Characterisation of sea-water intrusion in the Pioneer Valley, Australia using hydrochemistry and three-dimensional numerical modelling

A. D. Werner · M. R. Gallagher

Abstract Sea-water intrusion is actively contaminating fresh groundwater reserves in the coastal aquifers of the Pioneer Valley, north-eastern Australia. A three-dimensional sea-water intrusion model has been developed using the MODHMS code to explore regional-scale processes and to aid assessment of management strategies for the system. A sea-water intrusion potential map, produced through analyses of the hydrochemistry, hydrology and hydrogeology, offsets model limitations by providing an alternative appraisal of susceptibility. Sea-water intrusion in the Pioneer Valley is not in equilibrium, and a potential exists for further landward shifts in the extent of saline groundwater. The model required consideration of tidal over-height (the additional hydraulic head at the coast produced by the action of tides), with over-height values in the range 0.5–0.9 m giving improved water-table predictions. The effect of the initial water-table condition dominated the sensitivity of the model to changes in the coastal hydraulic boundary condition. Several salination processes are probably occurring in the Pioneer Valley, rather than just simple landward sea-water advancement from "modern" sources of marine salts. The method of vertical discretisation (i.e. model-layer subdivision) was shown to introduce some errors in the prediction of water-table behaviour.

Résumé L'intrusion de l'eau de mer est en train de contaminer activement les réserves d'eau souterraine potable dans les aquifères côtiers de la vallée de Pioneer au nord-est de l'Australie. Un modèle en trois dimensions de l'intrusion de l'eau de mer a était réalisé en utilisant le code MODHMS pour étudier les processus à l'échelle régionale et faciliter l'évaluation de stratégies de gestion du système. Une carte piézomètrique de l'intrusion de l'eau de mer, réalisée grâce à l'étude de l'hydrogéochimie, l'hydrologie et l'hydrogéologie, compense les limites du modèle en permettant une évaluation alternative de la vulnérabilité. L'intrusion de l'eau de mer dans la vallée de Pioneer n'est pas en équilibre et un potentiel existe pour des déplacements plus à l'intérieur des terres de l'étendue des eaux souterraines salées. Le modèle devait prendre en compte les surélévations dues aux marées (la charge hydraulique supplémentaire au niveau de la côte produite par l'action des marées), avec des valeurs de surélévations de l'ordre de 0.5–0.9 m entraînant de meilleures prédictions du niveau de la nappe. L'effet de l'état initial de la nappe était prédominant sur la sensibilité du modèle par rapport aux changements de la condition hydraulique aux limites au niveau de la côte. Plusieurs processus de salinisation doivent probablement avoir lieu dans la vallée de Pioneer et non pas uniquement une simple avancée d'eau de mer dans les terres à partir de sources "modernes" de sels marins. La méthode de la discrétisation verticale (subdivision en couches dans le modèle) s'est révélée être à l'origine d'erreurs dans la prédiction du comportement de la nappe.

Resumen La intrusión de agua de mar está contaminando las reservas de agua subterráneas de agua dulce en los acuíferos costeños en Pioneer Valley, noreste de Australia. Se ha desarrollado un modelo tridimensional de intrusión de agua de mar mediante el uso de código MODHMS para explorar procesos de escala regional y para asistir la evaluación de estrategia para el manejo del sistema. Un mapa de potencial de intrusión de agua de mar, producido mediante el análisis de hidroquímica, hidrología e hidrogeología balancea las limitaciones del modelo al proporcionar una asesoría alternativa de susceptibilidad. En Pioneer Valley la intrusión de agua del mar no está en equilibrio y existe el potencial de movimiento en la extensión de agua subterranea salada desde el mar hacia la tierra. El modelo requirió considerar la carga hidráulica adicional en la costa producida por la acción de las mareas (sobre-altura de la marea), con una sobre-altura en el rango de 0.5–0.9 m, locual produjo mejores predicciones de la mesa de agua. El efecto de la condición inicial de la mesa de agua dominaba la sensitividad del modelo a

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A. D. Werner (✉)
Department of Natural Resources and Mines,
Natural Resource Sciences,
Indooroopilly, Brisbane, 4068, Australia
e-mail: adrian.werner@nrm.qld.gov.au
Tel.: +61-617-38969144

M. R. Gallagher
Department of Civil Engineering,
University of Queensland,
St Lucia, 4072, Australia

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cambios en la condición de límite hidráulico de la costa. Es probable que múltiples procesos de salinización estén ocurriendo en Pioneer Valley, en lugar de un avance simple de agua de mar hacia la tierra de fuentes “modernas” de sales marinas. Se observó que el método de discretización vertical (subdivisión de capas del modelo) introduce algunos errores en las predicciones de cambios en el comportamiento de la mesa de agua.

Keywords Saltwater/freshwater relations · Numerical modelling · Coastal aquifers · Salination · Australia

Introduction

Sea-water intrusion is a widespread and common problem in developed coastal aquifer systems. The need to plan and manage coastal groundwater reserves has led to an abundance of sea-water intrusion studies and a wide range of approaches to management modelling. All regional-scale sea-water intrusion modelling studies adopt broad simplifications to salination phenomena that are often related to the scale of the problem, due in part to the large computational burden associated with density-coupled groundwater flow and salt transport simulation (Diersch and Kolditz 2002). Typically, modelling assumptions represent a balance between system complexities represented in the model and model-size or computational efficiency. Simplifications may also reflect the sparseness of water quality, hydrogeological and geochemical information, which is invariably insufficient to capture all the intricacies of salination processes occurring over an entire groundwater basin.

Common approaches to sea-water intrusion management modelling include the application of two-dimensional sectional models (e.g. Souza and Voss 1987; Yakirevich et al. 1998; Sherif and Hamza 2001; Zhang et al. 2004), vertically integrated planar models (e.g. Sherif and Singh 2002), sharp-interface models (e.g. Guvanasen et al. 2000; Mantoglou 2003; Park and Aral 2004), and density-independent models (e.g. Kabbour et al. 2005). These approaches simplify sea-water intrusion by neglecting one or a combination of the following: pumping-induced radial flow, water-density variations, vertical groundwater flow, vertical salinity gradients, hydraulic property heterogeneities in the vertical direction and dispersive salt transport. These simplifications are not necessary in three-dimensional, density-dependent, dispersive-transport modelling, although similar data and conceptualisation limitations to those of less complicated models still apply.

Three-dimensional sea-water intrusion modelling of large aquifers has recently become a more practical option due to the evolution of computers and the availability of numerically efficient codes. Gingerich and Voss (2005) used the US Geological Survey’s 3D SUTRA code (Voss and Provost 2002) to explore changes to the sea-water-freshwater transition zone in response to pumping in the Pearl Harbour aquifer, Hawaii. Langevin (2003) applied the SEAWAT code (Guo and Langevin 2002) to study rates of discharges to Biscayne Bay, Florida with consideration given to density-dependent groundwater flow. Langevin et al. (2003) describe applications of the codes MOCDENS3D (Oude Essink 1998) and MODHMS (HydroGeoLogic Inc. 2003) to three-dimensional sea-water intrusion modelling of coastal aquifers in the Netherlands and South Florida, respectively.

In this study, the MODHMS code is applied to the problem of sea-water intrusion in the coastal plain aquifers of the Pioneer Valley, north-eastern Australia as shown in Fig. 1. The hydrology of the Pioneer Valley aquifers has been modified through groundwater pumping and prolonged periods of drought, causing hydraulic imbalances between coastal saline water bodies and the groundwater system (Bedford 1978; Murphy and Sorensen 2000;

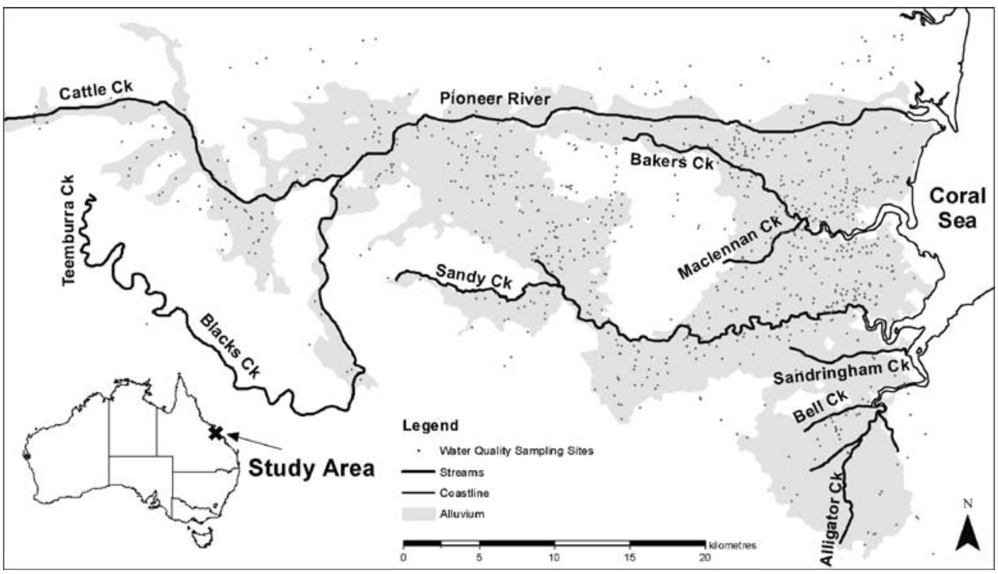

Fig. 1 Locality map of the Pioneer Valley study area, northern Queensland, and water quality sampling sites

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Werner 2004). The result has been a landward shift in the extent of high-salinity groundwater (Murphy and Sorensen 2000; Werner et al. 2005). Planning and management of the Pioneer Valley groundwater resources therefore requires an enhanced understanding of the key sea-water intrusion processes and the development of management tools for predicting sea-water intrusion changes (NR&M 2003).

This paper outlines the methodology adopted for the construction of a three-dimensional sea-water intrusion model of the Pioneer Valley using the MODHMS code. Various aspects of the model are evaluated, including the vertical discretisation approach, the coastal boundary conditions and the initial water-table conditions. The improved understanding of Pioneer Valley sea-water intrusion processes resulting from hydrochemical analyses and numerical modelling is described, and the benefit of complementing numerical modelling with alternative analyses is also highlighted.

Description of the study area

The Pioneer Valley is situated 400 km north of the Tropic of Capricorn in northern Queensland, Australia (Fig. 1). It has a tropical climate characterised by a distinct summer wet season (December–March), and high average rainfall (1551 mm/year) and evaporation (2010 mm/day) (Werner 2004). Land use in the region is dominated by a sugarcane monoculture, which utilises groundwater reserves in both alluvial and fractured-rock aquifers for irrigation.

Production bores in the coastal plain access water predominantly from unconsolidated alluvial and fluvial sediments deposited by the Pioneer River, Sandy Creek and Bakers Creek, and their predecessors. Murphy et al. (2005) describe the coastal plain sediments as Quaternary-aged inter-bedded sequences of clays, sandy clays, sands, clayey sands and gravels overlying mostly Palaeozoic rocks. Generally, up to three upward-fining sequences are evident (Bedford 1978). Sand dune and marine mud deposits are apparent near the coastline and within estuarine fringes (Murphy et al. 2005).

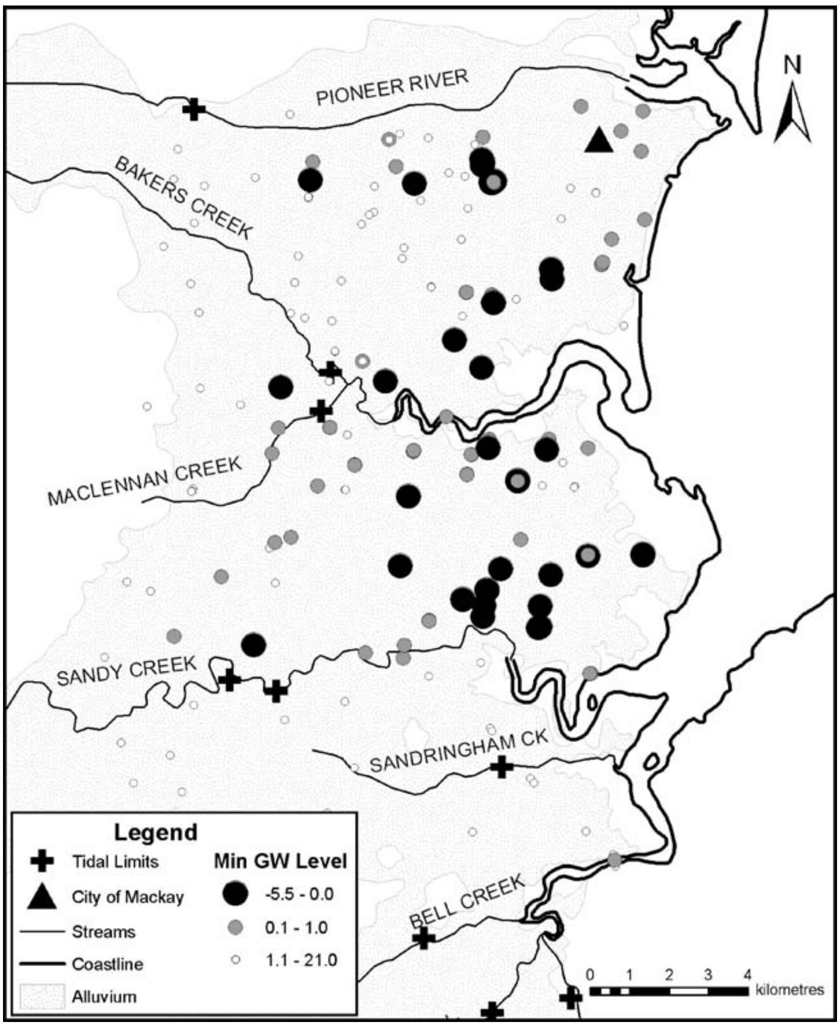

Fig. 2 Minimum-recorded groundwater levels (m AHD) in the Pioneer Valley coastal plain

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The Coral Sea bounds the Pioneer Valley to the east and is macro-tidal, having a 6 m range during spring tides (Gourlay and Hacker 1986). The large tides and relatively flat topography of the coastal plain have resulted in estuarine tidal limits extending up to 16.5 km inland, and estuarine sea-water intrusion contributes significantly to coastal aquifer salination (Werner 2004). The macro-tidal conditions are expected to raise the effective hydraulic heads representing the coastline and estuaries in the model above mean sea level (MSL), due to non-linearity effects and seepage face development on beaches and within estuaries (e.g. Nielsen 1990). The magnitude of any tidal over-heights (i.e. the additional average hydraulic head, above mean sea level resulting from the action of tides) will depend on the beach morphology and local hydrogeology (e.g. Nielsen 1999; Ataie-Ashtiani 2001). No estimates of Pioneer Valley tidal over-heights are available at present due to limited available field data, although the model was used to explore the influence of coastal boundary head changes on sea-water intrusion prediction.

Conceptualisation

The Pioneer Valley alluvial aquifers are fairly shallow, being less than 40 m from ground surface to basement, and are considered unconfined (Bedford 1978; Murphy and Sorensen 2000). Rainfall recharge is the primary influx to the groundwater system, with water-table observations showing a rapid response to rainfall (Bedford 1978; Murphy et al. 2005). During periods of reduced groundwater abstraction and aquifer recharge, water-table mounds develop between the groundwater discharge (sink) features: streams, estuaries and the ocean (Murphy et al. 2005). Water-table levels in observation bores indicate that excessive groundwater pumping has historically caused considerable modification to the groundwater hydrology in the area between Sandy Creek and the Pioneer River (Werner 2004; Murphy et al. 2005), as indicated by the abundance of minimum-recorded water-table levels below MSL depicted in Fig. 2. Note that groundwater levels are given in units of metres Australian

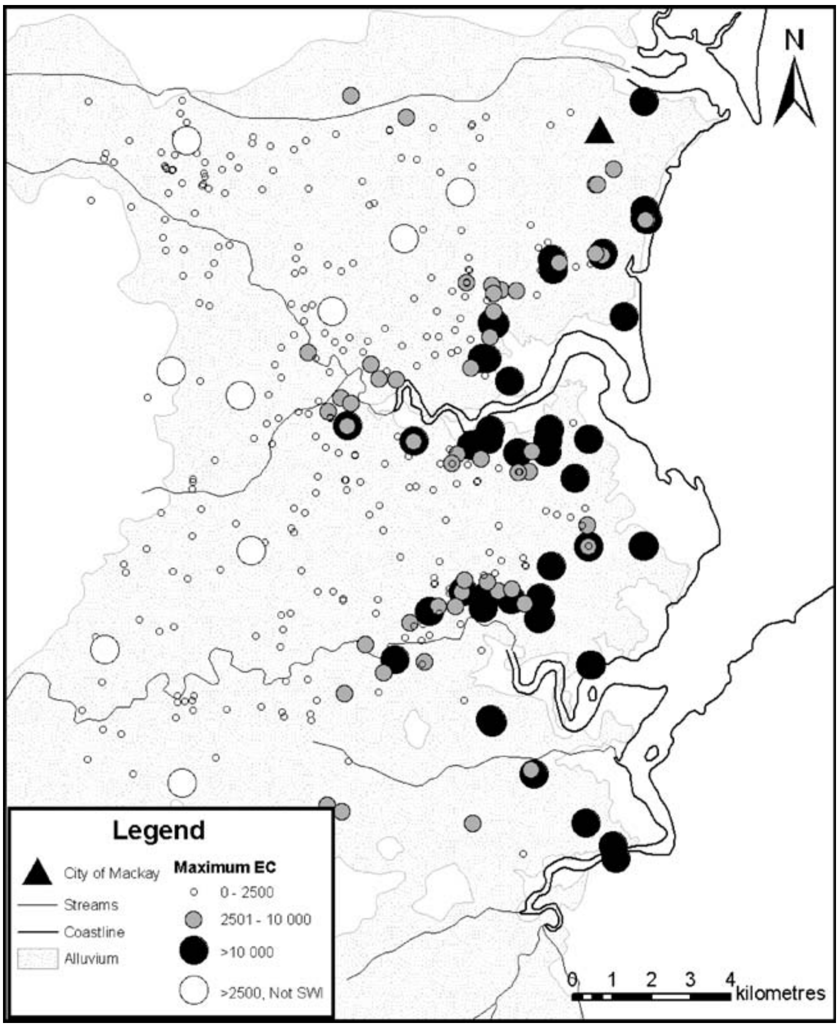

Fig. 3 Maximum-recorded EC values (in micro-Siemens per centimetre: μS/cm) in the Pioneer Valley coastal plain. >2500, Not SWI indicates salination processes other than sea-water intrusion

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Height Datum (m AHD), whereby a level of 0 m AHD is approximately equal to mean sea level (MSL).

The impact of the modified hydrology on sea-water intrusion extent is difficult to quantify in the absence of modelling. However, prolonged lowering of the water table below effective hydraulic heads of estuaries and the ocean constitutes an imbalance in the hydraulic potential, and is considered to increase the susceptibility of the aquifer to landward propagation of sea-water intrusion extent. It should be noted that a level of 0.3 m AHD is roughly the density-corrected MSL at the coastline. Average estuary water levels at tidal limits (Fig. 2) have been estimated to range between 0.7 and 1.5 m AHD (Murphy et al. 2005) in the absence of significant stream flows. These head estimates do not account for any tidal over-heights.

The salinity-state of the Pioneer Valley aquifers is monitored through an observation bore network. Electrical conductivity (EC) is the predominant indicator of Pioneer Valley groundwater quality, with water chemistry being measured sporadically. The distribution of water quality sampling sites is illustrated in Fig. 1. The extent of groundwater salination in the Pioneer Valley coastal plain is represented by the distribution of maximum-recorded groundwater EC measurements, as given in Fig. 3, which shows that the predominant source of groundwater salinity is associated with the ocean and estuaries. Observation bores that appear to be influenced by salination processes other than sea-water intrusion are differentiated in Fig. 3 as “>2500, Not SWI”.

The landward extent of sea-water intrusion appears to be advancing, as indicated by recent increases in groundwater EC (in μS/cm) at the fringe of the sea-water intrusion extent shown in Fig. 4. Two EC contours (1,500 and 10,000 μS/cm) are given that represent an interpretation of sea-water intrusion extent in 2004 by Werner et al. (2005), who attempted to isolate the extent of sea-water intrusion propagating from “modern” surface salinity sources (i.e. contours do not reflect salination by relic sea-water mobilisation or non-marine sources). Therefore, isolated occurrences of increased salinity at some distance inland of the sea-water intrusion extent (as

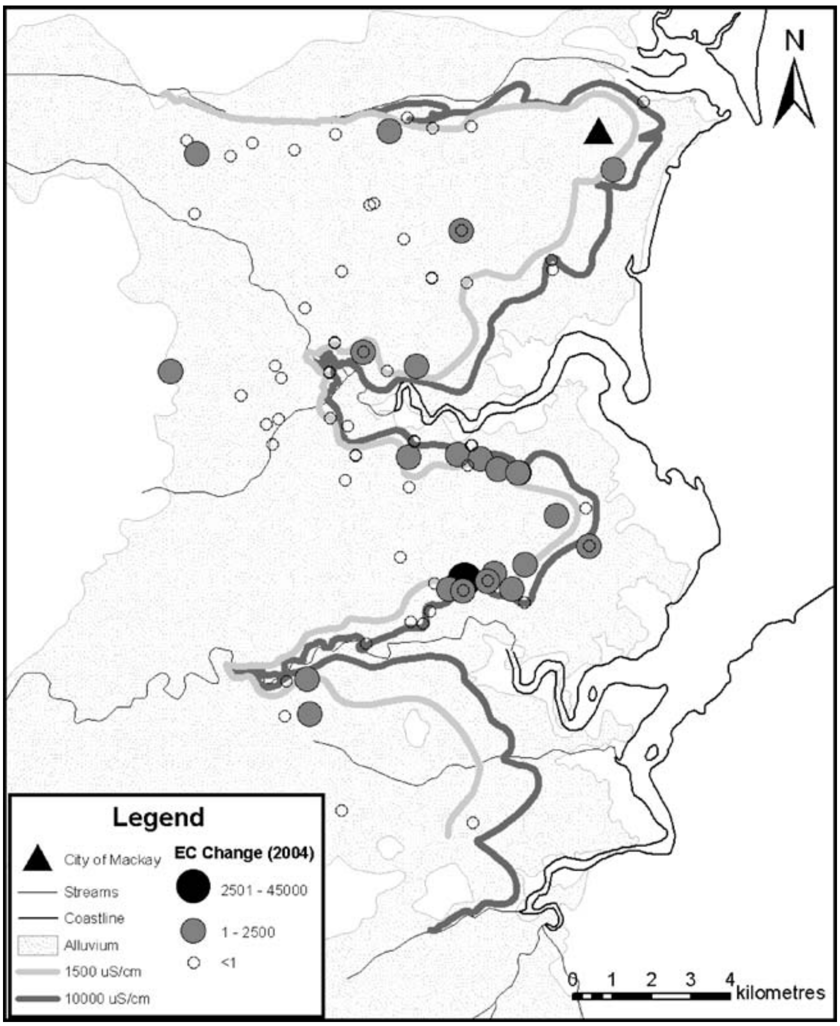

Fig. 4 Increases in the maximum-recorded EC that occurred during 2004

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interpreted by Werner et al. 2005) are attributed to alternative salination processes. The mobility of sea-water intrusion in the Pioneer Valley suggests that an equilibrium condition has not been reached, and no such steady-state condition may prevail given seasonal and long-term variations in land-use and climatic stresses as reported by Murphy et al. (2005).

Pioneer Valley groundwater salination has also occurred through other mechanisms such as basement rock dissolution (Bedford 1982), agricultural activities (Baskaran et al. 2002) and relic sea-water mobilisation (Murphy and Sorensen 2000; Werner 2004). Sites of elevated EC not attributed to sea-water intrusion are highlighted in Fig. 3. Distinguishing sea-water intrusion from other processes is a necessary precursor to sea-water intrusion management and modelling (Gassama et al. 2003; Kim et al. 2003; Post 2004). Numerical modelling requires interpretation of sea-water intrusion extent for the assignment of initial salinity conditions and to allow comparisons between model predictions and field observations. Where highly saline groundwater is adjacent to estuaries and the ocean, sea-water intrusion is likely to be the predominant salination process. However, other parts of the aquifer are susceptible to the combined effects of terrestrial salination (e.g. basement dissolution) and sea-water intrusion, as indicated by groundwater quality observations of Bedford (1978, 1982), Murphy and Sorensen (2000) and Werner et al. (2005).

A methodology similar to those used by McMahon (2004) and Park et al. (2005) was employed to provide insight into salt origins and confirm the interpretations of sea-water intrusion extent by Werner et al. (2005) (Fig. 4). The approach involved analyses of hydrochemical indicators and is best described through illustration of the results, as shown in Figs. 5 and 6. In summary, the methodology involved mapping several different ionic ratios to distinguish distributions of chemically similar groundwater, thus inferring salinity sources. Only the water chemistry of the largest EC sample from each bore was considered. Bores with maximum-recorded EC values greater than 2,500 μS/cm are distinguished in Fig. 6. The datasets pertaining to each ionic ratio were partitioned using distinguishing values calculated from inflection points on cumulative probability curves, plus the value for sea-water (Fig. 5). Several ionic ratios were analysed and mapped to characterise sea-water intrusion and other salination processes, but only the results of the Ca:HCO_3+CO_3 analysis are given in this paper as an illustrative example and for brevity.

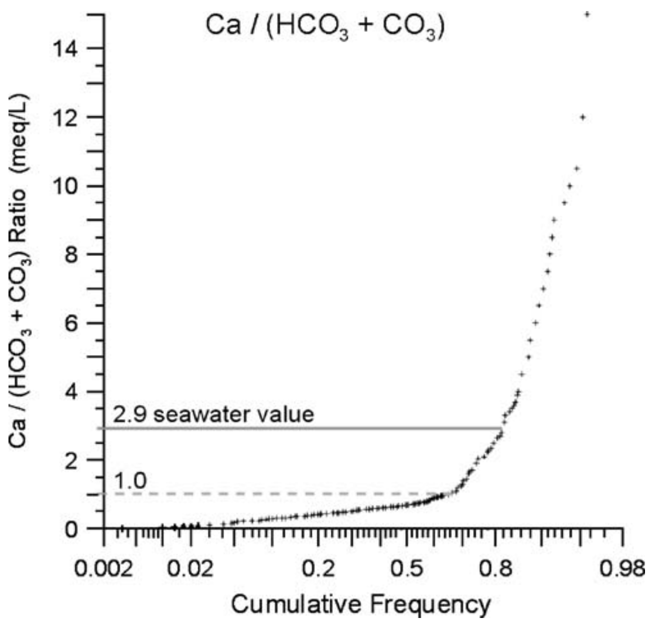

Fig. 5 A cumulative probability plot of the ratio Ca:(HCO_3+CO_3), showing an inflection value of 1.0 and the sea-water value of 2.9 (from Hem 1989)

A distinct chemical signature of groundwater within the region affected by sea-water intrusion in terms of the ratio Ca:HCO_3+CO_3, is shown in Fig. 6, thus supporting the interpretation of Werner et al. (2005). While the cause of this clear differential in Ca:HCO_3+CO_3 values within and outside of the sea-water intrusion extent is not discussed in detail here, such contributing factors may include: carbonate precipitation/dissolution, cation exchange reactions, mineral hydrolysis, and mixing with calcium-dominant groundwater (Bedford 1982; Richter and Kreitler 1993; Jones et al. 1999). McMahon et al. (2005) give a more complete discussion of ionic ratio analyses for the Pioneer Valley coastal plain groundwater.

It should be noted that the maps included in this paper do not reflect vertical variations in groundwater salinity, although large vertical salinity gradients (typically with freshwater overlying saline water) have been observed and simulated using cross-sectional numerical models (Werner 2004). Salinity maps (e.g. Fig. 3) are designed to highlight the maximum EC measured within the alluvium thickness. It is usually the case that the occurrence of elevated salinities at any depth within the alluvium renders the entire aquifer profile unusable for high-yield pumping due to the shallowness of alluvial deposits. From the perspective of groundwater resource management, planar depictions of sea-water intrusion extent are generally sufficient. However, the sea-water intrusion model is three-dimensional (rather than vertically integrated), because flow and transport in the vertical direction and the depth-variability of horizontal flow, salinity and density are likely to be necessary considerations following modelling by Werner (2004) and others (e.g. Oude Essink 2001; Langevin 2003; Gingerich and Voss 2005).

The results of the current sea-water intrusion conceptualisation were combined with the findings from other Pioneer Valley studies (Bedford 1978; Murphy and Sorensen 2000; Werner 2004; McMahon et al. 2005; Werner et al. 2005) to develop a sea-water intrusion-potential map given in Fig. 7. The map reduces the reliance on numerical model predictions by providing an interpretation of sea-water intrusion susceptibility in the Pioneer Valley that is independent of modelling. It is anticipated that the numerical model may produce

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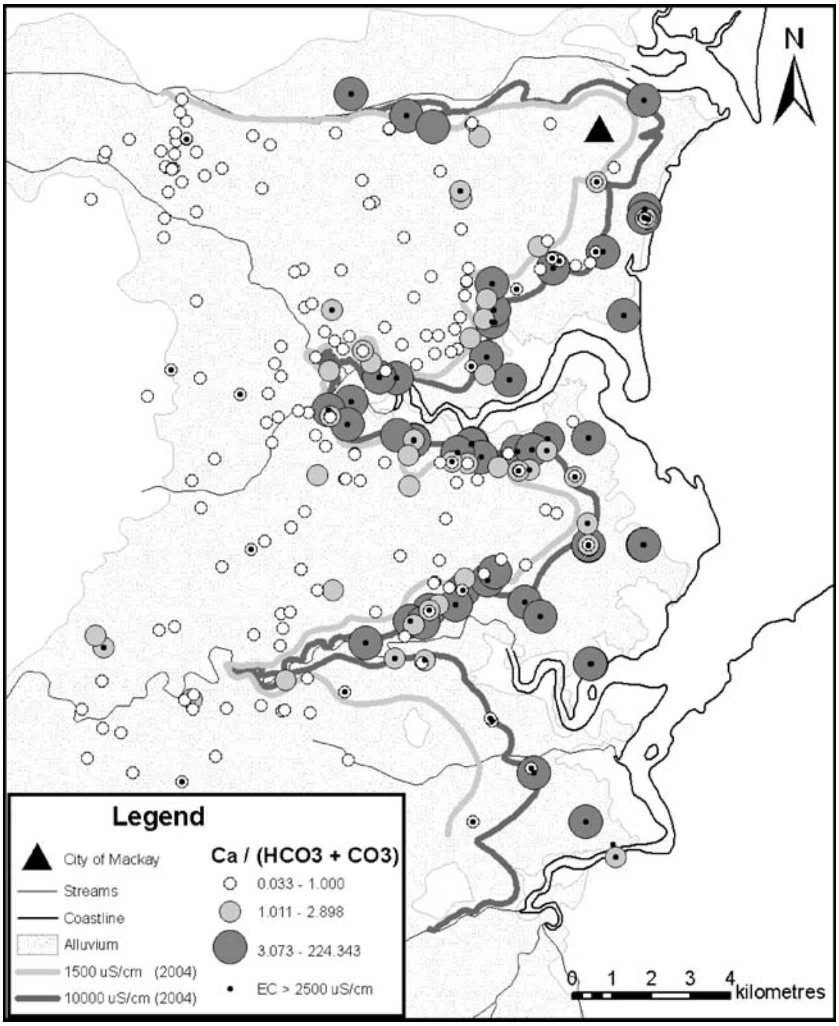

Fig. 6 Distribution of Ca:(HCO_3+CO_3) from maximum-EC samples

misleading predictions of salination trends in areas where relic sea-water mobilisation or other salination processes are occurring, and an alternative to numerical modelling is required to illustrate potential salination issues in those areas. By depicting the conceptual interpretation in this format, resource managers can easily assess monitoring requirements. Construction of the map considered three main system characteristics: the aquifer basement shape and the hydrogeology (e.g. Abarca et al. 2002), recent interpretations of sea-water intrusion extent (Werner et al. 2005) and evidence of pumping-induced groundwater depressions (Fig. 2 and Murphy et al. 2005). It should be noted that the map is entirely interpretative and not meant to depict the relative probability of sea-water intrusion advancement. Further, the distribution of field observations is highly variable, and therefore the accuracy of the map is dependent on the quantity, quality and timing of available field data, which are sparsely distributed south of Sandy Creek and near the mouth of the Pioneer River, but are reasonably distributed elsewhere (Fig. 1).

Numerical model

When the saltwater–freshwater transition zone extends greatly in both an areal and vertical extent, the density-dependent miscible flow and transport modelling approach first described by Henry (1964) is preferable to the assumption of two-phase fluid flow separated by a sharp interface known as the Ghyben-Herzberg relationship. See Reilly and Goodman (1985) among others for a historical overview of these approaches. Therefore, for coastal aquifers at a regional scale such as the Pioneer Valley aquifer, only numerical models that cast saltwater intrusion as a density-driven mixed-type process were considered.

MODFLOW, the modular, cell-centred, finite-difference code for three-dimensional saturated flow (McDonald and Harbaugh 1988) has previously been adapted to produce three-dimensional density-dependant modelling codes such as SEAWAT (Guo and Langevin 2002), MOC-DENS3D (Oude Essink 1998), the SWI Package (Bakker and Schaars 2003) and MODHMS (HydroGeoLogic Inc.

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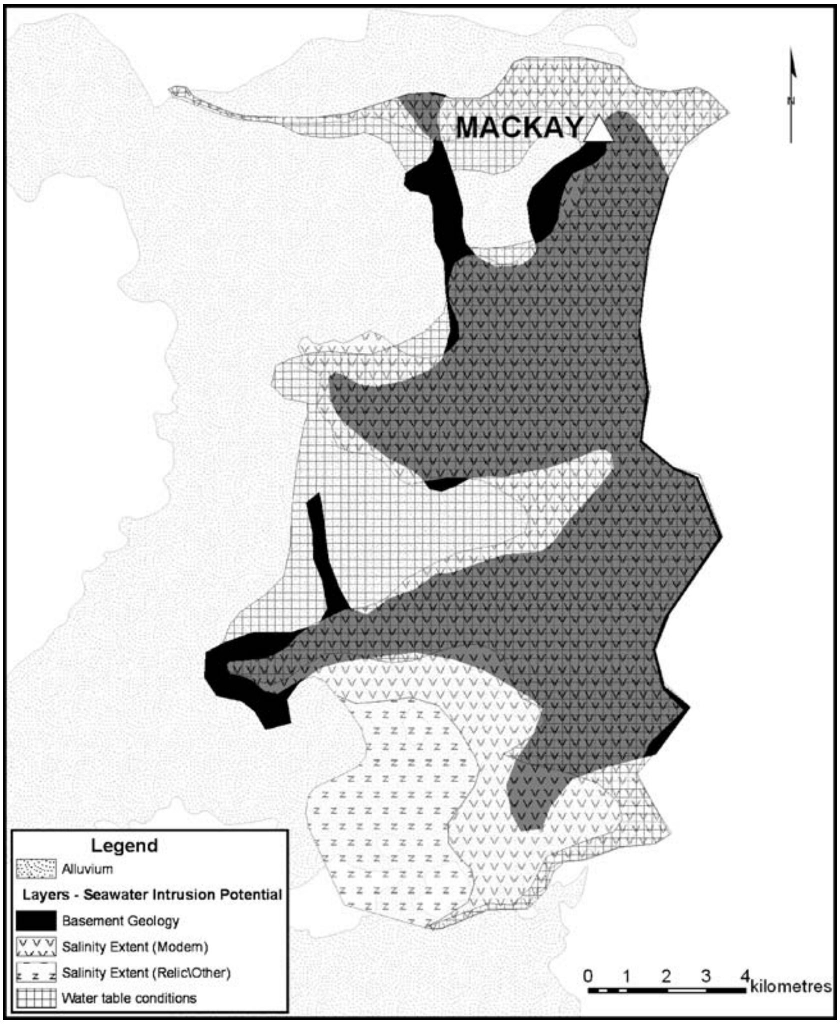

Fig. 7 A map of the interpreted sea-water intrusion potential. The *grey area* is where the basement geology area is overlapped by the salinity extent areas

2003). A verification of the density-dependent flow component of three of these codes (SWI, MOCDENS3D, and SEAWAT) by Bakker et al. (2004) concluded that they could be used to model accurately the movement of interfaces between immiscible fluids, and have little or no numerical dispersion. However, in an effort to minimise the considerable computational impost of a regional-scale density-dependant flow and transport model, compromises are often made in the form of coarse grid discretisation, whereby large dispersivity values are required to maintain numerical stability, as noted in Diersch and Kolditz (2002).

While satisfactory agreement of appropriate model codes with benchmarking problems featuring small-to-moderate density effects (e.g. Henry 1964) is achievable, Johannsen et al. (2002) showed that three-dimensional variable density problems require very fine, structured meshes for systems with more pronounced density effects. Also, Schincariol et al. (1994) found that minor changes to the dispersion parameter field or spatial and temporal discretisation could give rise to the propagation of numerical errors only ameliorated by fine mesh and time-steps. In response to such limitations, model telescoping and subsequent grid refinement (in terms of vertical discretisation) was undertaken to manage these numerical effects in addition to the adoption of adaptive time-stepping, in accordance with the requirements of the applied numerical solution methods (described in section Modelling methodology).

The advantages of integration with MODFLOW are numerous and as such, were considered a prerequisite for saltwater intrusion code selection. For example, existing sub-regional and site-specific model data sets could be employed with little or no modification; an almost unlimited degree of heterogeneity within the model domain could be accommodated, combined with the ability to interface with MODFLOW modules for simulation of various features of the hydrogeological system.

Following a review of the available codes, MODHMS was preferred as the platform for saltwater intrusion modelling due principally to its numerical robustness, in conjunction with software support provided directly from the code developer. Moreover, improved (or new) MOD-

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FLOW formulations for well discharge, surface and overland flow, unsaturated zone movement and adaptive time stepping incorporated into MODHMS, provided additional flexibility and rigour.

The governing equation for flow of a mixture fluid of variable density in an aquifer can be written in terms of an equivalent freshwater head in Eq. (1) below (HydroGeoLogic Inc. 1994).

$$S_{\mathrm{w}}S_{\mathrm{s}}\frac{\delta h}{\delta t}+\phi\frac{\delta S_{\mathrm{w}}}{\delta \mathrm{t}}+S_{\mathrm{w}}\phi\frac{\delta\eta^{\mathrm{T}}c^{\mathrm{T}}}{\delta t} = \frac{\delta}{\delta x_{\mathrm{i}}}\left[K_{\mathrm{ij}}\left\{\frac{\delta h}{\delta x_{\mathrm{j}}}+\eta^{\mathrm{T}}c^{\mathrm{T}}\frac{\delta z}{\delta x_{\mathrm{i}}}\right\}\right]-W \quad (1)$$

where:

x and z are Cartesian coordinates (L)
K_{ij} are the principal components of hydraulic conductivity along the x, y, and z axes, respectively (LT^{-1})
h is the equivalent freshwater hydraulic head (L)
W is a volumetric flux per unit volume and represents sources and/or sinks of water (T^{-1})
ϕ is the drainable or effective porosity
w is the active fluid phase (which is water for most typical simulations of coastal aquifer systems)
S_w is the degree of saturation of water, which is a function of the pressure head
S_s is the specific storage of the porous material (L^{-1})
$\eta^T c^T$ represents the total density factor (see below)
t is time (T)

The term $\eta^T c^T$ in Eq. (1) is the additional buoyancy term required by the flow equation for density-dependent simulations. The total density factor is the sum of the density factors of each of the component species whose density effect is significant. Further description of the numerical approach to density-dependent flow in MODHMS is provided in HydroGeoLogic Inc. (2003).

In addition to the flow Eq. (1), a second partial differential equation is required to describe solute transport in the aquifer as a result of advection and hydrodynamic dispersion. The advective-dispersive equation to describe salt transport is (Huyakorn et al. 1987):

$$\frac{\delta}{\delta x_{\mathrm{i}}}\left(D_{\mathrm{ij}}\frac{\delta c}{\delta x_{\mathrm{j}}}\right)-v_{\mathrm{i}}\frac{\delta c}{\delta x_{\mathrm{i}}}=\phi\frac{\delta c}{\delta t}+q_{\mathrm{r}}c \quad (2)$$

where:

c is solute concentration in the active phase (ML^{-3})
D_{ij} is the apparent hydrodynamic dispersion tensor (L^2T^{-1})
v_i represents the seepage velocity (LT^{-1})
q_r is the volumetric flow rate of sources, per unit volume of porous medium ($L^3T^{-1}L^{-3}$).

Groundwater flow causes the redistribution of solute concentration, which in turn alters the density field and ultimately, influences groundwater flow patterns. Therefore, the movement of groundwater and the transport of solutes in the aquifer are coupled processes, and the two equations must be solved jointly.

Modelling methodology

To the authors' knowledge, the only other published example of MODHMS application to sea-water intrusion modelling is that of Langevin et al. (2003), who describe a case study of sea-water intrusion in the Southwest Florida Water Management District. The model development approach taken by Langevin et al. (2003) is somewhat similar to the methodology applied here, although this paper describes model limitations in greater detail. Given the lack of previous MODHMS applications to sea-water intrusion problems, the code was initially verified against the popular benchmarking problem of Henry (1964). MODHMS was in good agreement with published solutions to the pressure and salinity distributions.

An abbreviation of the various stages of model construction is illustrated in Fig. 8. The groundwater flow aspect (i.e. hydraulic properties, boundary conditions and aquifer stresses) of the Pioneer Valley sea-water intrusion model is based predominantly on the MODFLOW (Harbaugh and McDonald 1996) model developed by Kuhanesan et al. (2005). A schematic of the Kuhanesan et al. (2005) model is given in Fig. 9, which shows the model grid, and MODFLOW well and river cells. Automated calibration of the MODHMS model was not possible due to long run-times, while considerably shorter run-times associated with the Kuhanesan et al. (2005) model allowed an intensive inverse modelling exercise to be undertaken to estimate hydraulic parameters. Hydrodynamic calibration prior to sea-water intrusion modelling has been undertaken previously (e.g. Sadeg and Karahanoglu 2001; Langevin et al. 2003), although neglecting solute transport predictions and observations from the calibration may result in higher calibration non-uniqueness (e.g. McKenna et al. 2003; Shoemaker 2004).

The Kuhanesan et al. (2005) flow model accounts for groundwater pumping, rainfall and irrigation recharge, river-aquifer and ocean-aquifer interactions, inflows from surrounding fractured rock aquifers, and surface drains. The finite-difference grid comprises a uniform cell size of 250 by 250 m and the entire aquifer is assumed to behave as an unconfined (water-table) system. The model hydraulic conductivity (K), specific yield (S_y) and riverbed conductance were calibrated using the advanced spatial parameterisation (ASP) technique of PEST (Doherty 2004). Kuhanesan et al. (2005) considered the model to be an acceptable representation of the Pioneer Valley groundwater flow system, as evidenced by the match between observed and simulated water-table behaviour.

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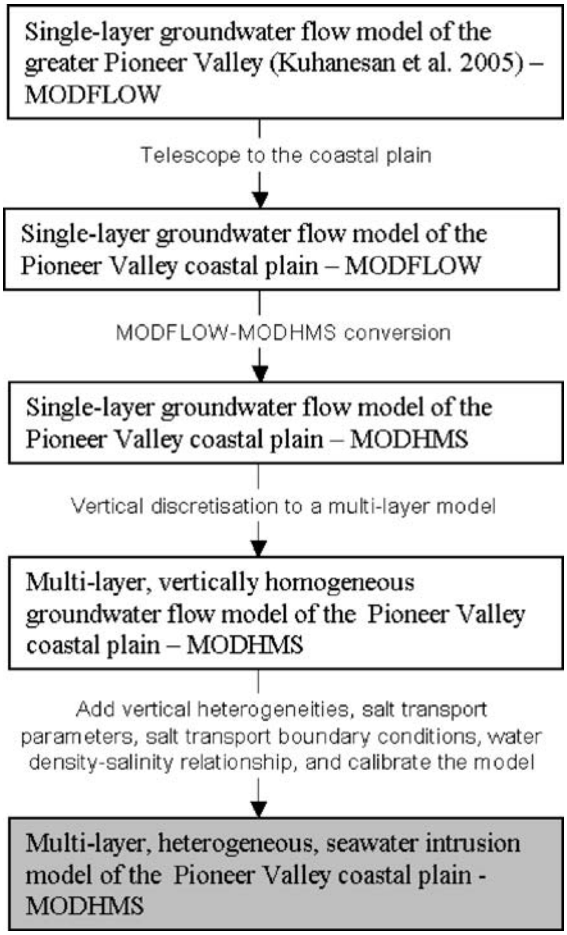

Fig. 8 A flowchart of the procedure for developing single-layer and multi-layer sea-water intrusion models

The Kuhanesan et al. (2005) flow model was telescoped (i.e. the model was reduced in areal extent) to the coastal plain (along the dissection line X-X in Fig. 9) for reasons of computational efficiency in sea-water intrusion simulations. It was considered necessary to subdivide the single-layer model to incorporate salinity gradients, heterogeneities, groundwater flow and salt transport in the vertical direction. Numerical modelling of Pioneer Valley sea-water intrusion in cross section by Werner (2004) and similar modelling studies (e.g. Neilson-Welch and Smith 2001) highlight the importance of depth-variability in sea-water intrusion processes.

The single-layer model was split into ten layers of equal, but spatially variable thickness that reflect the shape of the topographic and aquifer basement surfaces. This method of vertical discretisation is similar to that adopted by Langevin et al. (2003). Vertical discretisation necessitated a change in layer-type from unconfined to "variably-saturated" to avoid cell drying and re-wetting problems common in MODFLOW based models (Langevin et al. 2003). The use of "pseudo-soil relations" in MODHMS (Panday and Huyakorn 2004) permitted the use of unconfined aquifer properties and avoided the high parameterisation, i.e. the assignment of multiple soil hydraulic parameters, usually associated with true variably saturated modelling (e.g. van Genuchten 1980).

Cross-sections through the 1-layer model and an equivalent ten-layer model are shown in Fig. 10 to illustrate the vertical discretisation. Cross-section alignment is identified as transect A-A in Fig. 9. In Fig. 10, shaded cells represent various boundary conditions and aquifer stresses (e.g. wells, drains, fixed head, etc.), although the intention is not to identify specific cell types along the given transect. Where cells are inactive (designated as black cells in Fig. 10, e.g. the right-hand boundary), the top and bottom of the aquifer were assigned arbitrary values for plotting purposes. The up-gradient boundary (left boundary) comprises time-variant, specified-head cells that are used to represent the "purged" portion of the model (i.e. the region west of the dissection boundary X-X shown in Fig. 9).

In modelling studies by Neilson-Welch and Smith (2001) and Werner (2004), vertical aquifer heterogeneities were necessary to adequately predict sea-water intrusion extent, although their studies differed in scale to the Pioneer Valley

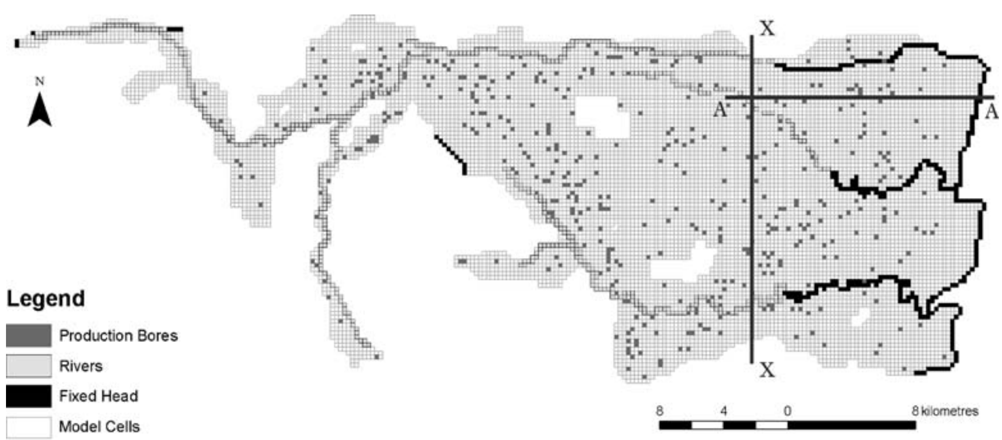

Fig. 9 An illustration of the Kuhanesan et al. (2005) groundwater flow model

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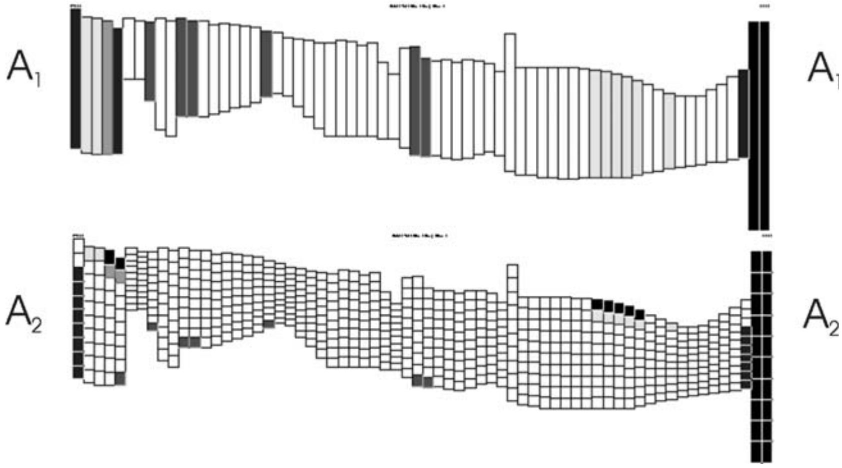

Fig. 10 Cross sections through row 17 of a single-layer telescoped model (A_1-A_1) and a ten-layer telescoped model (A_2-A_2), located as A-A in Fig. 9. *Black cells* represent inactivity and *shaded cells* represent various boundary conditions and aquifer stresses

situation. Comparisons between vertically homogeneous and vertically heterogeneous models of Pioneer Valley sea-water intrusion also showed differences in predictions, and therefore vertical heterogeneities were incorporated into the model using depth-varying K and effective porosity (ϕ).

A generic vertical heterogeneity model (GVHM) was used that reflects general descriptions of the coastal alluvium (Bedford 1978; Murphy and Sorensen 2000; Murphy et al. 2005) as consisting of up to three upward-fining sequences (i.e. more coarse-grained materials; sands and gravels are found in the lower part of the aquifer), in the absence of any regional-scale interpretation of the complex inter-fingering of alluvial deposits. The GVHM was applied universally and was used to modify the vertically homogeneous K-distribution such that the resulting vertically heterogeneous K-distribution had approximately the same transmissivity distribution as the original model. Thus, application of the GVHM is expected to retain the hydrodynamically calibrated state of the original flow model of Kuhanesan et al. (2005). Vertical heterogeneities in K were established using GVHM "proportionality constants", which provided an approximation of the vertical distribution in relative K from the representative stratigraphy. Proportionality constants below the average water-table elevation at each cell were normalised to 1.0 and multiplied by calibrated K values to produce a vertically heterogeneous representation of the aquifer of virtually identical transmissivity to the homogeneous model. The proportionality constants or layer-values of relative K defined by the GVHM are given in Table 1, which also details profiles of ϕ and horizontal-to-vertical K-anisotropy values applied as constants throughout the model. The values in Table 1 were adopted after a manual calibration that involved extensive model testing using various literature values of aquifer hydraulic properties (e.g. Carsel and Parrish 1988; Driscoll 1989; Weight and Sonderegger 2000).

Sea-water intrusion model calibration involved a rigorous qualitative assessment and was based on the results of sensitivity analyses, in which several model parameters/aspects were systematically varied and the influence on sea-water intrusion prediction was observed. In the sensitivity analyses, a 12-year simulation was adopted, representing the period July 1991–June 2003, as the original 5-year time frame used in calibrating the Kuhanesan et al. (2005) model was not considered of adequate duration. Sea-water intrusion varies gradually (van Dam 1999) and sufficiently long periods are necessary to analyse temporal trends. The initial salinity conditions were based on an interpretation by Werner et al. (2005).

Salt transport parameters such as porosity and the longitudinal, transverse and vertical components of dispersivity (i.e. α_L, α_T, α_V) were initially assigned literature values (e.g. Hunt 1998; Brady and Kunkel 2003) and then modified within practical constraints to provide a better match between observation and prediction—a common practice in sea-water intrusion modelling (e.g. Bond and Bredehoeft 1987; Neilson-Welch and Smith 2001; Pattle Delamore Partners Ltd 2002; Hassan et al. 2003). This process is described in more detail in the following section. Calibration also explored variations to the coastal boundary heads and initial water-table conditions, and involved revisions of the original conceptualisation that resulted in

Table 1 Parameter values used in the generic vertical heterogeneity model (GVHM)

Layer	Proportionality constants from the GVHM	ϕ	$K_{horizontal}$:$K_{vertical}$
1	2	0.15	1
2	2	0.18	1
3	5	0.22	2
4	5	0.22	2
5	15	0.30	3
6	4	0.22	2
7	2	0.18	1
8	1	0.12	1
9	50	0.30	20
10	30	0.25	10

K is the hydraulic conductivity (L/T) and ϕ is the effective porosity

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Table 2 Differences between the original (un-calibrated) and final (calibrated) sea-water intrusion models

Model characteristic	Original model value or approach	Final model value or approach
Coastal boundary head	0 m AHD	0.8 m AHD
Initial water-table conditions	Same as Kuhanesan et al. 2005	The last time-step from the 12-year simulation (1991–2003), which was modified for the new coastal boundary head
K	Same as Kuhanesan et al. 2005, i.e. vertically homogeneous and isotropic	Based on Kuhanesan et al. 2005 with vertical heterogeneities and vertical anisotropy (see Table 1)
Dispersivity (α_L, α_T, α_V)	(40, 8, 1 m)	(100, 10, 0.1 m)
ϕ	$1.5\times S_y$	Layer-constant values (see Table 1)
Mangroves, small estuaries, tidal drains	Not considered	Included as surface salt sources (i.e. using a solute transport boundary condition)
Mackay city domestic use	Not included	Estimates of domestic use applied to the model
Southern boundary inflows	Same as Kuhanesan et al. 2005	Reduced by factors of 0.01 and 0.001 to reflect model K values at the boundary

the addition of mangrove flats, small estuaries and tidal drains to the conceptual model. Sensitivity analyses provided indication of the most suitable parameter values, albeit with limited consideration given to the parameter-interdependence associated with multi-parameter optimisation. That is, *optimal* values from sensitivity analyses were not globally optimal, but were dependent on the other parameter values adopted in each sensitivity analysis.

Results and discussion

Calibration results

The changes to the sea-water intrusion model incurred through calibration are summarised in Table 2, and improvements to sea-water intrusion predictions (in terms of the 12-year salinity distribution at the base of the aquifer) are depicted in Fig. 11. The calibration phase of

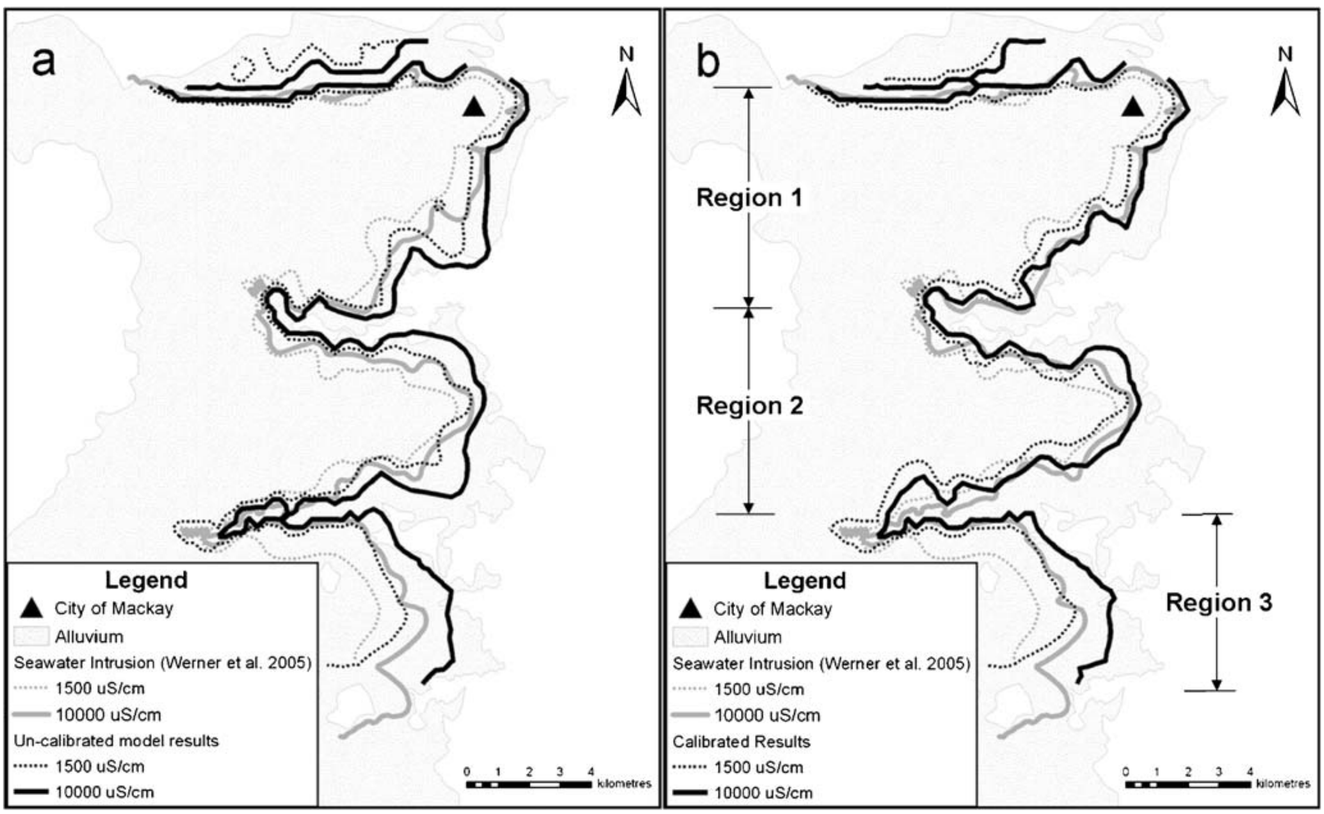

Fig. 11 A comparison between observed salinity contours (*grey lines*) and predicted salinity contours (*black lines*) from the **a** un-calibrated model and **b** calibrated model. The coastline is not shown

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model development significantly improved the match between observation and simulation of sea-water intrusion, as evidenced by the closeness of the salinity contours in Fig. 11b, compared to those in Fig. 11a. Throughout the majority of the Pioneer coastal plain, the match is considered adequate, although in some areas significant discrepancies between observation and simulation could not be overcome through calibration. Observations of salinity trends in region 3 (Fig. 11b) were especially difficult to reproduce through model modifications. In this area, groundwater salination is probably occurring through alternative processes such as relic sea-water mobilisation or water–rock interactions, as suggested by Werner et al. (2005). Other discrepancies between simulation and observation of sea-water intrusion are also evident in regions 1 and 2 (Fig. 11b), although mostly in the position of the lower salinity (1,500 μS/cm) contour.

The calibration match (i.e. Fig. 11b) was achieved partly through the representation in the model of small tidal waterways (e.g. tidal drains, small estuaries), and areas of occasional tidal inundation adjacent to mangrove forests such as sand-flats and mud-flats. Initially, these features appeared to contribute significantly to the extent of sea-water intrusion. However, relic sea-water deposits resulting from prehistoric sea-water inundation of much of the coastal plain (Gourlay and Hacker 1986) may occur in the same coastal margin. Limited groundwater sampling in these regions makes it difficult to differentiate salt sources or salination processes, although improvements in the calibration match suggest that surface salinity sources are at least partially influencing sea-water intrusion extent. Water resource management strategies for both forms of salination may be the same given the shallowness of the alluvium, although further hydrochemical and hydrogeological analyses are warranted to better understand Pioneer Valley salination processes in these areas.

Calibration of the model was not aimed at reproducing any localised observations of vertical salinity gradients, although generally, it is common to encounter increasing salinity with depth in areas subject to advancing sea-water intrusion extent (Werner 2004). Examples of simulated vertical salinity gradients, including those in areas where salinity-inversion (i.e. sea water above fresh groundwater) is caused by the partially penetrating estuaries, are illustrated in Fig. 12. Simulated salinity patterns show a general trend of increasing salinity with depth, as observed in field observations, although a more rigorous analysis is required to ascertain whether the model provides a reasonable representation of vertical flow and transport effects. It is likely that dispersion parameters and the grid resolution will influence predictions of vertical salinity gradients (e.g. Diersch and Kolditz 2002), and further investigation of the effects of these characteristics on model accuracy is warranted.

Coastal boundary head and initial water-table conditions

The macro-tidal characteristics (>6 m spring tidal range) of the ocean and estuary boundaries, and the shallow-sloping beach morphology of the Pioneer Valley are expected to produce a significant tidal over-height (e.g. Nielsen 1990, 1999). The Kuhanesan et al. (2005) model neglects the effects of tidal over-heights due to difficulties in quantifying the magnitude and variability of this effect for the Pioneer Valley system. Preliminary sea-water intrusion simulations (i.e. pre-calibration) indicated that the Kuhanesan et al. (2005) coastal head was indeed under-estimated, with predictions giving unrealistic sea-water intrusion trends (i.e. under-prediction of sea-water intrusion).

The importance of neglecting any tidal over-height is expected to be somewhat compensated for by the process of calibrating the Kuhanesan et al. (2005) model. Calibration modifies model hydraulic parameters (e.g. K and S_y) to match water-table observations, and as such, aquifer parameters near the coast may partially account for any error in the elevation of the coastal boundary head. Only a

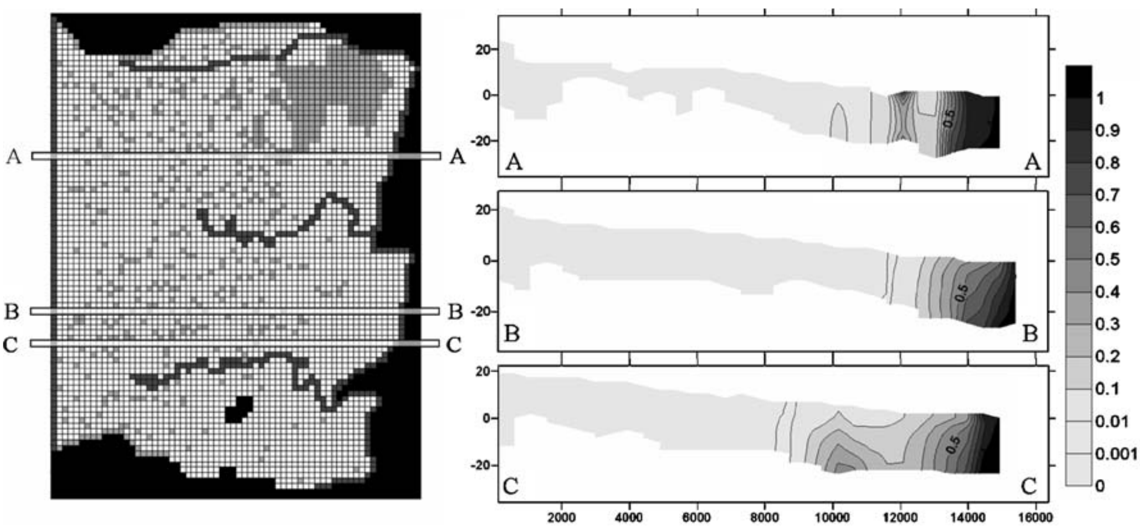

Fig. 12 Profiles of salinity distributions (relative salinity units used, whereby 1.0 is sea water). The vertical axis scale is m AHD

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true indication of the impacts of errors in the coastal boundary head is possible through re-calibration using different boundary values. This may be the focus of future work, but in the interim, a sensitivity analysis of coastal boundary heads on sea-water intrusion prediction has been conducted.

The results of two different comparisons of boundary head effects, reported in terms of salinity distributions in layer 10 (aquifer base) at the end of simulations, are illustrated in Fig. 13. Figure 13a represents a 5-year simulation period (1998–2003) and the changes in sea-water intrusion extent predicted using two different boundary heads of 0 m AHD and 1.5 m AHD. The initial water-table distribution of the Kuhanesan et al. (2005) model was adopted in both 5-year simulations. Figure 13b shows results from two 200-year simulations that again use coastal heads of 0 and 1.5 m AHD, but the initial water-table distributions approximately represent steady-state conditions, i.e. the hydraulic heads after 48 years of constant aquifer stresses correlate to the respective boundary heads. Aquifer stresses (recharge, pumping, etc.) in the 200-year simulations were taken as average values from the 12-year simulation (July 1991–June 2003) described previously.

The results given in Fig. 13b indicate that modifying the coastal hydraulic head produces only minor changes to Pioneer Valley sea-water intrusion predictions, when an initially stable hydraulic condition is adopted. The Pioneer Valley flow system is essentially a flux-driven system, with distributed recharge being the predominant inflow mechanism and comparatively few hydraulic head controlling features in the coastal plain other than the coastline and estuaries (Kuhanesan et al. 2005; Murphy et al. 2005). As such, modifications to the model's coastal head have only minor impacts on predicted hydraulic gradients, which are the principal controllers of sea-water intrusion extent in a system of fixed hydraulic conductivity and constant groundwater-sea-water density differences (e.g. Glover 1964). The 200-year simulation results also provide some indication of areas potentially more susceptible to sea-water intrusion advancement in the Pioneer Valley under recent management practices. This is because the stresses used were representative of average conditions between 1991 and 2003. Given the differences in the predicted sea-water intrusion extents after 5 years (Fig. 13a) and after 200 years (Fig. 13b), combined with recent evidence of sea-water intrusion encroachment (e.g. Fig. 4), the system is probably not currently in a state of equilibrium.

Adopting initial hydraulic conditions that were hydraulically unstable (i.e. sharp hydraulic gradients near the coastal boundary that resulted from modifications to the coastal boundary head, based on the Kuhanesan et al. 2005 initial heads) induced large differences in sea-water intrusion predictions after 5 years in region 2 (Fig. 13a). This result highlights the importance of specifying stable initial hydraulic head distributions in short-term sea-water intrusion simulations. It is likely that automated calibration of sea-water intrusion models needs to somehow ensure an initially stable or equilibrium hydraulic condition if simulation periods are relatively short.

Long-term simulations show the apparent insensitivity of sea-water intrusion predictions to coastal boundary heads (Fig. 13b), in the absence of the "initial condition effects" as illustrated in Fig. 13a. Nevertheless, it is imperative that accurate boundary head values are used in

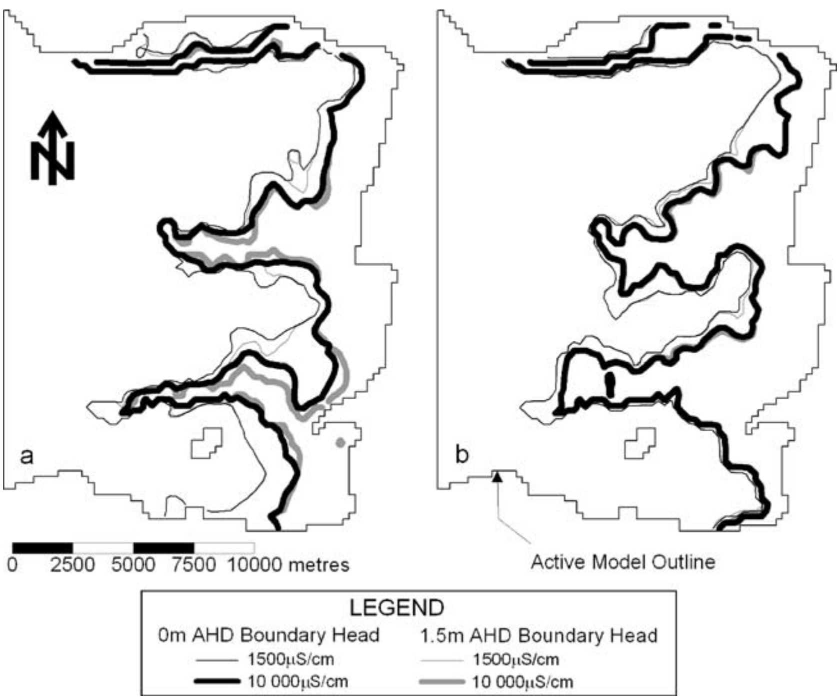

Fig. 13 Comparison between boundary head effects using **a** two 5-year simulations and **b** two 200-year simulations

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the Pioneer Valley sea-water intrusion model to best reproduce relationships between water-table conditions and sea-water intrusion trends. Such relationships are essential for analysing water resource management decisions, which are likely to require estimation of the relationship between water-table distributions and potential sea-water intrusion movements. For example, the model may be used to approximate water-table levels in monitoring bores, which are used by resource managers to "trigger" management actions such as pumping restrictions or changes in annual water allocations, and the prediction of any such trigger levels is likely to depend on the accuracy of the assumed coastal boundary head.

The results of a sensitivity analysis into coastal hydraulic head and initial conditions, aimed at evaluating a range of boundary and initial conditions in terms of coastal water-table predictions are summarised in Table 3. Differences (errors) between observation and simulation for the 12-year simulation period are given for four different initial conditions and seven different boundary hydraulic heads that included the initial Kuhanesan et al. (2005) distributions. The initial water-table conditions specified as original in Table 3 were those used by Kuhanesan et al. (2005). Initial conditions designated as 12-year, 24-year and 48-year were obtained by running the Kuhanesan et al. (2005) simulation 1, 2 and 4 times consecutively, and adopting the final hydraulic heads. Positive average errors represent simulated water levels higher than observed water levels. Any changes to the initial conditions gave higher water-table prediction errors; an expected outcome given the hydrodynamically calibrated state of the original model. Therefore, while adopting stable initial hydraulic conditions (e.g. the 48-year initial conditions) reduced the overall error in salinity predictions, a trade-off was incurred in the form of increased water-table prediction error.

The average water-table error in the 12-year Kuhanesan et al. (2005) model, which neglects tidal over-heights, indicates that predicted coastal hydraulic heads are lower than observed heads by 0.39 m on average, suggesting the model coastal boundary head is indeed too low. Raising the coastal boundary head and adopting the same initial conditions produced an improvement in the discrepancy between predicted and observed coastal hydraulic heads, with a minimum error obtained using a coastal head of 1.0 m AHD. The models with modified boundary heads were not re-calibrated, and therefore the most appropriate boundary head may be between 0.8 and 1.2 m AHD (i.e. 0.5 and 0.9 m above density-adjusted MSL), given the similar magnitude of errors within this range of boundary heads. The results suggest that the assumed coastal boundary head of 0.3 m AHD, i.e. density-adjusted MSL, adopted by Kuhanesan et al. (2005) is significantly under-estimated.

Errors in water-table predictions

Trade-offs between the predictability (i.e. the level of calibration) of salinity and hydraulic head distributions are inherent in the calibration of models of coupled salt transport and groundwater flow (Hassan et al. 2003). Calibration of the Pioneer Valley sea-water intrusion

Table 3 Changes to water-table predictions with modifications to boundary heads and initial conditions

Boundary head (m AHD)	Initial water-table conditions	Average error (m)	Average absolute error (m)	Root-mean-square error (m)
0.3	Original	−0.39	0.67	0.99
0.3	12-year	−0.79	1.09	1.89
0.3	24-year	−0.80	1.16	2.01
0.3	48-year	−0.78	1.18	2.03
0.5	Original	−0.37	0.65	0.98
0.5	12-year	−0.76	1.08	1.88
0.5	24-year	−0.77	1.15	2.00
0.5	48-year	−0.75	1.17	2.03
0.8	Original	−0.26	0.62	0.95
0.8	12-year	−0.63	1.03	1.84
0.8	24-year	−0.63	1.11	1.96
0.8	48-year	−0.62	1.13	1.99
1.0	Original	−0.15	0.61	0.94
1.0	12-year	−0.50	1.00	1.78
1.0	24-year	−0.50	1.07	1.90
1.0	48-year	−0.48	1.09	1.93
1.2	Original	−0.04	0.62	0.94
1.2	12-year	−0.36	0.99	1.74
1.2	24-year	−0.35	1.06	1.86
1.2	48-year	−0.34	1.08	1.89
1.5	Original	0.13	0.68	0.98
1.5	12-year	−0.14	1.01	1.68
1.5	24-year	−0.13	1.08	1.81
1.5	48-year	−0.12	1.10	1.84
2.0	Original	0.41	0.85	1.13
2.0	12-year	0.26	1.12	1.55
2.0	24-year	0.24	1.22	1.77
2.0	48-year	0.26	1.24	1.81

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model was undertaken essentially as two separate phases, with salinity calibration following the hydrodynamic calibration of Kuhanesan et al. (2005). This two-phase process was expected to have reduced the accurate prediction of hydraulic head distributions, and therefore the groundwater flow aspect in the final sea-water intrusion model will have deviated from its originally calibrated state. Errors in water-table predictions were expected to be mostly caused by MODFLOW-MODHMS conversion (including changes in layer-type and solution approach), the addition of density-dependency, vertical discretisation, the single-layer-to-multi-layer translation of aquifer stresses and boundary conditions (e.g. rivers, drains, specified heads, etc), and the addition of vertical heterogeneities.

Errors in water-table prediction resulting from each phase of model construction were explored to establish relative contributions to error. To illustrate changes to water-table predictions, hydraulic head contours were generated at each stage of sea-water intrusion model development and calibration, and three sets of intermediate results are given in Fig. 14. Kuhanesan et al. (2005) results are compared to (1) a single-layer, telescoped, MODHMS model of groundwater flow; (2) a multi-layer, vertically homogeneous, telescoped, MODHMS model of groundwater flow; and (3) multi-layer, vertically heterogeneous, telescoped, MODHMS model of sea-water intrusion.

Figure 14 shows that water-table predictions were indeed altered by the transformation of the Kuhanesan et al. (2005) model to a telescoped, multi-layer, heterogeneous sea-water intrusion model. The largest reduction in accuracy of water-table prediction occurred due to vertical discretisation, which followed the layering approach used by Langevin et al. (2003). This result is attributed to the high-variability in the shape of the aquifer, as defined by the basement and ground surfaces (e.g. Fig. 10), the finite-difference approximation adopted in MODHMS, and the vertical discretisation approach. It is likely that horizontal layering (i.e. equal cell volumes) would reduce vertical discretisation errors. However, such an approach would require virtually twice the number of model layers (and therefore a greater numerical burden) to retain a similar vertical resolution to that achieved using the current approach of layer subdivision. Model testing using different vertical discretisation approaches is warranted to establish the relative efficiencies and accuracies of approaches, although generally, the water-table predictions from the existing calibrated sea-water intrusion model are considered acceptable.

Conclusions

Sea-water intrusion is actively contaminating groundwater in the Pioneer Valley, and is able to be distinguished from other salination processes through hydrochemical mapping. More specifically, the regions of groundwater affected by modern sea-water intrusion were spatially demarcated using an ionic ratio mapping technique for the largest EC sample per bore.

Conceptualisation of sea-water intrusion is a necessary precursor to numerical model development by providing an alternative method of assessment that complements model predictions. A sea-water intrusion potential map is used to convey the results of conceptualisation, by interpreting the level of susceptibility on the basis of hydrochemical mapping, aquifer basement morphology and modified groundwater hydrology resulting from anthropogenic influences.

The staged approach to model development involving both MODFLOW and MODHMS (whereby hydrodynamic calibration preceded the construction of the sea-water intrusion model) was efficient, although some errors were introduced by the vertical discretisation approach of layer-

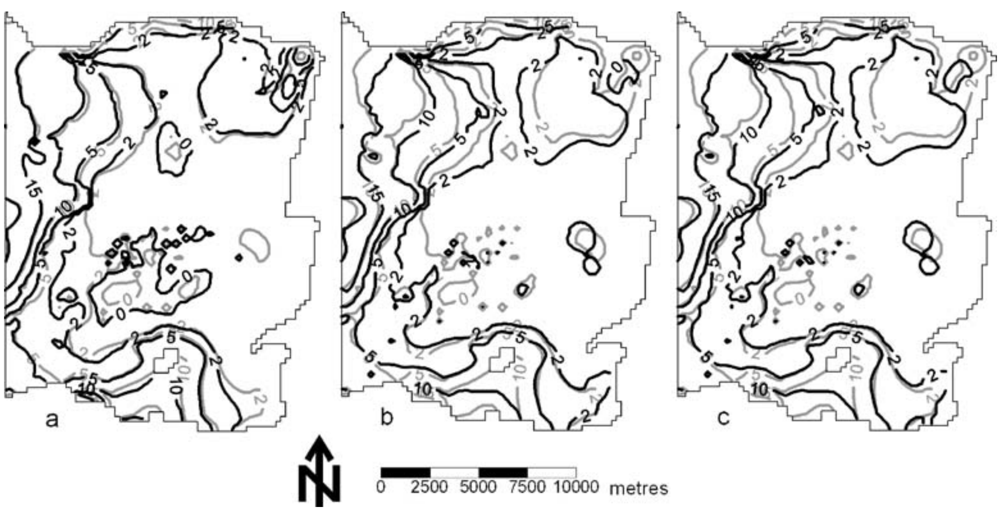

Fig. 14 Comparison between final water-table predictions from the Kuhanesan et al. (2005) model (*grey contours*) and MODHMS models (*black contours*) at three different stages of sea-water intrusion model development. See text for description of the stages at **a**, **b** and **c**

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subdivision. Water-table predictions were improved by raising the coastal hydraulic head above the original density-corrected MSL value of 0.3 m AHD, with an increase of 0.5–0.9 m giving optimal results. Higher coastal hydraulic heads were necessary to account for tidal over-heights, which were neglected in previous groundwater flow modelling.

Calibration of the sea-water intrusion model to regional salinity interpretations indicated that some salinity problems in the coastal aquifers are not attributable to seawater intrusion in the form represented in the numerical model. Further, adequate calibration of the model required that areas of occasional tidal inundation be represented as salt sources, although distinguishing the relative contributions of various salt sources to observed salinity trends requires further investigation of the distribution and mobility of relic sea-water deposits. However, the model is considered an adequate tool for assessing relative changes in the extent of sea-water intrusion caused by altering resource management practices. Given that seawater intrusion appears to be actively encroaching on fresh groundwater resources, water resource management measures are warranted to alleviate negative hydraulic gradients, although extensive salinity and water-table monitoring will be necessary to gauge the effectiveness of any remediation strategies.

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