeks were also simulated using the Cauchy boundary condition; however, the creek bottom elevation was assigned as the reference hydraulic head to allow for free

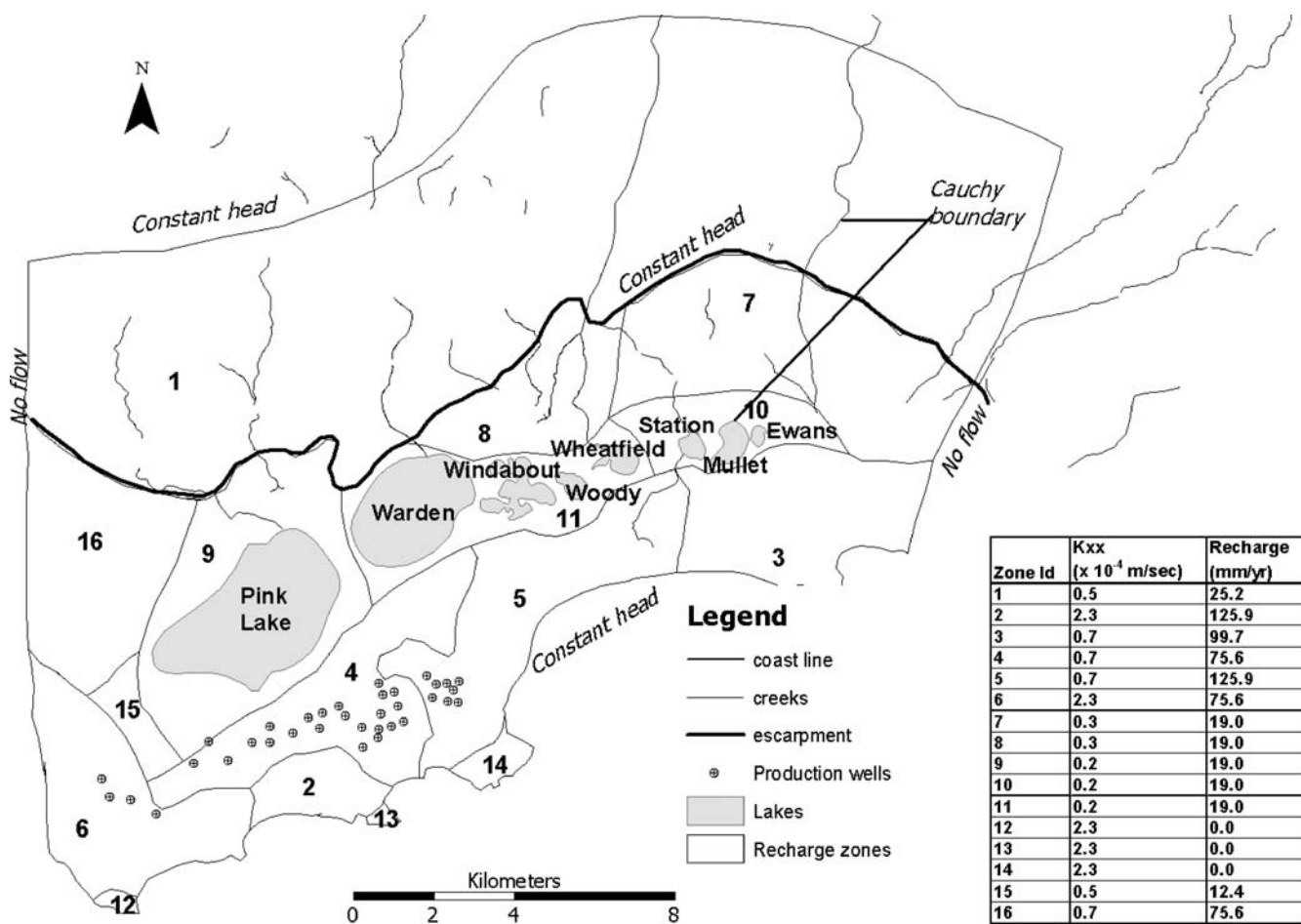
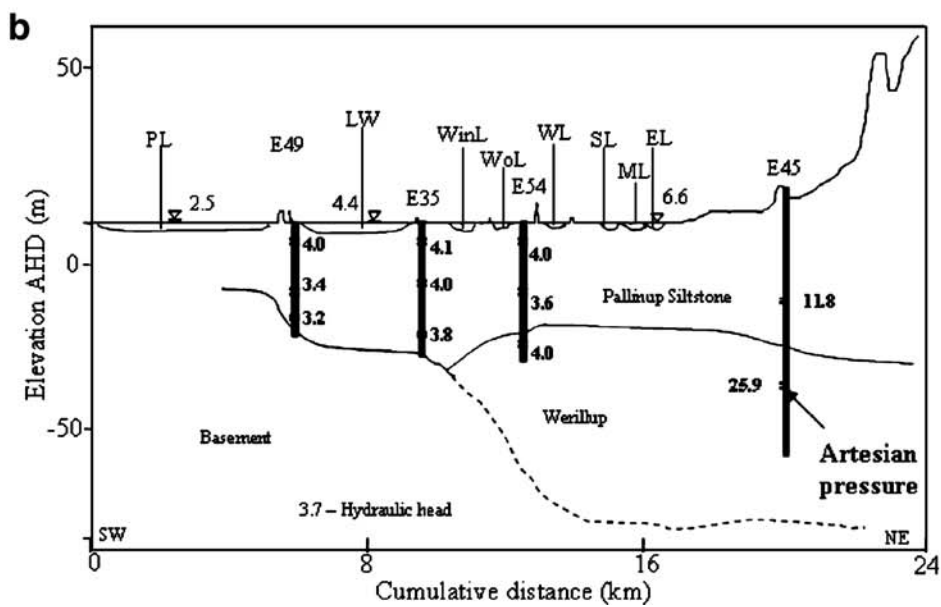
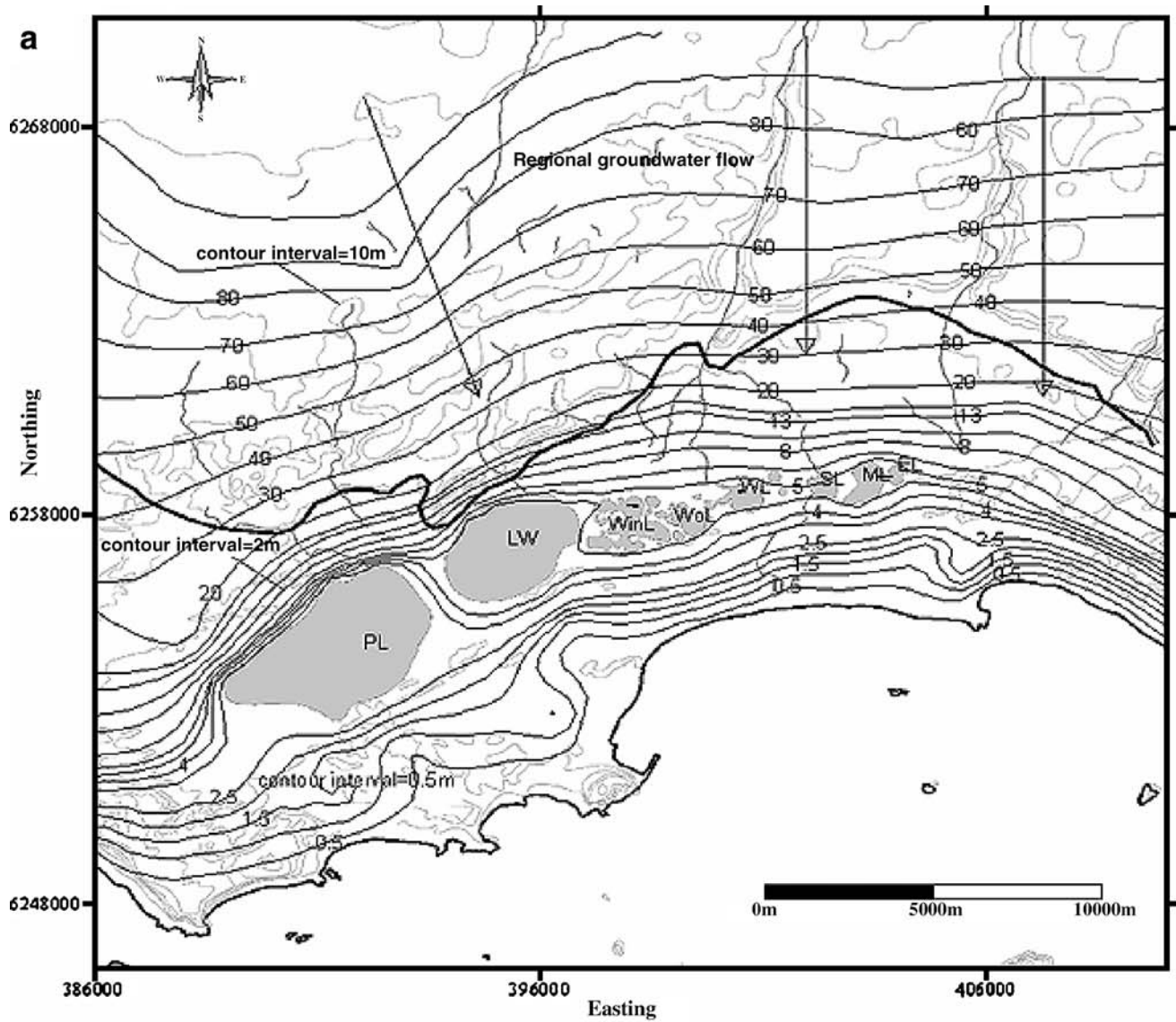


Fig. 3 Rainfall recharge zones for layer 1 (superficial deposits) and model boundary conditions. Kxx horizontal hydraulic conductivity



exit into the surface feature. This boundary condition allows simulated creeks to both receive water from the aquifer (gaining conditions) and to contribute water to the aquifer (losing conditions). The escarpment was represented as a seepage zone, utilizing a Dirichlet-type boundary condition $h=z$ (elevation) combined with a constraint condition of maximum flux=0 to ensure a free outflow of water from the model, but no inflow. Boreholes E19 and E53 in the escarpment region agreed with the above condition (i.e. groundwater level is at the same elevation as the surface elevation).

The hydraulic properties for the system were determined from previous aquifer test analyses (Baddock 1998), lithologic data, and slug tests (Table 2). Drilling logs within the wetlands system correlate poorly and indicate that the lateral and vertical extent of the layers is highly variable. Therefore, rather than discretize the aquifer into many arbitrary areas of varying horizontal hydraulic conductivity (K_h), layer 1 was subdivided into 16 zones (Fig. 3). The zones were chosen on the basis of soil type and pumping tests conducted within the coastal plain (Baddock 1998), and slug tests within the wetlands system. The geometric mean of the values within each zone was used as model input for K_h . For the other layers, the inverse distance weighting interpolation scheme was adopted to regionalize the limited measured K_h values. The interpolation was cross checked with the geology of

the study area and it was determined that K_h values were consistent with the geology. The vertical hydraulic conductivity was not measured in the field, however, as the study area represents a sequence of alternating strata of sand, silt and clay deposits, the vertical hydraulic conductivity (K_v) is expected to be significantly lower than the horizontal hydraulic conductivity (Zheng and Bennett 2002). Six different anisotropy ratios (K_h/K_v) were tested in the model calibration (Table 3).

Rainfall is the principal source of groundwater recharge in the study area (Baddock 1998). A study performed on the coastal plain indicated that rainfall recharge ranged from 5 to 30% of annual rainfall (Baddock 1998). Recharge varies considerably due to differences in soil type, topography and relief. The distribution of recharge zones in the study area were categorized based on areas with a shallow water table, vegetation cover, built-up areas and dunes. The chloride mass balance approach (Eq. 2; Wood and Sanford 1995) was adopted to estimate the groundwater recharge for the study area and used along with the results from Baddock (1998). The recharge value incorporated in the model for each zone is shown in Fig. 3 with maximum recharge occurring in the coastal plain.

$$q = (P)(Cl_{\text{wap}})/Cl_{\text{gw}} \quad (2)$$

Table 3 Calibration results of observed and modeled anisotropy ratio (K_h/K_v) for selected groundwater observation points representing the different lithologic layers

K_h/K_v	Bore ID	Observed head (m AHD)	1 Model (m AHD)	2 Model (m AHD)	3 Model (m AHD)	10 Model (m AHD)	X ^a Model (m AHD)
Layer 1 coastal plain	3/93	2	1.8	1.8	1.8	1.8	1.8
	4/93	3.3	3.8	3.8	3.7	3.9	3.9
	25/97	1.8	1.8	1.8	1.8	1.8	1.8
	26/97	0.5	0.9	0.9	0.9	0.9	0.9
Layer1 wetlands system	E05	4.1	4.3	4.3	4.3	4.6	4.6
	E06	3.8	4	4	4	4.2	4.2
	E09	4.1	3.8	3.9	3.9	4	4
	E11	5	6.3	6.3	6.3	6.4	6.3
	E12	5.4	7.4	7.4	7.4	7.4	7.4
	E35a	4.2	4.2	4.2	4.2	4.3	4.2
	E40a	5.4	5.9	6	6	6.3	6.3
	E49a	4	3.6	3.6	3.6	3.6	3.6
	E52a	15	14.3	14.4	14.3	14.4	14.4
	E54a	4.2	3.9	4	4	4.2	4.1
Layer 2	E35b	4	4.2	4.2	4.2	4.3	4.2
	E40b	5.5	5.4	5.4	5.4	5.7	5.7
	E45a	15	15.9	16.1	16.1	16	16
	E48	43.4	40.1	40.3	40.3	40.9	40.8
	E49b	3.4	3.6	3.6	3.6	3.6	3.6
	E52b	15.3	14.4	14.5	14.4	14.5	14.5
	E54b	3.6	3.9	3.9	3.9	4.1	4.1
	E45b	23.4	16.5	17.7	17.7	23.6	23.6
Layer 4	E50	3.7	3.4	3.5	3.5	3.9	3.9
	E54c	4.2	3.8	3.9	3.9	4.4	4.4
Layer 5	E35c	3.7	4.2	4.2	4.2	4.3	4.2
	E49c	3.9	3.6	3.6	3.6	3.6	3.6
	E53	25.1	24.9	25	25	25.1	25
	E55	3.9	5	5.1	5.1	5.2	5.1

^a Denotes varying K_h/K_v values that were used in the different lithologic layers for a single simulation and the assigned values are as follows: layers 1 and 2=2, layers 3 and 4=10; layer 5=3

Where q is the recharge rate (mm yr^{-1}), P is average annual precipitation (mm), Cl_{wap} is the weight-average chloride concentration in precipitation (mg L^{-1}), Cl_{gw} is the average chloride concentration in groundwater (mg L^{-1}).

There are uncertainties in the recharge estimates within the wetlands system because the water bodies within the system (zones 7, 8, 9, 10 and 11) exhibit varying chloride concentrations (Table 1 and Fig. 1) and the estimated recharge may not reflect the true recharge rate. However, the chloride mass balance approach provides estimates of a range of recharge values which can be verified in the model calibration. The recharge rate within urbanized areas (zones 4 and 5 see Fig. 3) is significantly higher, which may reflect losses from the municipal water supply and infiltration from storm sewers.

The groundwater within the study area is abstracted for domestic and town supply. Local water authority wells which supply water to the town of Esperance are located in the south west of the study area. A total of 31 pumping wells from this area are incorporated in the model, with the pumping rates ranging from 0 to $769 \text{ m}^3 \text{ day}^{-1}$. The domestic wells (powered by wind mills) to the north of the study area are mainly for local consumption and none of these wells are metered. The abstraction is expected to be minimal and therefore will not have a large impact on the simulation results.

Steady-state model calibration

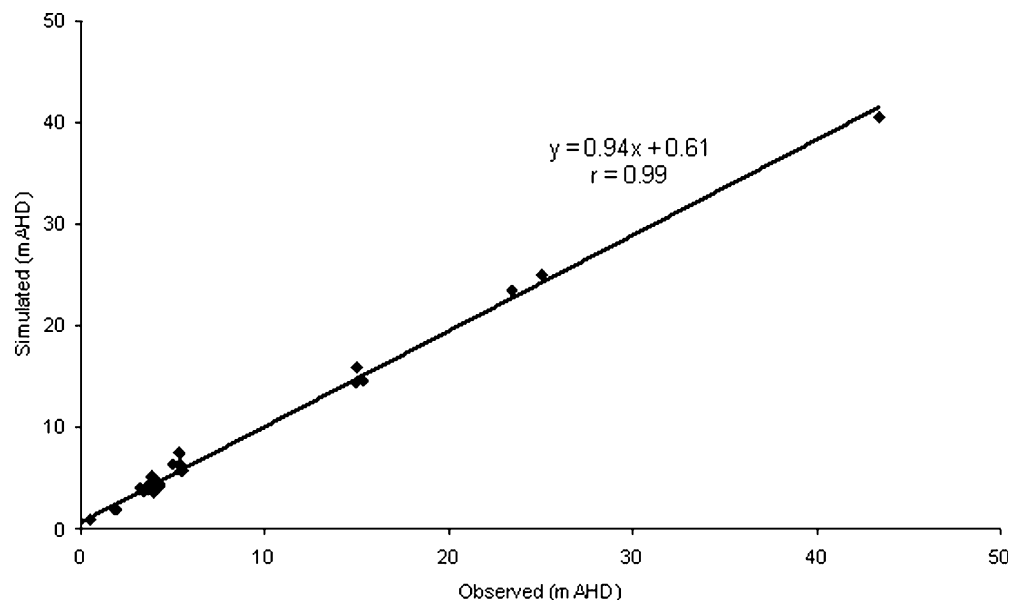
The steady-state model calibration was carried out to minimize the difference between the simulated and observed groundwater levels of the 28 bores distributed over the study area. The groundwater levels have only been monitored since 2001 and due to this fact, it was not possible to establish a good time-averaged field measurement to justify the steady-state condition for the area. The water levels measured in summer (2001) were used as a

basis to represent the observed groundwater levels. Additionally, this period also corresponds to the beginning of the groundwater level monitoring. Model calibration was done by a trial-and error process during which initial estimates of model parameters were adjusted until a satisfactory match between observed and simulated groundwater level was achieved. Among the input parameters, the hydraulic conductivity values are one of the most poorly constrained due to limited aquifer analyses carried out in this area. The analysis of lithological variations of the old drill records and the recent drill program within the wetlands system (Marimuthu et al. 2005), indicates that the hydraulic conductivity values can be varied up to 10% of the field values for all the layers during model calibration to get a good match of the simulated and observed groundwater levels (Fig. 5). Storage parameters are not modified during steady-state calibration as the storage properties of the aquifer are forced to zero at steady state.

The anisotropy ratio of hydraulic conductivity (K_h/K_v) was initially set to 1 and several sensitivity simulations were conducted to determine the optimal value for the system. The simulations indicate that changing the anisotropy ratio has no significant change in regards to the agreement between the simulation and observed values in layer 1; however, some differences have been observed in the other layers (Table 3).

The transfer coefficients for the Cauchy boundary conditions for the lakes and creeks are also unknown, and are very difficult to parameterize even with extensive field investigations. They were estimated based on the $\left(\phi_h^{\text{in}} = \frac{K^{\text{in}}}{d}\right)$ where d and K^{in} are the estimated thickness (L) and hydraulic conductivity ($L T^{-1}$) values of the lake and creek-bed sediments respectively. The thickness and hydraulic conductivity of lake-bed sediments were estimated from lake-bed cores obtained from another investigation (Wilson 2003), and are in the range of 0.15 to 0.3 m thick

Fig. 5 Comparison of simulated and observed groundwater level (m AHD) under steady-state calibration



and 4×10^{-3} to 9×10^{-3} m/sec, respectively. The transfer coefficients were varied between 1×10^{-6} to 100×10^{-6} m/sec during the calibration process to estimate the optimal value. The groundwater flow values from each simulation were calibrated with the water balance of the lake:

$$\frac{dV}{dt} = G_i + P + S_i - G_o - E = 0 \quad (3)$$

Where G_i and S_i are groundwater flow and surface runoff rates ($L^3 T^{-1}$), respectively, G_o is the groundwater outflow rate ($L^3 T^{-1}$), P and E are the precipitation and evaporation rates ($L^3 T^{-1}$) respectively (Bureau of Meteorology, Esperance), V is the volume of water in the lake (L^3), and t is the time. G_i and G_o are determined through the budget analyzer of the flow model and the evaporation rate from the lake is assumed equal to $0.7 \times$ evaporation rate (Penman 1948). The surface runoff rates were obtained from the stream gauges (Coramup and Bandy creeks).

There is a reasonably good match between the simulated and observed heads in most of the boreholes of the study area (Table 4). The overall root mean square (RMS) error was 0.85 m and the correlation coefficient between the simulated and measured water levels was 0.99 (Fig. 5). Errors are generally spread across the model area, although there are some areas with consistently

higher simulated water levels (i.e. E11, E12, E40a and E55), the largest difference being 2.88 m. These differences are likely due to site-specific factors such as local variations in hydraulic conductivity and local recharge effects. Due to their unknown characteristics or to limited model resolution, these local heterogeneities could not be incorporated into the model.

Overall, the steady state model succeeds in capturing the observed groundwater levels within a reasonable range; however, the steady state model only represents stresses at a dynamic equilibrium condition. To observe changes in hydraulic head with time for the field conditions being modeled the steady state model simulation may be inadequate. Hence, a transient model was used to determine the general effects of time-varying hydraulic properties (i.e. recharge and pumping) on groundwater-flow patterns in the aquifer and how these effects may vary within different areas of the aquifer. Model parameterization drawn from the steady state was used for the transient model.

Transient model calibration

The same model domain, boundary condition type, and aquifer properties represented in the steady-state model were used for the calibration of the transient model. The

Table 4 Calibration of observed and simulated groundwater levels

	Bore ID	Easting	Northing	Observed head (m AHD)	Modeled head (m AHD)	Difference (m)	Square difference
Layer 1	3/93	391526	6250551	1.95	1.84	0.11	0.01
Layer 1	4/93	388864	6250747	3.25	3.94	-0.69	0.47
Layer 1	25/97	397029	6252674	1.82	1.83	-0.01	0.00
Layer 1	26/97	394619	6250483	0.53	0.89	-0.36	0.13
Layer 1	E05	400997	6258222	4.12	4.47	-0.35	0.12
Layer 1	E06	400392	6258281	3.78	4.14	-0.37	0.14
Layer 1	E09	399457	6257573	4.13	3.94	0.19	0.04
Layer 1	E11	396531	6258639	5.00	6.32	-1.31	1.72
Layer 1	E12	397359	6258987	5.36	7.44	-2.08	4.34
Layer 1	E35a	397100	6258221	4.23	4.22	0.01	0.00
Layer 1	E40a	399311	6259068	5.39	6.25	-0.87	0.75
Layer 1	E49a	393835	6256485	3.98	3.62	0.37	0.14
Layer 1	E52a	399145	6260968	14.98	14.38	0.59	0.35
Layer 1	E54a	399832	6257716	4.23	4.09	0.14	0.02
Layer 2	E35b	396965	6258066	4.03	4.22	-0.20	0.04
Layer 2	E40b	399176	6258913	5.49	5.67	-0.19	0.04
Layer 2	E45a	406686	6260413	15.00	15.82	-0.82	0.68
Layer 2	E48	398949	6263074	43.38	40.80	2.88	8.28
Layer 2	E49b	393787	6256304	3.41	3.61	-0.20	0.04
Layer 2	E52b	399145	6260968	15.33	14.48	0.84	0.71
Layer 2	E54b	399697	6257561	3.62	4.01	-0.39	0.15
Layer 4	E45b	406688	6260406	23.40	23.42	-0.02	0.00
Layer 4	E50	399285	6256706	3.69	3.87	-0.19	0.04
Layer 4	E54c	399697	6257561	4.24	4.35	-0.11	0.01
Layer 5	E35c	396965	6258065	3.67	4.22	-0.55	0.31
Layer 5	E49c	393787	6256306	3.89	3.61	0.28	0.08
Layer 5	E53	393302	6259011	25.08	24.97	0.11	0.01
Layer 5	E55	392799	6256857	3.86	5.07	-1.21	1.46
						RMS error	0.85
						Mean	-0.14
						Variance	0.43
						SD	0.65

SD standard deviation

model was simulated in transient conditions for a time interval of 3 years over the period 2001 to 2003. The monthly recharge rate was calculated as the percentage of the annual recharge rate based on monthly precipitation. The recharge rates were varied within 10–20% of the estimated values and more weight is given to winter precipitation. This range is thought reasonable due to uncertainties in the estimation of recharge within the wetlands system. Additional support is provided by the stable isotope analysis within this region indicating that groundwater is mainly recharged by winter precipitation (Marimuthu et al. 2005).

A specific yield of 0.02 was estimated from soil tests performed within the wetlands system (zones 1, 7, 8, 9, 10, 11, 15 and 16, see Fig. 3). For other zones, an estimated value of 0.2 was assigned to layer 1 (Baddock 1998). During the calibration process, the value of specific yield was allowed to vary by up to 10% to encompass variability due to geologic heterogeneity that was not captured in the slug test analysis. A uniform storage coefficient of 0.0002 was assigned to the layers underlying layer 1. It was determined that the model was comparatively less sensitive to specific storage in the deeper layers. The averaged monthly lake levels for the period 2001 to 2003 were used as the reference hydraulic head for the time-dependent lake-transfer boundary conditions. The hydraulic head predictions that resulted from the steady-state model were used as the initial condition for each transient simulation.

The calibration was carried out to reproduce the observed hydraulic heads for the period 2001 to 2003 (Fig. 6). The trial and error process by which calibration of the transient model was achieved included 50 trials until a good match was achieved between simulated and observed heads over space and time. Model parameters were refined during the calibration of the model by varying both the storage property and in some instances the hydraulic conductivity. If during transient calibration the hydraulic conductivity required modification, the steady-state model was re-run using the revised hydraulic conductivity. The revised hydraulic head predictions that resulted from re-running the steady state model were then used as the initial condition for further transient calibrations.

The model effectively reproduces the general temporal trends in hydraulic heads as seen in the observed hydrographs (Fig. 6); however, in some areas, the modeled hydraulic head is higher than the observed (i.e. E 40a, E11 and E55). The goodness of fit of the transient simulations and observed monthly water levels was examined using the root-mean-squared residual errors (RMS). The results ranged from 0.12 to 2.92 m. The comparison between observed and simulated heads indicates that the transient model represents general hydrologic conditions observed in the field and was considered to be calibrated satisfactorily (Fig. 7). The simulated flow pattern (as deduced from hydraulic head contour plots) of the calibrated steady state and transient flow models are similar to the observed flow pattern with the exception of a groundwater mound

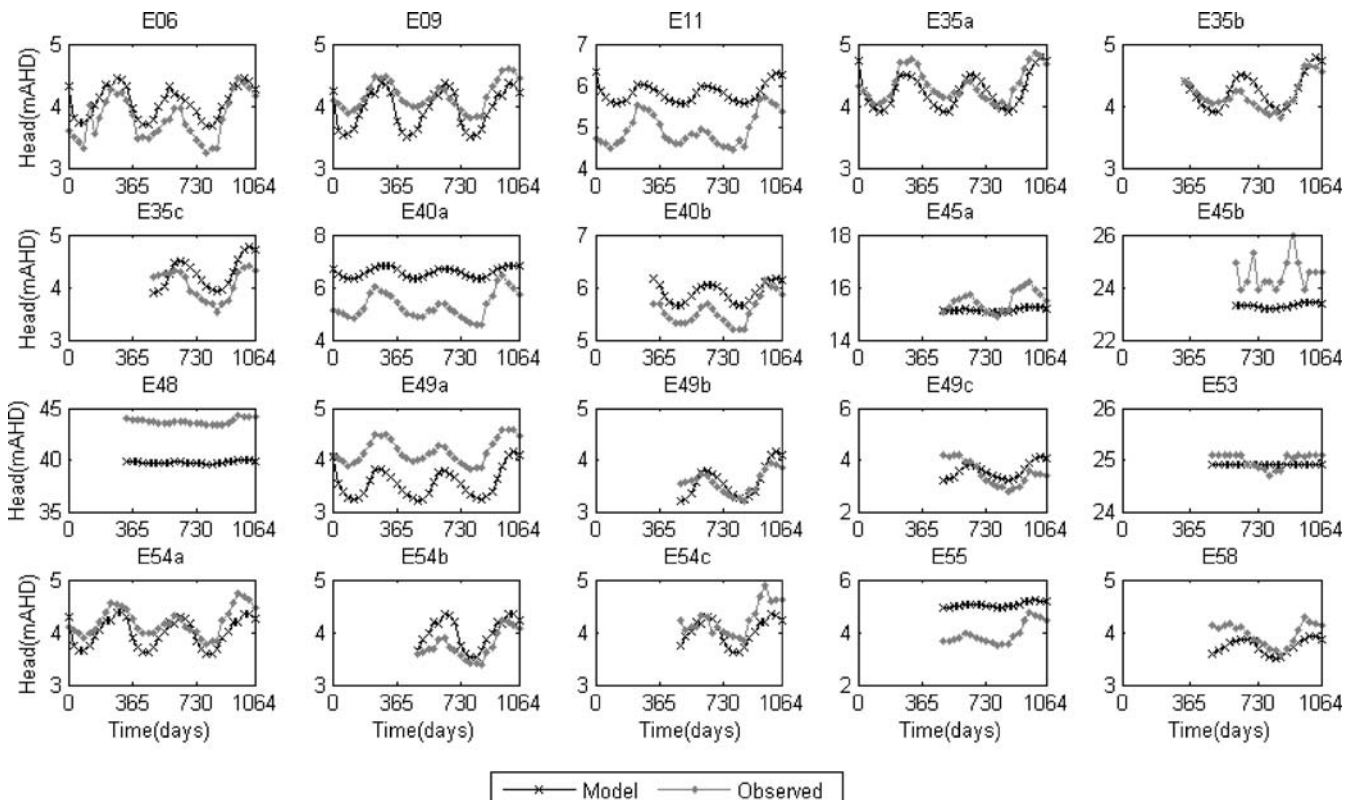
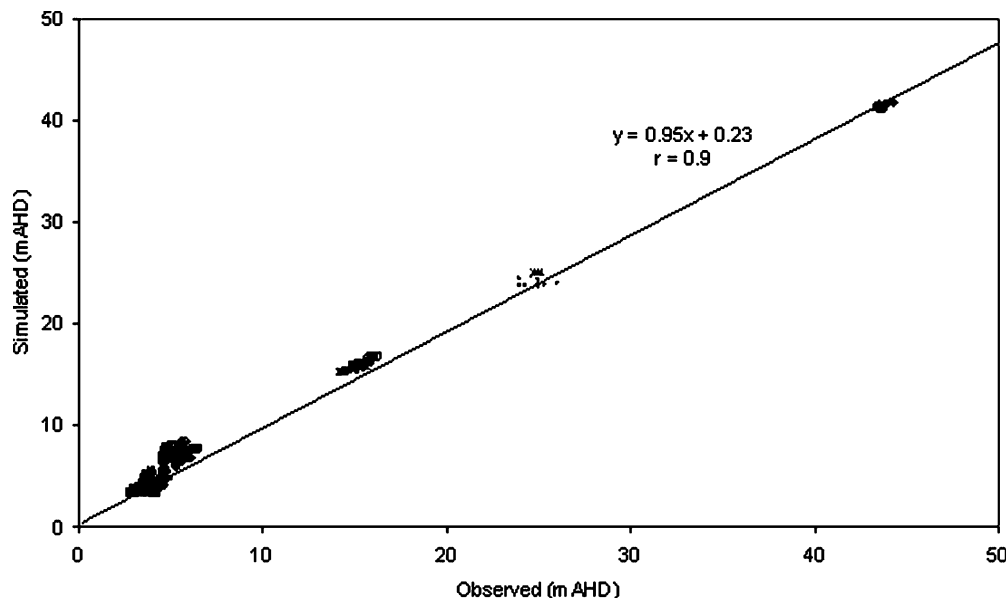


Fig. 6 Simulated and observed monthly groundwater level (m AHD) under transient calibration. The model was simulated for a time interval of 3 years over the period January 2001 to December 2003

Fig. 7 Comparison of simulated and observed groundwater levels (m AHD) under transient simulation



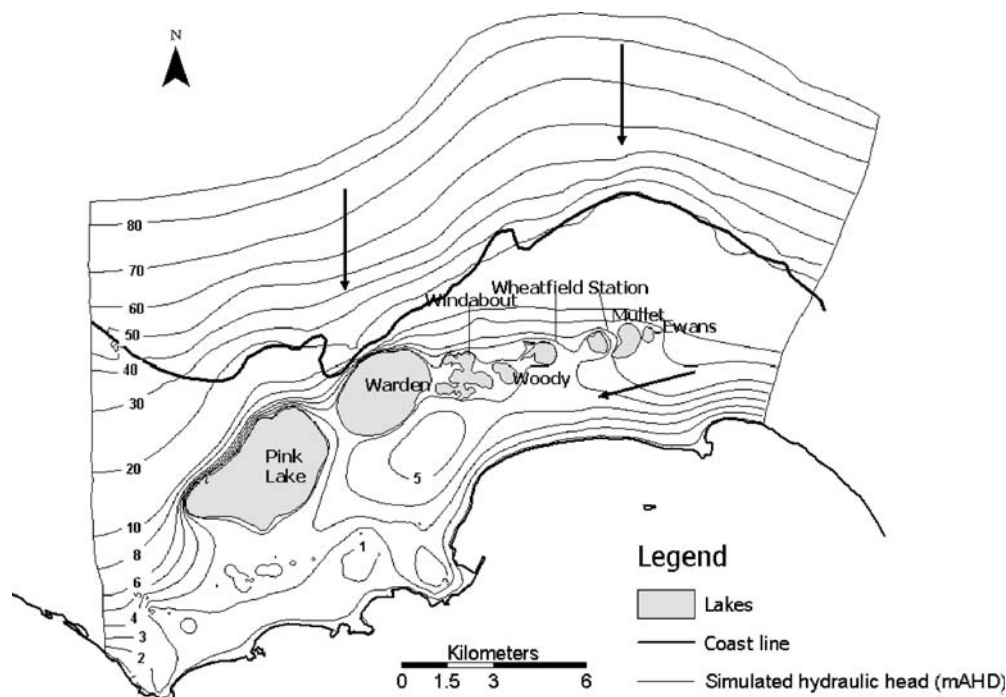
between Lake Warden and the coastal plain which exists in the numerical results (Figs. 4a and 8). Groundwater flow within the wetlands is NE–SW in the eastern side and E–W within the middle portions, with Pink Lake acting as the discharge point for the flow (Figs. 4b and 8). The calibrated flow models were also able to mimic the local hydraulic head variations of the layers within the wetlands system (Table 4). For example, the large hydraulic head difference observed between layers 2 and 4 (E45a and b) was captured reasonably well in the models which also indicate that the deeper formation is recharging the surficial formation to the east of the wetlands system. Similarly, small variations and changes in hydraulic

gradients are also observed in the middle part of the wetlands system. These agree well with the findings of previous hydraulic, chemical and isotopic study (Marimuthu et al. 2005).

Particle tracking

The flow path and travel time of groundwater flow within the system was determined by an advective particle-tracking simulation on the calibrated steady-state groundwater flow model. The three-dimensional particle tracking post-processing program (FEFLOW) uses the output from

Fig. 8 Simulated hydraulic head of Lake Warden wetlands system for steady state. Arrow denotes groundwater flow



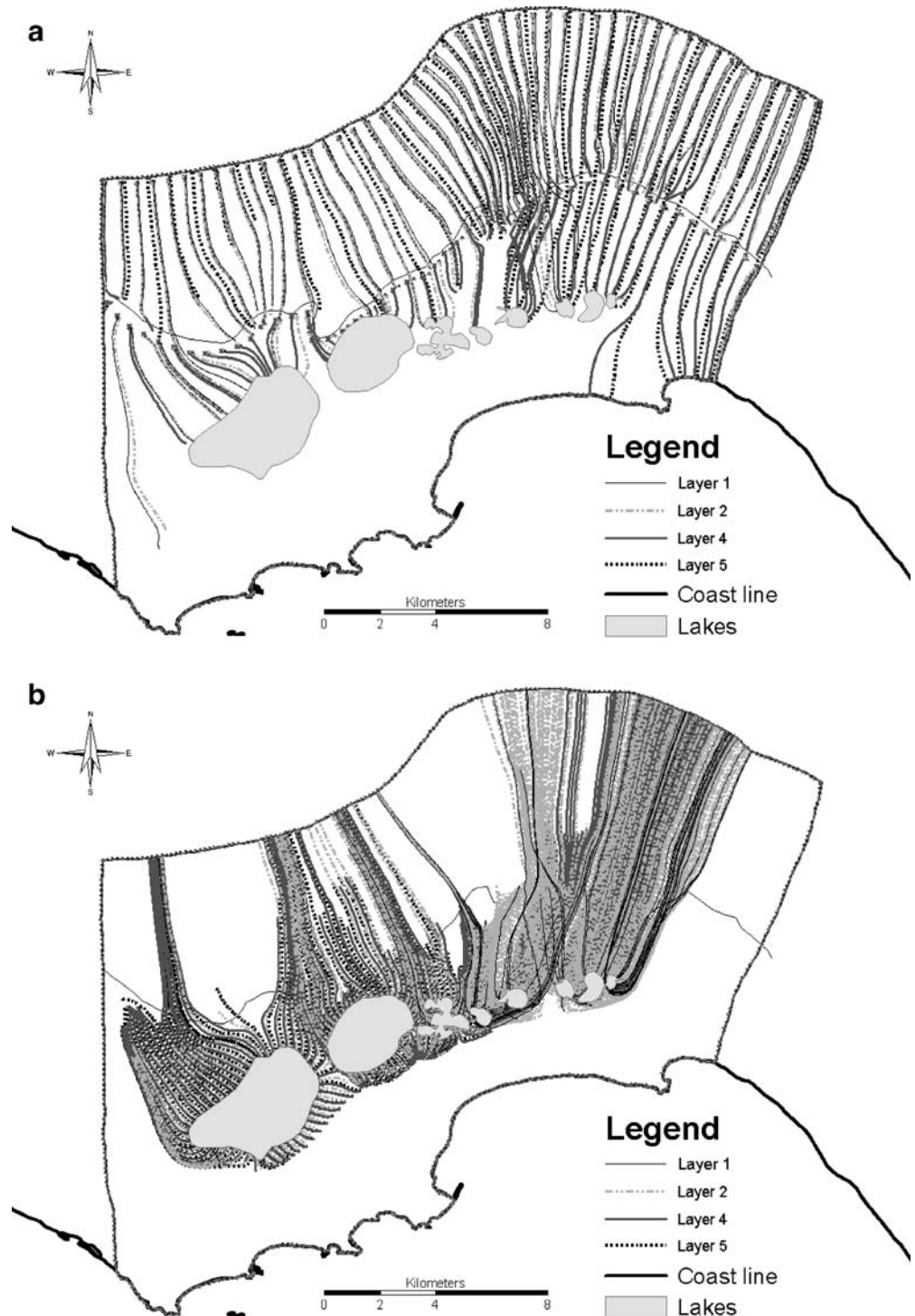
groundwater flow simulations (in the form of the velocity field) to simulate the direction of particles of groundwater flow and their travel times.

Three particle-tracking simulations were performed using the calibrated steady-state model. Simulation 1 tracked groundwater particles forward from the northern boundary (specified constant head) to determine the regional groundwater flow patterns (Fig. 9a). A large number of particles

were introduced around the edges of the lakes in simulation 2 to delineate the connectivity between the lakes and the regional flow path. Reverse particle tracking was utilized in simulation 3 to determine the point of origin of the water entering the lakes (Fig. 9b).

The particles introduced at the northern boundary of layers 1, 2, 4 and 5 travel down gradient to the escarpment, with a limited number of particles moving

Fig. 9 Simulated pathlines in the Lake Warden wetlands system by particle tracking approach: **a** Particles tracked forward from the northern boundary (simulation 1) and **b** particles tracked backwards from the lakes (simulation 3) to determine the point of origin of the water entering the lakes



towards the lake system (Fig. 9a). Another series of particles were therefore introduced along the escarpment to provide better resolution within the central portions of the system. For these particles, flow paths ending within the lakes are clearly evident (Fig. 9a), with the exception of the eastern side of the wetlands, where flow paths end at the coast, in particular for layers 4 and 5 (Fig. 9a). The particle-tracking simulations depict a regional flow field that is discharging to the escarpment in the shallower layers, and discharging to the lakes and to a lesser extent the coast in the deeper layers. Given the hydraulic parameters of the subsurface, however, the contribution from the regional N–S flow, in particular on the western side of the wetlands system, is expected to be small to the lakes. The volume of groundwater flow is expected to be greatest on the eastern side of the wetlands system (Fig. 9a and b) which is underlain by thick sedimentary sequences including the observed paleochannel trending N–NE.

The flowlines determined from the particle-tracking simulations are conceptually similar to the model developed in Marimuthu et al. (2005), in that lake water levels and recharge/discharge to and from the lakes within the wetlands system are constrained by both the regional and local groundwater flow systems. The lakes on the eastern side of the wetlands are in hydraulic connection with the N–NE flow system, while in the middle and west, E–W flow predominates and Pink Lake acts as the discharge point for the flow within the wetlands system (Figs. 4, 8 and 9b), while receiving little in the way of regional north south flow. The results of simulation 2 (not shown), indicates that the three lakes on the eastern side of the wetlands system (Station, Mullet and Ewans) are hydraulically connected (Fig. 9b); however, they are not hydraulically connected to the lakes on the middle and western side of the wetlands system (Wheatfield, Woody, Windabout, Lake Warden and Pink Lake).

The advective particle-tracking simulations have corresponded well with observed head data which suggests that the conceptual model is correct, and the flow-model results have quantitatively defined the direction and rate of groundwater movement except in the area of the simulated groundwater mound. In addition, the delineation of the regional and local flow system is also in agreement with the findings of isotopic composition of the two different systems; the regional groundwater flow above the escarpment and the local groundwater flow within the wetlands. Utilization of the advective flow model for detailed work within the wetlands system is questionable, given the scale of the parameters used in its development. There is always the issue of uniqueness when dealing with models calibrated through hydraulic-head measurements alone. Successfully matching an additional calibration target to the model will give more confidence in predictions when using the model at the local (single lake) scale. The conclusions drawn from the flow model, therefore, have been tested for consistency and accuracy by using a transport model and the deuterium composition results from the field program.

Transport model

The water bodies within the Lake Warden wetlands system display varying isotopic compositions (Table 1) due to different degrees of evaporation and mixing (Marimuthu et al. 2005). The different isotopic composition of the water bodies can be used to identify zones of inter-mixing, with the degree of intermixing subject to groundwater flux and the leakage from the surface water bodies. The simulation of deuterium composition within the groundwater flow system has been performed to provide additional confidence that the groundwater flux has been assessed reasonably well in the flow model. The mean deuterium concentration was inferred from temporal and spatial variations in deuterium of the different water bodies within the system.

The simulation of deuterium concentration was undertaken in the finite element flow and transport model (FEFLOW). The concentration was represented by transport of discrete particles by groundwater flow and each particle represents a certain mass of concentration (i.e. the relative concentration of deuterium ($\delta^2\text{H}$) in the water molecules). The transport of the discrete particles is governed by the following equation:

$$\frac{\partial C}{\partial t} \varepsilon = \frac{\partial}{\partial x_i} \left(q_i^f C - D_{ij} \frac{\partial C}{\partial x_j} \right) \quad (4)$$

Where C is the concentration (M L^{-3} ; mass per volume), ε is the effective porosity, q_i^f is the Darcy flux (L T^{-1}) and D_{ij} is tensor of hydrodynamic dispersion ($\text{L}^2 \text{T}^{-1}$). Some assumptions were made in the transport modeling process: the conservative tracer (deuterium) exhibits no adsorption, degradation and chemical reaction, hence, the retardation factor (R) is set to 1. In addition, the isotopic fractionation in the lakes was not considered in this model, as the input values (measured concentration) of the lakes were incorporated as a boundary condition.

The simulation results for stress period day 455 (April 2002) from the transient flow simulation were selected and used as the initial condition for the flow and transport model. This corresponds with the beginning of the water sampling for the chemical and isotope analysis. Isotopic concentration is expressed as the difference between the measured ratio of the sample over the measured ratio of the VSMOW reference (Vienna Standard Mean Ocean Water; Clark and Fritz 1997):

$$\delta^2 H_{\text{sample}} = \left(\frac{R_{\text{sample}}}{R_{\text{reference}}} - 1 \right) 1000 \quad (5)$$

Where $\delta^2 H_{\text{sample}}$ is the isotopic composition of deuterium, and R_{sample} and $R_{\text{reference}}$ are measured ratios of the sample and reference. The isotopic composition is expressed using the delta (δ) notation ($^0/_{00} \equiv$ parts per thousand) and a positive value indicates higher abundances than the VSMOW reference and a negative value indicates lower abundances than the VSMOW reference. The delta value

from this method is expressed as both a negative and positive value, so excluding use in that form in a transport model. Hence R_{sample} values have been used directly, multiplying with 10,000 as the following example, to obtain values in a reasonable range for the convenience of modeling and it will be referred as deuterium concentration (mg L^{-1}).

$$R_{\text{sample}} = \left(\frac{-24.00}{1000} + 1 \right) (0.00015575) \quad (6)$$

Where -24.00 is the isotopic composition of deuterium, and R_{sample} and 0.00015575 are measured ratios of the sample and reference, respectively.

$$\begin{aligned} \text{Deuterium concentration} &= (10,000)(R_{\text{sample}}) \\ &= (10000)(0.000152012) = 1.520 \text{ mg L}^{-1} \end{aligned}$$

The measured isotopic composition of groundwater collected on April 2002 was utilized as the basis for the initial concentration field. The inverse distance weighted (IDW) interpolation scheme was adopted to generate initial values for all corresponding model layers. The IDW interpolation method is based on a weighted averaging process where nearby samples exert a greater influence than distant samples. It was determined that the distribution of interpolated concentration values represent the observed values.

The northern and southern borders were assigned as fully penetrating type I specified mass-boundary conditions (Dirichlet boundary conditions). The values assigned to the Dirichlet boundaries reflect the mean deuterium concentration of regional groundwater (1.51 mg L^{-1}) for the northern boundary and the mean deuterium concentration of coastal plain groundwater for the southern boundary (1.52 mg L^{-1}). Conversely, the eastern and western borders were treated as no-flow boundaries. No mass-boundary condition has been assigned to the escarpment, as the constraint condition set in the flow model allows free outflow of water from the model, and does not allow inflow.

The aerial recharge is imposed as the prescribed mass flux (Neumann boundary condition).

$$D_{ij} \frac{\partial C}{\partial x_j} n_i = q_2 \quad (7)$$

Where D_{ij} is hydrodynamic dispersion ($L^2 T^{-1}$), n corresponds to the normal unit vector (positive outward), C is the deuterium concentration ($M L^{-3}$), and q_2 is the mass flux ($M L^{-2} T^{-1}$). The spatial variability of recharge was taken into account and the aerial mass flux was defined as ($q_2 = RC_p$), where R is the recharge rate ($L T^{-1}$) utilized in the flow model, and C_p is the monthly mean weighted deuterium concentration in precipitation ($M L^{-3}$). The precipitation samples were collected at the Bureau of Meteorology station, Esperance.

Lake boundary conditions were incorporated into the transport model by using a Neumann boundary condition. To evaluate the flux function for the boundary condition, the lake was partitioned into its individual nodes, and the nodal areas normalized to the elemental area. The fluid flux represented by each node is calculated from the flow model, and used to determine the mass flux into the system from the lake:

$$\sum_{i=1}^n \frac{q_i}{A_i} C_m = q_2 \quad (8)$$

Where q_i is the balance flux at each lake node ($L^3 T^{-1}$), C_m is the monthly mean weighted deuterium concentration ($M L^{-3}$) of a lake; A_i is the mean area for each node (L^2) in the lake, n is the number of nodes in the lake, and t is the time.

An average effective porosity of 0.3 was assigned to layers 1, 2 and 4; and 0.1 for layers 3 and 5 respectively (Table 5). The values were based on similar aquifer material found in the literature (Fetter 2001). As a check on the sensitivity of the calibrated model, three transport simulations were performed by varying porosity values up to $\pm 15\%$ of the estimated values. The differences in the simulation results were negligible.

The transport model was calibrated to seasonally observed isotope compositions. The significance of dispersion was considered during the calibration and the dispersivity values used were obtained from the literature. Dispersivity values for use in field scale transport simulation are inherently difficult to measure in the field and are not well defined physically (Gelhar et al. 1992; Zheng and Bennett 2002). Dispersivity values are therefore often used as a model fitting parameter (Anderson and Woessner 1992). Most reported values of longitudinal dispersivity (α_L) fall in the range from 0.1 times the scale of the system and for a system greater than 1 km in extent,

Table 5 Transport model parameters, the thickness of the aquifers are reported in Table 2

Layer	Aquifer/unit	Effective porosity	Longitudinal dispersivity α_L (m)	Transverse dispersivity α_T (m)	Hydrodynamic dispersion (D_{ij}) $\text{m}^2 \text{ s}^{-1}$
1	Superficial	0.3	100	5	10^{-9}
2	Pallinup Siltstone	0.3	100	5	10^{-9}
3	Confining layer	0.1	100	5	10^{-9}
4	Werillup Formation	0.3	100	5	10^{-9}
5	Weathered zone	0.1	100	5	10^{-9}

it is reasonable to use $\alpha_L \sim 100$ m (Fetter 1993; Javandel and Doughty 1984) and transverse dispersivity (α_T) to 20% of the α_L values (Gelhar et al. 1992).

As a check on the sensitivity of the calibrated transport model, three transport simulations were performed using three different dispersivity values and some of the simulated plots that represent different layers of the model are presented in Fig. 10. Changes in longitudinal dispersivities by an order of magnitude have no significant impact on the simulations. Phillips et al. (1989), who used stochastic theory to analyze the influence of longitudinal dispersion in large sedimentary aquifers, also concluded that effects of longitudinal dispersion do not exert a significant influence on environmental tracer distribution. However, results are sensitive to transverse dispersivities especially in areas where vertical flow is predominant (Plots E50 and E54c see Fig. 10).

During the calibration process, the value of source concentration was allowed to vary by $\pm 12\%$ to encompass variability due to the analytical precision of the deuterium analysis ($\pm 3\text{‰}$). Small differences were observed in the simulations results mainly in the high permeable zone (e.g. E54b, E54c, and E50); however, significance differences were observed in most of the areas if the source concentration varied above $\pm 12\%$.

The model and observed results of some of the boreholes (e.g. E35b, E50 and E55) show that there is

far more leakage of enriched lake water into the lower layers than was originally thought, based on the selection of model parameters. After a series of calibration suites with dispersivity, porosity and source concentration (not shown), it was concluded that the influential parameter regarding the modeled deuterium concentration was the vertical hydraulic conductivity. The hydraulic conductivity of layers 3 and 4 were varied until simulated and observed concentrations matched within a reasonable range (the new hydraulic conductivity values were bounded to ensure they were still within the range of values of what might be expected for the sediment type). The improved calibration results are also presented in Fig. 11.

The final calibrated transport model simulated deuterium concentration for each of the 16 calibration points for the seasonal observation points (May 2002–November 2003), the results are shown in Fig. 11. The simulation results (within the analytical precision (3‰) of the analysed samples) are in agreement with the observed values but some variations are noticeable (e.g. E35c, E42, E45b, E48, E49c, E52 and E54c). Overall the transport model was able to represent the spatial and temporal variations of deuterium concentration within the wetlands system which suggests that the model has captured successfully the mixing processes hinted at by the observed isotopic composition of the wetlands system (Marimuthu et al. 2005).

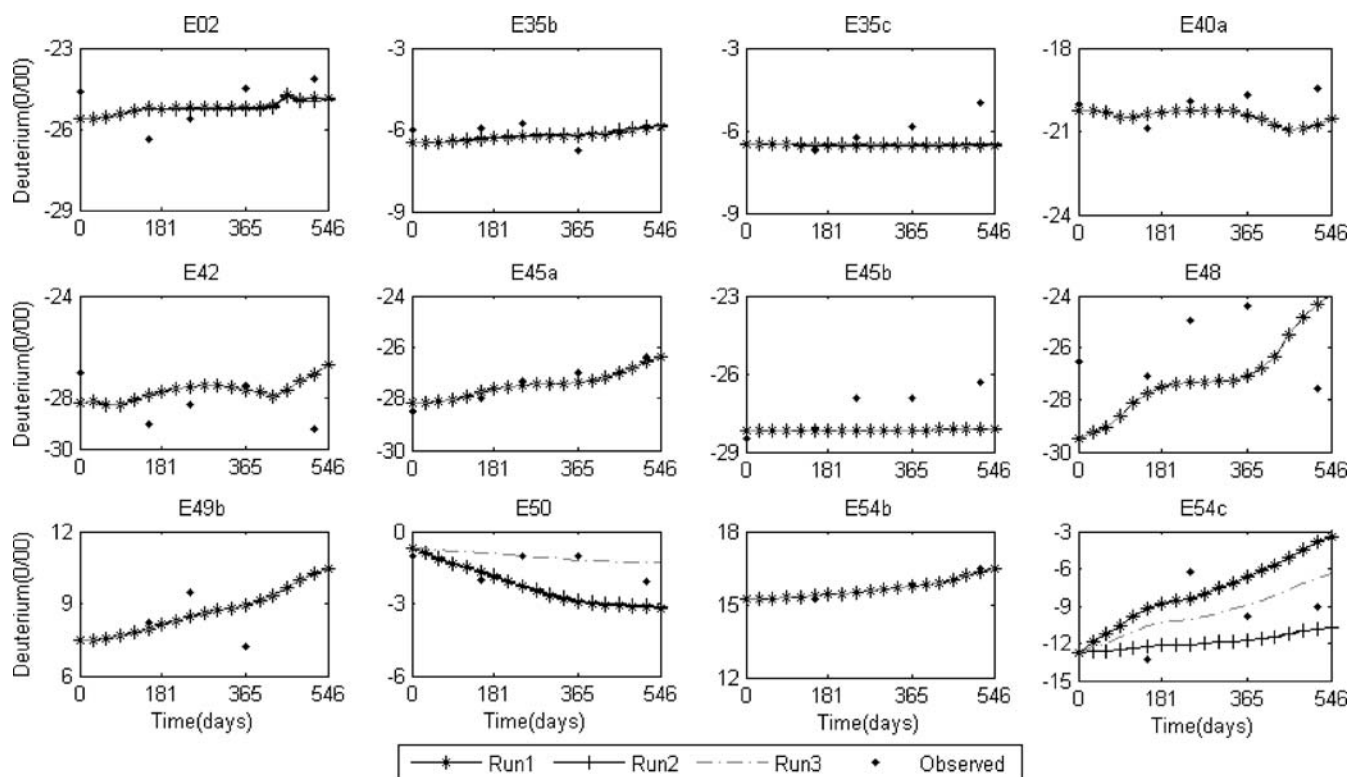


Fig. 10 Simulated and observed deuterium composition. Varying dispersivities (Run1- $\alpha_L=100$ m and $\alpha_T=5$ m; Run 2- $\alpha_L=50$ m and $\alpha_T=2.5$ m; Run 3- $\alpha_L=5$ m and $\alpha_T=1$ m). Refer to Fig. 1 for the calibration point locations. Note: Simulated and observed deuterium concentration expressed as delta notation (‰)

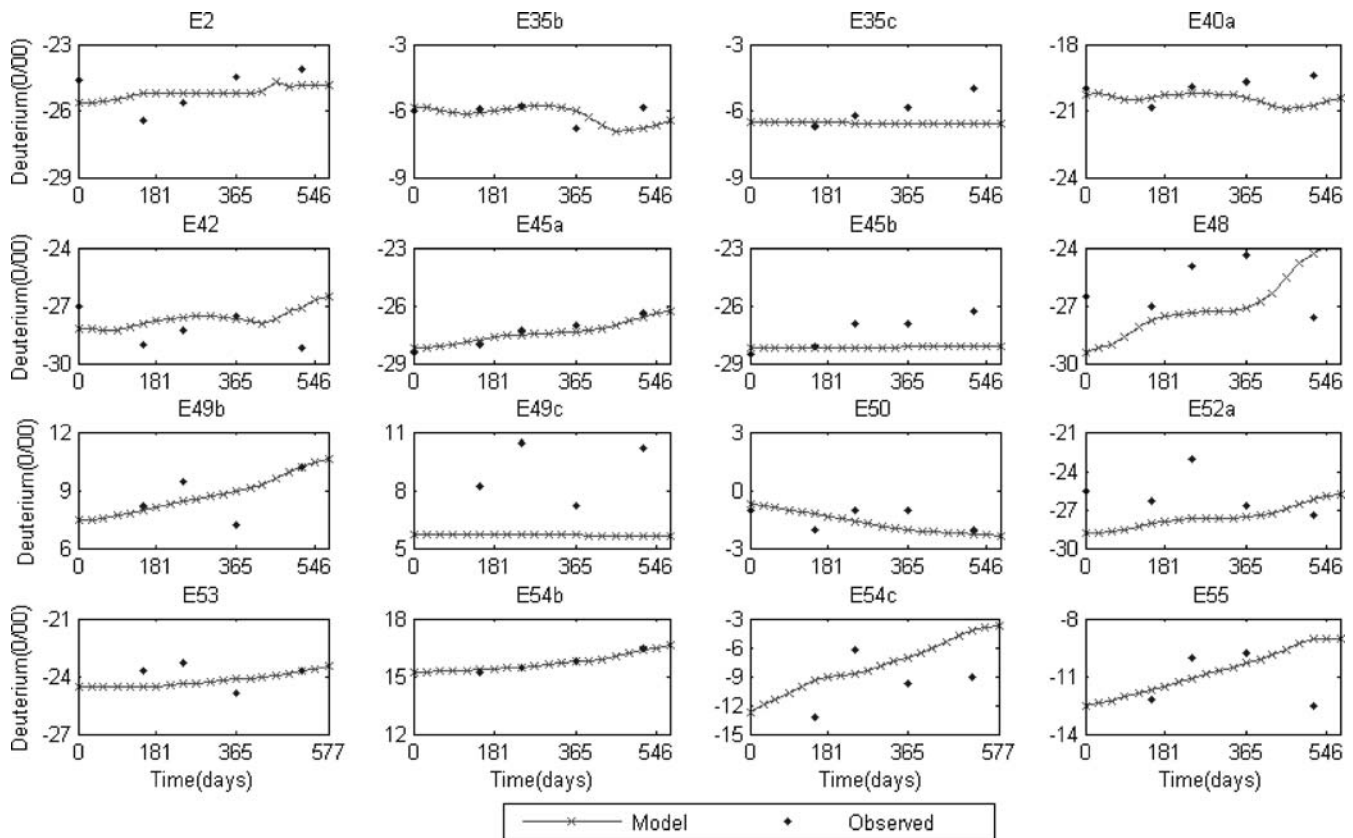


Fig. 11 Simulated and observed deuterium composition using the final calibrated transport model. Note: Simulated and observed deuterium concentration expressed as delta notation ($^0_{\text{‰}}$)

Summary and discussion

This study has presented an integrated approach utilizing multiple calibration targets, steady state and transient stresses, particle tracking analysis and isotopic compositions (deuterium), to calibrate a three-dimensional finite element model. Additionally, the simulation interface module of the FEFLOW (Diersch 2002) was used to integrate the time varying isotopic composition in a complex environment such as the Lake Warden coastal wetlands system.

The flow model was calibrated for both steady state and transient conditions (3 years) utilizing traditional hydraulic information only. There was fairly good agreement between the simulated and observed heads (Figs. 5 and 6) and the observed flow patterns are similar to simulated flow patterns (Figs. 4a and 8). Errors are generally spread across the model domain, with some areas having simulated water levels consistently higher (the largest difference being 2.1 m). These differences are probably due to local heterogeneities in the aquifer system. Due to their unknown characteristics or to limited model resolution, these local heterogeneities could not be incorporated in the model.

The flow-path analysis supports the earlier conceptual model work (Marimuthu et al. 2005) that showed the wetlands as being a minor component of the overall flow

system, and acting as a sink for the N–S groundwater flow. Although the path analysis has captured the general flow systems within the study area, full confidence in the understanding of the interaction of flows within the wetlands system is constrained by sparse hydraulic data and the complexity of the site. To improve the confidence in the model's ability to be utilized for detailed flow path analysis as well as the full understanding of the interactions of the flows within the wetlands system, and to verify the uniqueness of the calibration, the spatial and temporal variations of deuterium composition were utilized as another calibration target.

The different isotopic composition of water bodies of the Lake Warden coastal wetlands system were used to identify zones of inter-mixing. For example, the deuterium composition of the regional groundwater is close to the weighted average composition of deuterium-depleted precipitation in winter ($-25^0_{\text{‰}} \pm 3^0_{\text{‰}}$) and the isotopic measurements along the NE–SW transect within the wetlands system (Fig. 1) display intermediate isotopic characteristics between the regional groundwater and lake water (Marimuthu et al. 2005). These results were used as the basis to determine how well the transport model captured the mixing zones beneath the lakes within the wetlands system based on the concentration front passing an observation location. The discussion will be focused along the NE–SW transect (Fig. 1).

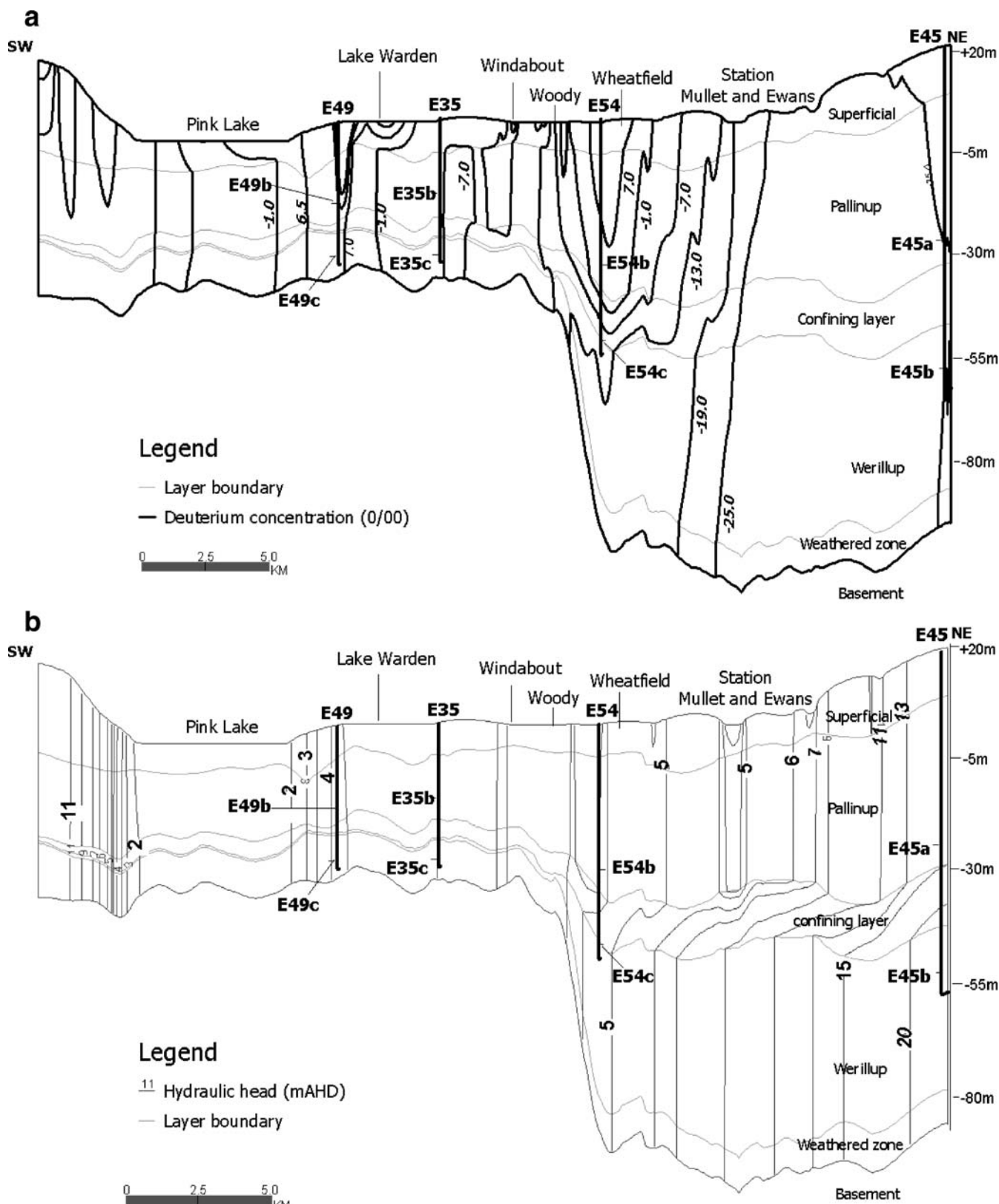


Fig. 12 NE–SW cross section for the wetlands system, displaying the simulated **a** deuterium composition and **b** hydraulic head. Refer to Fig. 1 for the transect location. Elevation in mAHD

The simulated distribution of deuterium composition along the NE–SW transect is presented in Fig. 12a. It is evident from the plot that the simulated deuterium composition in the upper aquifer (superficial) is highly enriched relative to the intermediate aquifer (Pallinup Siltstone). Conversely, the intermediate aquifer is highly enriched relative to the deeper aquifer (Werillup Formation). The exception to this is in the location of borehole E35, where the deuterium compositions are identical in the intermediate and deep aquifers. A thorough analysis of the transect indicates that enrichment is not continual along the transect. For instance, the deuterium composition from piezometers located on the east (upgradient) side of the wetlands system (E45a and E45b), is very similar to that of regional groundwater. Piezometers located in the middle part of wetlands system (E54b and E54c) indicate enriched deuterium composition. Piezometers on the eastern side of Lake Warden (E35a and E35b), however, display less enriched deuterium composition relative to the middle part (E54); but on the western side of Lake Warden relatively enriched deuterium composition was observed (E49b and E49c).

These findings indicate that the enrichment is due to groundwater flux and that leakage from the surface water bodies, and the transport model was able to capture the processes. The equipotential lines along the transect

indicate the presence of deep circulation of local groundwater within the vicinity of E54 (Fig. 12b), implying that the depth of circulation ultimately influences the distribution of the deuterium composition. The sensitivity analysis on source concentration also indicates that significant differences were observed if the source concentration was varied beyond $\pm 12\%$, mainly in sampling locations such as E54b and E54c. Locally recharged surface water, with a comparatively short residence time, was the dominant source for enrichment deuterium within this region, as the enriched water mixed with regional groundwater in the Pallinup Siltstone aquifer. This finding also clearly indicates that advection is the main process controlling transport within the system.

As a demonstration of the importance of calibration to multiple targets, two transport simulations were performed. Simulation 1 was performed with the fully calibrated flow model using the same transport parameters that were used as in the final calibrated transport model except the flow model maintained the original hydraulic conductivity distribution. The final calibrated transport model was used for the second simulation. A cross section comparing the results for the NE–SW transect is presented in Fig. 13. A noticeable difference between the simulations occurs in the vicinity of piezometer E54. The findings also illustrate that the distribution of deuterium

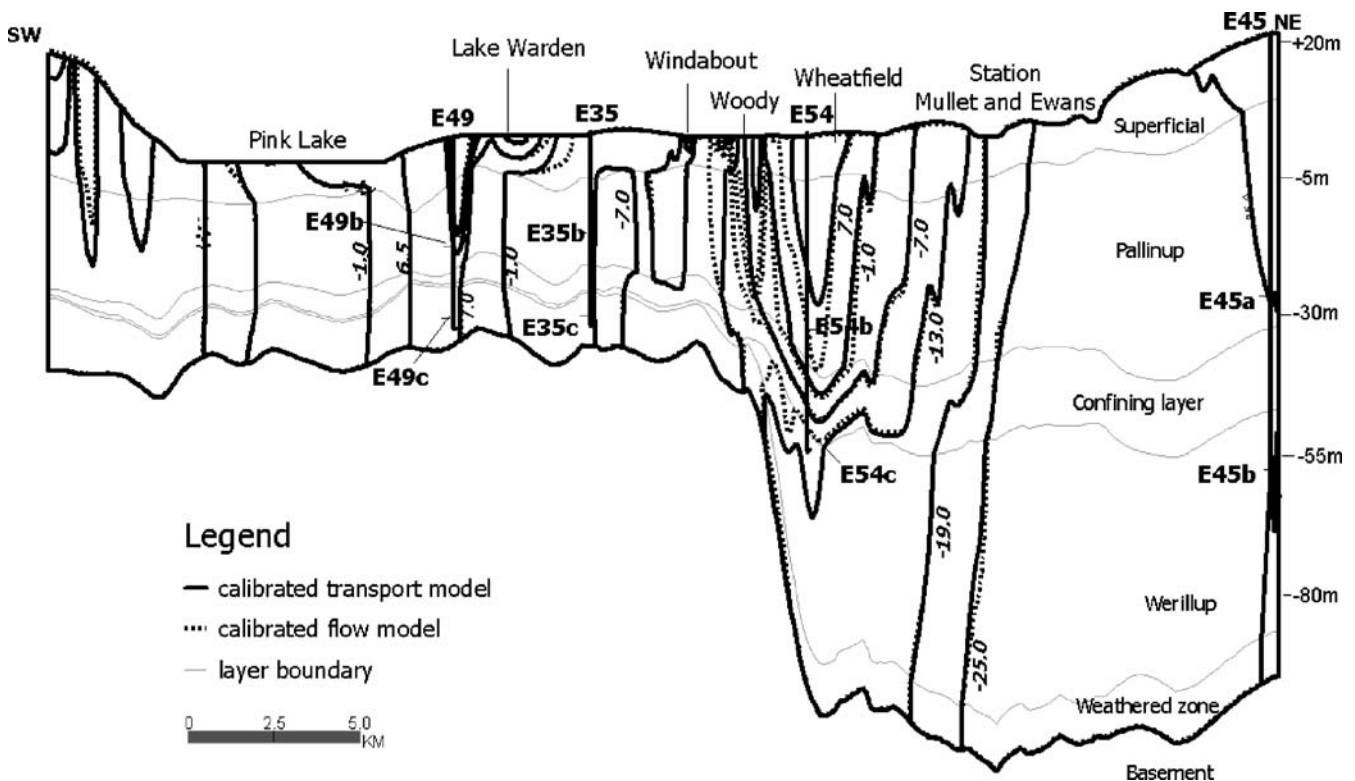


Fig. 13 Comparison of the simulation that was performed with the fully calibrated flow model and final calibrated transport model in the NE–SW cross section of the wetlands system, and the deuterium composition. Refer to Fig. 1 for the transect location

composition within the wetlands system has provided an independent means to quantify the hydraulic conductivity of the aquifer.

Although, the transport model was able to capture the varying deuterium composition both temporally and spatially within the wetlands groundwater system, a number of potential limitations should be considered. The simulated lower concentration in some of the boreholes may indicate that simulated groundwater fluxes generally are higher and travel times faster than in the real system (E35b, E40b and E49c). Another possibility for this discrepancy is aquifer heterogeneity; the hydraulic parameters obtained from the site were limited, and the estimated transport parameters could also further compound the problem.

The results from the final calibrated transport model show that there are no significant differences in the hydraulic head from the original flow-model results on the northern part and coastal plain of the study area. However, some differences were observed within the wetlands system. The results clearly show that some improvement in the flow model has been achieved when flow-path information and deuterium composition were used together to calibrate the model. The end result is a final calibrated groundwater flow model from which quantitative estimates of groundwater contribution to the Lake Warden wetlands system can be obtained with greater confidence. The estimation of the groundwater component is essential to assist in the mitigation of the effects of non-seasonal floods which occur in the region.

The flow-model calibration procedure utilizing hydraulic head only as calibration targets provides good agreement between the simulated and observed heads as discussed previously, but is subject to non-uniqueness. It is also possible to obtain very similar simulated head distributions by any number of combinations of values for various input parameters such as boundary conditions, hydraulic conductivity and recharge in particular in an environment where limited borehole information were available (Zheng and Bennett 2002). As an alternative to the use of deuterium compositions as a second calibration target set, the flow-model calibration could be further improved if additional point measurements (boreholes) are considered within the study area. The choice of approach may be limited by economic factors; additional point measurements may not be feasible or economical. Due to such cost constraints, other viable alternatives need to be explored in order to improve model calibration.

A number of researchers have shown that in situations where field data are limited, additional information such as tracer data (Harrington et al. 1999; Kim et al. 1999; Krabbenhoft et al. 1990; Sanford et al. 2004) have improved the flow-model calibration. In addition, the utilization of multiple tracers has also improved the understanding of the system and can be used as a basis to check on the correctness of numerical models since each tracer provides a feed back or iterative process based on comparisons of independent estimates of travel time (Reilly et al. 1994). However, there are some limitations

on the usage of multiple tracers, in particular, their natural occurrence and analytical uncertainties (Harrington et al. 1999; Kim et al. 1999; Krabbenhoft et al. 1990). The other major factor hampering the utilization of multiple tracers is the availability of financial resources to experiment with them concurrently.

This study has adopted the use of a common tracer and shown that the application of deuterium composition in a complex environment such as the Lake Warden wetlands system has provided additional confidence to the flow model calibration. The use of isotopes in hydrogeology has been gaining wider recognition in recent years, prompted in part by improvements that have brought down the cost of stable isotope analysis. For example, the cost of analysis of a water sample for deuterium and oxygen –18 in 2005 was approximately one third what it was in 1995. For a relatively small additional investment for comprehensive isotope analysis (compared with the cost of installing boreholes), the understanding and effective management of lakes and groundwater resources can be improved.

The application of stable isotopes in hydrogeology and modeling, however, has its own limitations. For example, their use in numerical simulation requires significant differences in the isotopic composition of source waters within the model domain. In addition, field studies for data gathering should incorporate all the water bodies within the system and be carried out for a reasonable length of time to represent the temporal variations of the flow system. As shown in this study, it is most suitable in an environment where the surface water–groundwater interaction is significant and at sites where little hydraulic data exist.

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References

- Anderman ER, Hill MC, Poeter EP (1996) Two-dimensional advective transport in groundwater flow parameter estimation. *Groundwater* 34(6):1001–1009
- Anderson MP, Woessner WW (1992) *Applied groundwater modeling: simulation of flow and advective transport*. Academic Press, San Diego
- Baddock LJ (1997) *Hydrogeology of the Esperance-Mondrain Island 1:250000*. Water and Rivers Commission, Perth
- Baddock LJ (1998) *Esperance Source Investigation Report 1977 Drilling Programme and Resource Assessment*. Water Corporation, Perth
- Clark I, Fritz P (1997) *Environmental isotopes in hydrogeology*. Lewis Publishers, Boca Raton, FL

- Department of Planning and Infrastructure (DPI) (2004) Coastal data, Online Department of Planning and Infrastructure. Available: <http://www.dpi.wa.gov.au/coastaldata/index.html>. Cited 20 February 2005
- Diersch H-JG (2002) Interactive, graphic-based finite element Simulation system FEFLOW for modeling groundwater flow, contaminant mass and heat transport processes. WASY Institute for Water Resources Planning and Systems Research Ltd., Berlin
- Fetter CW (1993) Contaminant hydrogeology. Macmillan, London
- Fetter CWJ (2001) Applied hydrogeology. Prentice Hall, Englewood Cliffs, NJ
- Gelhar LW, Welty C, Rehfeldt KW (1992) A critical review of data on field-scale dispersion in aquifers. *Water Resour Res* 28 (7):1955–1974
- Harrington GA, Walker GR, Love AJ, Narayan KA (1999) A compartmental mixing-cell approach for the quantitative assessment of groundwater dynamics in the Otway Basin, South Australia. *J Hydrol* 214:49–63
- Javandel IC, Doughty CFT (1984) Groundwater transport: handbook of mathematical models. American Geophysical Union, Washington, DC
- Keating EH, Bahr JM (1998) Using reactive solutes to constrain Groundwater flow models at a site in northern Wisconsin. *Water Resour Res* 34(12):3561–3571
- Keidser A, Rosbjerg D (1991) A comparison of inverse approaches to groundwater flow and transport parameter identification. *Water Resour* 27(9):2219–2232
- Kim K, Anderson MP, Bowser CJ (1999) Model calibration with multiple targets: a case study. *Groundwater* 37(3):345–351
- Krabbenhoft DP, Anderson MP, Bowser CJ (1990) Estimating groundwater exchange with lakes, calibration of a three-dimensional solute transport model to a stable isotope plume. *Water Resour Res* 26(10):2455–2462
- Marimuthu S, Reynolds DA, Salle CLGL (2005) A field study of hydraulic, geochemical and stable isotope relationship in a coastal wetlands system. *J Hydrol* 315:93–116
- Morgan KH, Peers R (1973) Explanatory notes on the Esperance-Mondrain Islan geological sheet, Western Australia. Western Australia Geological Survey, East Perth
- Myers JS (1985) The Fraser Complex: a major layered intrusion in Western Australia. Report 14, Western Australia Geological Survey, East Perth
- Myers JS (1995) Geology of Esperance 1:1000000 sheet. Western Australia Geological Survey, East Perth
- Penman HL (1948) Natural evaporation from open water, bare soil and grass. *Proc Roy Soc London A* 193:120–145
- Phillips FM, Tansey M, Peters LA, Cheng S, Long A (1989) An isotopic investigation of groundwater in the central San Juan Basin, New Mexico: carbon-14 dating as a basis for numerical flow modeling. *Water Resour Res* 25:2259–2273
- Portniaguine O, Solomon DK (1998) Parameter estimation using groundwater age and head data, Cape Cod, Massachusetts. *Water Resour Res* 34:637–645
- Reilly TE, Plummer LN, Phillips PJ, Busenberg E (1994) The use of simulation and multiple environmental tracers to quantify groundwater flow in a shallow aquifer. *Water Resour Res* 30 (2):421–433
- Sanford WE, Plummer LN, McAda DP, Bexfield LM, Anderholm SK (2004) Hydrochemical tracers in the middle Rio Grande Basin, USA: 2. Calibration of a groundwater flow model. *Hydrogeol J* 12(4):1–40
- Street G, Abbott A (2004) Interpretation of airborne electromagnetic survey over Lake Warden Catchment Esperance, Western Australia, Department of Conservation and Land Management, Geraldton, Western Australia
- Wilson W (2003) A preliminary assessment of the recent environmental history of the lake Warden Wetlands Esperance, Western Australia. Technical Report for the Department of Conservation and Land Management, Geraldton, Western Australia
- Wood WW, Sanford WE (1995) Chemical and isotopic methods for quantifying groundwater recharge in a regional, semiarid environment. *Groundwater* 33:458–468
- Zheng C, Bennett GD (2002) Applied contaminant transport modeling. Wiley, New York
- Zhu C (2000) Estimate of recharge from radiocarbon dating of groundwater and numerical flow and transport modeling. *Water Resour Res* 36(9):2607–2620