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Assessment and Prediction of Saline Sea Water Transport in Groundwater Using 3-D Numerical Modelling

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Abstract This paper presents the application of a three-dimensional numerical model to the Al-Raudhatain and Umm A-Aish fresh water aquifers located in north Kuwait. The two aquifers have been polluted by saline sea water imported to extinguish the oil well fires during the Gulf war. A timevariant salinity transport model was calibrated simultaneously with the transient groundwater flow system to assess the impact of saline sea water. Variably saturated flow and transport were modelled. The results of the salinity transport model suggest that although the fresh water–saline water interface, as defined by the 1500 mg/L contour, has moved towards the centre of the lens, in some areas upgradient of the fresh water recharge, the extent of the fresh water lens has actually increased slightly in the down-gradient areas. After 23 years (simulation period 1990–2013), the areal extent of the total dissolved solids plume is estimated at 27 and 29% of the Al-Raudhatain and Umm A-Aish fresh water bodies, respectively. Under the scenarios assumed, there are large masses of salts stored in the soil profile that will leach over time to the water table. The total dissolved solids concentrations are predicted by the model to decrease to 4500 mg/L from 7800 mg/L, after 73 years (simulation period 1990–2063) from the moment the saline sea water was added. The predicted total dissolved solids concentration simulation provides a worst-case scenario of the likely extent of contaminant movement in groundwater in the two fresh water fields. Solute transport modelling has become increasingly important tool for interpreting groundwater quality data and processes relevant to natural and contaminant aquifer systems to a wide range of real-world groundwater quality problems. Further data, from drilling sampling and other testing and experimentations should help clarify the assumptions made and assist in updating the solute transport modelling effort which helps to provide insights into the past and present behavior, and allows to predict water quality management scenarios.

Keywords Groundwater. Numerical modelling . Plume . Salinity. Contamination . Kuwait fire impacts. Gulf war

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1 Introduction

Groundwater is an important source of water supply in many parts of the world. As groundwater use has increased, issues associated with the quality of groundwater resources have likewise grown in importance. Water quality analysis is one of the most crucial aspects in the study of water resources. The hydrochemical study reveals quality of water that is suitable for drinking, agriculture and industrial purposes (Daniels et al. [2016](#page-22-0); Hamid and Behzad [2012](#page-23-0)).

For many years, attention has been directed to contamination from point sources such as landfills and hazardous waste-disposal sites. The natural chemistry of the groundwater is largely controlled by the dissolution of the geologic materials through which the water flows. Contaminants enter groundwater from sources at the ground surface through chemical weathering soil leaching, decaying vegetation, etc. These dominant processes depend on the geological and geochemical conditions, as well as the chemical and biological characteristics of the contaminant. More recently, concerns have increased about non-point sources of contamination (e.g., application of fertilizers and wastewater sludge in agricultural areas, use of pesticides, irrigation with wastewater, and acid rain) and about the overall quality of groundwater resources (Gulgundi and Shetty [2016;](#page-23-0) Vishal and Leung [2015](#page-23-0); Zheng [2009](#page-24-0); Yihdego [2015](#page-24-0)). It is stated that the chemical composition of groundwater is affected by several diverse factors like topography, rock and soil compositions, rainfall pattern and temperature in the region, soil microbial diversity, land use pattern and several other anthropogenic processes, such as excess groundwater extraction for various applications. This has led to considerable interest in the design of investigative studies and monitoring programs to describe groundwater quality over regions that may range from tens of square kilometers to an entire country (Deceuster and Kaufmann [2012;](#page-22-0) Teles et al. [2006](#page-23-0); Yang et al. [2016\)](#page-23-0).

The contaminants affecting water quality are commonly spatially dispersed and may be widespread and frequent in occurrence. The fate of chemical constituents in groundwater is determined by their reactivity and migration capacity in the soil. The protection and enhancement of the quality of groundwater resources is an environmental concern of high priority. Deterioration of groundwater quality may be virtually irreversible, and treatment of contaminated groundwater can often be expensive. Detection of groundwater contamination is complicated by the out-of-sight nature of groundwater (Gulgundi and Shetty [2016;](#page-23-0) Vishal and Leung [2015](#page-23-0); Yihdego et al. [2016b](#page-24-0)). Commonly, neither the sources nor the effects of contamination are easily observed or measured. Many contaminants are colorless, tasteless, and odorless. The degree of threat posed by groundwater contamination depends on many factors, including the concentrations of the contaminants, their toxicity (individually or in combination), the volume of affected groundwater, the uses of water from the aquifer, the population affected by these uses, and the availability of an alternative water supply. The sources of components that determine groundwater quality are numerous and diverse. These components can enter groundwater in an aquifer through many different routes (Kwarteng et al. [2000](#page-23-0); Kwarteng [1999](#page-23-0); Yihdego and Webb [2016](#page-24-0)).

The scale of gulf war damage to Kuwait was enormous, ranging, among several others, from destruction caused by oil fires, oil spills and saline sea water to economic decline for the Kuwaiti oil industry (Al-Sulaimi et al. [1993\)](#page-22-0). The selection of appropriate remediation design requires assimilating and analysing available data into understandable and technically supportive representation of site conditions. Numerical models are

sophisticated tools which simplify the process of solving multiple mathematical algorithms on large data sets within a prescribed framework used to simulate site conditions (Yihdego and Becht [2013](#page-23-0); Yihdego et al. [2016a\)](#page-23-0). The current study employs numerical transport modelling to characterize and predict the extent and migration of the pollution.

1.1 Regional Climate and Hydrogeology

Kuwait's only two fresh water aquifers, the Al-Raudhatain and Umm Al-Aish, are located in the northern portion of the country in the Al Jarha Governorate, near the Raudhatain and Sabriyah oil fields, beneath the topographic depression associated with the Al-Raudhatain-Umm Al-Aish drainage basin (Fig. 1). These fresh water aquifers are unique in that their recharge process reflects the rapid infiltration of surface water runoff and their proximity to the oil field makes them very vulnerable to contamination. The damage caused from the destruction of oil wells during the Gulf War of 1991 and sea water used to control and extinguish oil fires has directly affected the aquifers.

Kuwait is an arid country, home to over 3.5 million people, characterised by long summers with extremely high temperatures and high humidity, short mild winters with low humidity, and high evaporation rates (Grealish et al. [1998](#page-23-0)), no fresh surface water supplies, and very limited renewable groundwater. High intensity rainstorms are common

Fig. 1 Location of the Al-Raudhatain and Umm Al-Aish Aquifers in Kuwait

and produce surface water runoff through the network of wadis which provide recharge to groundwater aquifers.

The bulk of Kuwait's groundwater is brackish (Omar et al. [1994](#page-23-0); Parson Corporation [1964](#page-23-0)). Total dissolved solids (TDS) is an important indicator of groundwater quality with values less than 1000 mg/L considered to represent 'fresh' water. Water supply relies on desalinated water, brackish groundwater and treated wastewater. As of 2011, about half of water supply was provided by desalination and the rest by a combination of mostly brackish groundwater and treated sewage effluent.

The geology of Kuwait consists of recent (Quaternary age) deposits and sediments unconformably overlying sedimentary rocks (Tertiary age) which host the groundwater aquifers. The regional dip of strata is about 2 m per km towards the north-east and this regular dip is interrupted by anticlines and other small structures which are present at the Raudhatain oil field. The Dibdibba Formation, confined to the northern part of Kuwait, comprises sands and gravels with minor clay and gypsiferous sandy clay beds. Hydrogeologically, the two fresh water aquifers of interest are situated beneath the shallow, elongated depression of the Al-Raudhatain – Umm Al-Aish drainage system (Fig. [1\)](#page-2-0), consisting of an extensive network of wadis and drainage lines (Yihdego and Al-Weshah [2016](#page-23-0)). The drainage system that leads to these two playas is the most pronounced of the seven main catchments or drainage systems within Kuwait. The catchment is about 110 km from south-west to north-east with a maximum width of about 55 km. The highest elevation of the catchment is 252 m above sea level (asl) at the south-west end and the lowest is about 30 m asl near the centre of the Umm Al-Aish depression. About 15 km to the west of the depressions, there is a 10 km wide wind eroded sand transport corridor (Kwarteng [1999](#page-23-0)), where most of the wadis have been eroded by the action of the north-west, south-east winds.

1.2 Groundwater Recharge and Flow Direction

Rainfall is the primary source of recharge to the fresh water lenses at Al-Raudhatain and Umm Al-Aish as indicated by isotopic studies reported in Ebrahim et al. [\(1993](#page-23-0)) and Robinson and Al-Ruwaih [\(1985\)](#page-23-0). The actual process leading to infiltration is subject to several theories based on limited evidence, and is discussed in detail in the Conceptual Model Report. The direction and gradient of flow within the Kuwait Group aquifers essentially follows the stratigraphic dip and is in a north-easterly direction. The gradient steepens in the south-east and reflects discharge to the Arabian Gulf. In the north-east, the gradient flattens and groundwater discharge is largely to coastal sabkhahs (salt flats). The rate of groundwater flow in the central part of the Al-Raudhatain well field (based on permeability, porosity and gradient) has been estimated at about 110 m/year (Parsons [1964](#page-23-0)). The inferred flow velocity using the flow line distance and the results of ^{14}C and 3 H age dating indicated a flow velocity of between 11 and 245 m/year (Parsons [1964](#page-23-0)). Using the groundwater gradients (0.0003–0.0006), flow directions were determined (SMEC [2014](#page-23-0)). There is an effective porosity of 0.2 and hydraulic conductivity range of 40 to 80 m/day (which are considered typical of the upper aquifers in Umm Al-Aish and Al-Raudhatain). These calculations gave an estimated groundwater velocity range of 20 to 90 m/year (SMEC [2006](#page-23-0), [2014](#page-23-0)).

The groundwater level for the Al-Raudhatain and Umm Al-Aish fresh water aquifers highlights the north-easterly flow direction. The direction and gradient of flow follows the stratigraphic dip eventually discharging to the Arabian Gulf.

The fresh water lenses at Al-Raudhatain and Umm Al-Aish are generally contained within the unconfined Aquifer. There is a distinct zonation in salinity with the freshest water being contained in the centre of the groundwater body, with a general increase in the salinity laterally away from the centre. The salinity change is gradual. The rate of change is from 500 to 3000 mg/L total dissolved solids and from 1000 to 5000 mg/L total dissolved solids over several kilometres for Al-Raudhatain and Umm Al-Aish, respectively. Salinity zonation also occurs with depth, with the magnitude of salinity change more rapid, from less than 500 to 7500 mg/L within 15 m (KISR [2009\)](#page-23-0). Between 1989 and 2005, groundwater salinity was observed to increase from historical readings. The rise in salinity has been linked to the Gulf War contamination. It is also likely that pumping has resulted in a decrease in the thickness of the fresh water lenses and drawing in more saline water. Also of concern are the widespread saline pits and the potential for contamination of recharge water with these salts. Salinity measurements of lake water in a pit near well P18 has an electrical conductivity (EC) of 400,000 μS/cm, indicating the presence of large areas of high-concentration salt in the catchment (KISR [2012,](#page-23-0) [2013](#page-23-0); SMEC [2006](#page-23-0)). Both the Al-Raudhatain and Umm Al-Aish basins are affected by high total dissolved solids water (Fig. 2), coming from brines associated with oil and seawater contamination.

There appears to be a significant areal extent of contamination within the Umm Al-Aish Basin and in the south-eastern portion of the Al-Raudhatain Basin. Contamination (in the form of saline water) seems to have penetrated 10 to 30 m below the water table, extending the impact of the contamination. There is large storage of salt and salty water

Fig. 2 Composite TDS concentration from 2012 (sample analysis by KISR. Note: Depth of screen Interval or aquifer from which the sample was collected was not indicated)

still in the catchment areas of Umm Al-Aish and Al-Raudhatain that will likely continue to contaminate overland flows in wadis and other parts of the catchments. This may lead to focused points of contaminated recharge to the fresh groundwater lenses. Aerial maps and on-ground reconnaissance has identified dozens of pits and oil lakes used to fight fires or drain oil.

Predictive analysis using mathematical models (KISR [2009;](#page-23-0) SMEC [2014\)](#page-23-0) underscored the possibility of large-scale contamination of the groundwater resources in the Umm Al-Aish basin, caused by ongoing movement of hydrocarbon pollutants toward the supply bores. Recent studies (SMEC [2006\)](#page-23-0) suggested that the groundwater in Umm Al-Aish area has been significantly affected by the hydrocarbon pollutants. It has been predicted (KISR [2009\)](#page-23-0) that these pollutants would move towards the Al-Raudhatain fresh water lens if no preventive and/or remedial measures were taken in the near future.

2 Methodology

2.1 Conceptual Hydrogeological Model

The conceptual model was constructed taking into account the key factors influencing the hydrogeology of the area of interest. These may include: recharge, discharge, flow direction, geology, and contamination in the local and regional context. The model is an approximation and presents the understanding of how the hydrogeological system is understood to work. Figure 3 presents the conceptual hydrogeological model used to develop the numerical model.

The Environmental Visualisation Software EVS-pro (C Tech Development Corporation [2013\)](#page-22-0), three- dimensional data presentation program has been used to build a hydrostratigraphic model using available data from boreholes (260) and geophysical

Fig. 3 Idealised conceptual model of the fresh water aquifer systems

surveys (downhole logging and time domain electromagnetic surveys) to build a database. The database allows for geo-statistical assessment of the data in both two (2-D) and three (3-D) dimensions.

2.2 Numerical Groundwater Model

2.2.1 Model Design

The groundwater model of the Al-Raudhatain and Umm-Al-Aish basins were undertaken using the MODFLOW-SURFACT numerical code (HGL [2013\)](#page-23-0). MODFLOW-SURFACT is a state of the art simulator that utilises vadose zone flow and transport equations to provide practical solutions to the analysis of flow and contaminant transport at various levels of complexity and sophistication as needed for site evaluation and closure. The variably saturated flow equation can be solved with standard retention functions or multimodal relative permeability curves for unsaturated flow in porous and fractured systems. The equation can further be solved with soil retention functions for confinedunconfined simulations. The variably saturated transport equation can be solved for unsaturated medium or can be used for confined-unconfined situations. It is highly advantageous to have the unsaturated and saturated simulation capabilities in a single code that may be used to analyse all stages within the lifecycle of a site investigation – from pilot point to closure. Benefits of the comprehensive simulation capability include:

- 1. Scalable solution in terms of detail of conceptualisation, ranging from simple evaluations to more complex and complete investigations;
- 2. Consistent approximations throughout the analyses as opposed to possible differences in results from different codes owing to differences in gridding structures, spatial and temporal discretisation approximations, and material property assignment schemes; and
- 3. Further, approximations involved in translating from one code to another are avoided.

Overcoming the difficulties and expanding the simulation capability of MODFLOW-MT3D solutions can be done using MODFLOW-SURFACT. This is a comprehensive simulator for set of equations for evaluating multicomponent contaminant transport within multiple phases in the subsurface by using the vadose zone flow and transport equations in unique ways to perform the wide range of analysis needed for understanding and managing contamination and remediation projects (Panday and Huyakorn [2008](#page-23-0)). MODFLOW-SURFACT includes three major classes of transport solution techniques (the standard finite-difference method, the particle-tracking-based Eulerian–Lagrangian methods, and the finite-volume third-order Total Variation Diminishing [TVD] method) in a single code. Since no single numerical technique has been effective for all transport conditions, the combination of these solution techniques, each having its own strengths and limitations, is believed to offer the best approach for solving the most wide-ranging transport problems with efficiency and accuracy. MODFLOW-SURFACT is used for the variably saturated three-dimensional groundwater flow and transport modelling, and is presently considered a code that complies with industry standards (HGL [2013](#page-23-0)). The flow and transport models were calibrated by using a manual iterative parameter approach and the parameter optimising program PEST (Doherty [2004](#page-23-0)).

The conceptual and hydrostratigraphic models have been used to design the numerical model layers, extent of the domain and hydrogeological cycle inputs. From the hydrostratigraphic model five layers were assigned to represent the seven lithological units on the Quaternary and Kuwait Group sediments.

3 Modelling Approach

3.1 Flow Model

The modelling approach was to develop a calibrated salinity dependent transport component to account for the saline contamination which was coupled with to allow assessment of remediation scenarios. The initial stage involves construction of the numerical model and calibration against known data. Calibration started with a steadystate flow model developed to study regional flow patterns in the aquifer and to calibrate recharge and hydraulic conductivity among others. The steady-state flow model looks at an average (long term) period and allows static calibration of, e.g., hydraulic properties, to a known or measured data set (Fig. [4](#page-8-0)). A transient flow model was then developed to assess seasonal recharge on groundwater and investigate their effects on flow patterns. A transient flow model allows for time dependent calibration of known changes, for example concentration or water levels over time. A density (salinity) dependent transport model was required to be coupled to the flow model as the density of the saline contamination (sea water) can drive flow and contamination movement within the groundwater system. The combined flow and transport model was then used to simulate remediation scenarios.

For the purpose of modelling the groundwater system, constant head boundaries were set along the north-east and south-west model limits and no flow boundaries were set along the northwest and south-east model boundaries. Constant head boundaries were set along the interpreted groundwater contours of 6.5 m asl along the northeast boundary and 11 m asl contour along the southwest boundary. The no flow boundaries along the north-west and south-east model limits coincide with the interpreted groundwater streamlines, which were no flow boundaries by definition. The base of the model was set as a no flow boundary. The groundwater level is below Layer 1 at the boundaries, therefore, two sets of boundary conditions have been applied. The boundary conditions in Layer 1 reflect the fact that the boundary condition is essentially dry, whilst in Layers 2 to 5 the boundary condition is wet (Al-Weshah and Yihdego [2016\)](#page-22-0).

In arid environments, such as in northern Kuwait, there is no true steady-state situation. This is because recharge only occurs in sudden intense events and the system is, therefore, always responding to or recovering from the last recharge event. Groundwater predominantly occurs from surface water infiltration following rainfall. A uniform recharge rate of 280.3 mm/year was applied in all recharge zones, based on the conceptual model assessment and model calibration. Selected areas, coinciding with the "flood" areas, as specified by Parsons ([1964](#page-23-0)) and KISR ([2012](#page-23-0)), were designated as recharge boundaries. This rate of recharge and the area over which the recharges was applied gives a total volume of recharge of $4680 \text{ m}^3/\text{day}$ into the model domain. The recharge value is similar to previous estimates by Parsons ([1964](#page-23-0)) and SMEC [\(2006\)](#page-23-0). Source recharge is assumed from using isotope, chemistry and hydrograph data.

Fig. 4 Plot of simulated steadystate groundwater table contours. Blue cells represent the constant head boundary and target bores are shown. Green target bores show 0.3 m maximum discrepancy (after Al-Weshah and Yihdego [2016](#page-22-0))

The aquifer properties adopted are based on the conceptual model, results of hydraulic tests, observations collected during purging of the monitoring wells and model calibration. For parameters where no data was available, industry accepted values and best estimates have been used. The model was calibrated using the adopted data. There were different hydraulic conductivities applied to each fresh water field as well as in the area of brackish water, beyond the extent of the model aquifers. The pumping test data was in agreement with the chemistry data and showed variable hydraulic conductivity with depth. The van Genuchten soil function (using upstream weighing) was employed to solve the variably saturated water flow equations, which calculates conductance in all directions including the vertical as per saturated conductance times a relative permeability. The functional expressions used to describe the relationship of relative permeability versus water saturation and the relationship of pressure head versus water saturation are described in Panday and Huyakorn ([2008](#page-23-0)).

3.2 Salinity Transport Model

The time-variant salinity transport model was calibrated simultaneously with the transient groundwater flow system (for the period March 1991 to July 2013). This includes variably saturated flow and transport. This was done prior to proceeding to simulate contaminant transport, as the hydraulic gradients and flow direction (and storage volume) are a significant control on contaminant migration.

The model simulated the period from 1991 onwards, at which point a large volume of saline water was injected, to simulate the seawater used to put out the oil fires, along with a pulse of contaminant, assumed to enter the groundwater system at this time. Based on the information concerning recharge events between 1991 and the present day, it was necessary to simulate further incidents of contamination along with fresh water recharge at the location of the contaminant sources.

During the modelling of salinity, it was observed that improving the convergence and stability of transport models required grid refinement in relation to the dispersivity values to maintain a Peclet number of less than one and regular grid geometry. The historical mass transport model for salinity could be significantly improved if data were available on the vertical distribution of salinity and the variation of salinity over time. This would allow a time-variant calibration of the mass transport model which, in turn, would expedite determination of mass transport parameters for salinity. Should appropriate data become available, it could be used to investigate the significance of seawater recharge in terms of the flow and transport models. The volume of seawater may be significant in terms of flow directions and hydraulic gradients.

This model is designed to simulate contaminant transport beginning at the oil fire events of March 1991 to July 2013. Therefore, the transient model consists of sequential runs, each with 1 month duration divided into 269 stress periods and 730 time steps of 12 h over this time period.

Initial heads for the steady-state model were set at 13 m asl across the domain. It was important to use a level slightly higher than the highest heads expected to result from the model as it aids model convergence by ensuring that no elements which should be saturated would start the model as dry elements. The initial heads for the transient-state model were the resulting heads from the steady-state model. These were a good starting point for the transientstate model, since this model represented the average conditions of the transient-state model.

A spatially-varying recharge condition based on simulated net infiltration is applied to the top model boundary, with a constraint of >35 mm/month (that is, there will be no recharge with rainfall of <35 mm/month). The recharge in the transient-state model was applied at the same locations as in the steady-state run. The time-variant recharge was applied as a percentage of average monthly precipitation (12%) to the recharge locations.

Extensive amounts of saline water were used for firefighting the oil well fires, about 6×10^6 m³ of seawater or brackish water (KISR [2009](#page-23-0)). A total of 361 seawater storage pits, or well head pits were excavated to support fire-fighting operations. Limited soil analysis has shown that these areas now have high total dissolved salts and sodium concentrations.

There was insufficient data available to model the effects on the salinity distribution of the oil-fire related seawater recharge of 1991. There was no data available on the volume of water, the rates at which it was entering the area, the groundwater concentrations over time, or the time-variant groundwater heads. An assumed recharge rate of $1000 \text{ m}^3/\text{day}$ was applied over the entire recharge areas of the depressions for this purpose.

The model recharge flow boundaries were set up to simulate the seawater recharge at the assumed rate of $1000 \text{ m}^3/\text{day}$ total among all locations of contamination sources, between March and November 1991. This was done to investigate the significance of seawater recharge in terms of flow and transport model (simultaneous calibration of the flow and salinity transport was carried out to attain this objective). The volume of the sea water may be significant in terms of flow direction, hydraulic and concentration gradients, and hence contamination migration.

3.2.1 Dispersivity

As there is no site-specific dispersivity data, the dispersivity values for the simulation of the contaminant transport were based on interpretations of data published by Gelhar et al. ([1992](#page-23-0)). The 59 field-scale tests, presented by Gelhar et al. [\(1992\)](#page-23-0), indicate a trend of increasing longitudinal dispersivity with the scale of observations, which is defined as the distance between the observation points and a source of contamination. However, this trend of increasing longitudinal dispersivity with distance is less apparent if the reliability of the tests is considered. At any given scale the values of longitudinal dispersivity range over two or three orders of magnitude, but the more reliable values tend to fall in the lower portion of this range. Gelhar et al. [\(1992\)](#page-23-0) concluded that there are no highly reliable longitudinal dispersion coefficients at scales greater than 300 m. However, the reliability of these estimates may be due to the fact that all reliable values were obtained from specifically designed well controlled dispersion experiments and these were limited to small scale tests only. The horizontal transverse dispersivities are typically from one third to almost three orders of magnitude lower than longitudinal dispersivities. Vertical transverse dispersivities are typically one to two orders of magnitude lower than horizontal transverse dispersivities.

With no site-specific data that could be used to assess dispersivities of the aquifer material in the model area, the longitudinal dispersivities (Table 1) were estimated from the dispersivity plots of Gelhar et al. [\(1992\)](#page-23-0).

The scale of the problem was determined by the distance between the most distant potential source of contamination and the model boundary (along the groundwater contour of 8 m asl). This distance is 7400 m in Umm Al-Aish and 10,300 m in Al-Raudhatain. According to the plots, the longitudinal dispersivity for such a scale can be approximately 100 m (in 10 to 200 m range); however, it has a low reliability value. The longitudinal dispersivity value adopted in the model was assumed to be between these two values at 40 m. Research also suggests that dispersivity may be smaller, but can only be assumed as such if detail is known of the heterogeneity of the aquifer systems, and in particular if the distribution of hydraulic conductivity is known at a relatively fine scale, which is not the case for this model. The ratio of the horizontal transverse to the longitudinal dispersivity was assumed to be 0.1. The ratio of the vertical transverse to the horizontal transverse dispersivity was also assumed to be 0.1. These

Material property	Value	Units	Justification	
Longitudinal dispersivity Horizontal transverse dispersivity Vertical transverse dispersivity	0.1 0.01	m m m	1/10 of estimated length of hydrocarbon plume 1/10 of longitudinal dispersivity 1/10 of horizontal transverse dispersivity	

Table 1 Transport material properties (Dispersivity)

ratios are commonly used in sedimentary aquifers where there are no other data indicating sitespecific dispersivities.

3.2.2 Sorption

Typically the movement of hydrocarbons (TPH) in soil and groundwater is slower (retarded) in relation to the movement of groundwater or water itself. The soil/water partitioning coefficient (Kd), is the parameter routinely used to describe the ability of the aquifer matrix to retard the movement of contaminants. The retardation is due in part to the sorption of the hydrocarbons onto the aquifer matrix. The concentration of organic carbon, typically expressed as fraction of organic carbon (foc), on the soil matrix has a major impact on this retardation. AACM International analysed 35 soil samples collected from all over Kuwait for foc (AACM and KISR [2001](#page-22-0)). Samples were collected from depths between 1 and 60 cm below the surface. The foc in those samples varied between 0.05 and 0.42%. The foc in soil samples collected near the fresh water fields varied between 0.09 and 0.15%. There are no data available for organic carbon concentrations either at depths greater than 0.6 m or in the saturated part of the aquifers. Considering the above, it was assumed that the organic carbon content of the unsaturated materials was 0.1%. Sampling of monitoring bores in May and August 2002 indicated that groundwater was aerobic (KISR [2013\)](#page-23-0). This implies that the organic carbon in the aquifer is low or that the remaining concentration of organic matter is not-easily degradable. In the former case, sorption would be low. The soil/water partitioning coefficient (Kd) is often written as follows (Eq. 2):

where

$$
R = 1 + Kd \times \rho_b/n \tag{1}
$$

$$
Kd = foc \times Koc \tag{2}
$$

where: Koc is an organic carbon partition coefficient; ρ_b is the bulk density of the soil/aquifer matrix; and n is the effective porosity.

The retardation of the organic components was developed on data of the Octanol/water partition coefficient and the Karickoff Kd approach. The fraction of natural organic carbon foc in the sediment was estimated to be 0.001. Retardation coefficient for TPH was set to 1.2 - this equates to a distribution coefficient (Kd) value of 5.62×10^{-6} m³/kg. Also found elsewhere, typical retardation coefficients were less than 1.2. This value is taken in subsequent simulations of TPH transport through the vadose zone and in groundwater.

3.3 Boundary and Initial Conditions

3.3.1 Model Boundary

Dirichlet (1st kind), Neumann (2nd kind) and Cauchy-type (3rd kind) boundary conditions can be specified for flow, mass and heat. These boundary conditions can be arbitrarily placed at nodal points. All boundary conditions (from 1st to 3rd kind) can be specified either as steadystate or as transient conditions. Furthermore, for each boundary condition, constraint formulations can be combined. They represent limitations of boundary conditions and result from the requirement that boundary conditions should only be valid as long as minimum and maximum bounds are satisfied (e.g., a Dirichlet-type concentration boundary condition should only be valid if the flow enters the boundary portion while a natural boundary condition has to be set up as soon the flow is released from the boundary).

Contaminants typically enter a groundwater system with a fluid source (recharge) that contains the contaminant. Consequently, a third-type solute boundary condition (Cauchy) is logical match - in which the source concentration is specified and associated with outflow. The concentration of the sea water was allowed to vary as a function of time. It was assigned as 36,000 mg/L for the first year since the source added and 20,000 mg/L for the rest of the simulation time.

For the purpose of modelling the groundwater system, constant concentration boundaries were set along the north–east and south–west model limits and no flow boundaries were set along the north–west and south–east model boundaries, as shown on Fig. [6.](#page-14-0) Constant concentration boundaries were set along the interpreted concentration contours of 12,000 mg/ L m along the northeast boundary and 5000 mg/L m contour along the south–west boundary. A value from 10,000 to 6500 mg/L was assigned along the south–east to east boundary. The no flow boundaries along the north–west and south model limits coincide with the interpreted concentration streamlines, which were no flow boundaries by definition.

3.3.2 Source of Contamination (Seawater)

Sources of contamination were based on the areal extent of drainage pits, wadis and fringes of dry and wet lakes. The location of the contaminated areas in relation to the fresh water bodies are shown in Fig. [5](#page-13-0) with respect to the model domain. The areas of potential sources overlying the two fresh water bodies were calculated as 2.17 km^2 for Umm Al-Aish and 2.45 km^2 for Al-Raudhatain (Fig. [6](#page-14-0)).

3.3.3 Initial Concentrations

The initial concentrations for the model were interpolated from total dissolved solids data set recorded over the period 1962 to 1991.

3.4 Spatial and Temporal Discretization

The model domain was a sub-regional area encompassing the two basins. The area modelled comprised a rectangle of 39.5 km by 14.7 km, totalling 580 km². The model limits have been set along groundwater contours, and streamlines, interpreted using groundwater level data from (October 2002), and a survey of the monitoring bores (from September 2002). The model domain extended at least 1.7 km from the Umm-Al-Aish bore field for the southern boundary, 4.7 km away from the Al-Raudhatain bore field to the north, north–east and east and 4.5 km for the north–west. The active part of the model grid was 532 km². The model grid contained 97,800 rectangular cells arranged in 163 rows with 120 columns and five layers. The model grid has been rotated 53.6° counterclockwise from the east to west direction to be sub-parallel to the orientation of the regional geology and groundwater contours. The cell size in the specific basins was 100 by 100 m and the peripheral domain had a cell size of 1700 by 757 m.

The active model consisted of five layers. For the purpose of modelling, Layer 1 which corresponded to Aquifer 1 was mainly unsaturated but was important for recharge and vadose zone source migration. Aquifers 2 and 3 were saturated, with Aquifer 2 containing the main majority of the fresh water lenses, and Aquifer 3 was predominantly saline. Modelling of the groundwater systems concentrated on Aquifers 2 and 3 which remained saturated throughout the model period.

Fig. 5 Location of contamination sources. Blue cells show the constant concentration boundary, black outlines show fresh water lenses and red outlines show contaminant areas

The transport simulations were conducted assuming that the only processes influencing transport were advection, dispersion and sorption or retardation (for total petroleum hydrocarbon), but no biodegradation was simulated.

The model grid refinement was set up in preparation for the application of the model to the saline and hydrocarbon contaminant transport problems since these simulations would require a more refined and more regular grid than the flow simulation. The grid Peclet number should be maintained at less than 1 in MODFLOW. The Peclet number Pe is given by (Eq. 3):

$$
Pe = \Delta x / \alpha_L \tag{3}
$$

where: Pe is the Peclet number (dimensionless); Δx is the Grid size length (m); and α_L is the longitudinal dispersivity (m).

The α_L was estimated for the two distinct mass transport problems to be investigated, salinity and hydrocarbon transport. In the absence of site-specific data, α_L was estimated using $\alpha_L = 0.1$ × domain length. For the salinity, the scale of the problem was estimated at around

5 km, based on the approximate dimensions of the fresh water lenses. This resulted in an estimated α_{I} of 500 m. Since the mass transport for salinity was simulated over the entire model domain, it was necessary to keep the grid size for the fresh lenses below this edge size.

The model was set up to run from March 1991 to July 2013 for historical matching, simultaneously with the transient flow model. The reasoning behind this was to allow 50 to 100 years of predictive remediation simulation time from the end of 2013. In this case, the initial period in model simulation has been the period of anthropogenic input of the contaminant to the environment (March 1991).

3.5 Model Calibration

Calibration was accomplished by applying a set of hydraulic parameters; boundary conditions and stresses that produce computer generated simulated pressure heads (or water level drawdown) to match the actual measured, within an acceptable range of error. Model

Layer	Effective porosity	Specific yield	Specific storage (m^{-1})
Layer 1	0.29	0.14	0.00028
Layer 2	0.15	0.12	0.00013
Layer 3	0.29	0.14	0.00028
Layer 4	0.15	0.12	0.00006
Layer 5	0.29	0.14	0.00028

Table 2 Summary of storage values adopted in the model

Fig. 7 Plot of simulated vs observed transient TDS concentration from 1991 to 2013

calibration was performed by manual (iterative trial and error) and automatic (inverse model using the Parameter Estimation by PEST) methods. A steady-state flow model was developed to assess the regional groundwater flow pattern and to calibrate the recharge and hydraulic conductivity parameters. A transient-state flow and transport model were then developed to assess salinity and hydrocarbon contamination.

In flow models, it is expected that the calibrated model will reproduce most of the observed heads within an acceptable level of error. However, it is not feasible for transport models to expect that the calculated concentrations will accurately match all variations observed in the

Fig. 7 (continued)

measured data, or even at a single observation bore. The aim is that the calculated concentrations should reproduce the major trends and locally averaged values (e.g., as discussed by Konikow [2011](#page-23-0)).

Effort was made to obtain a better match by modifying the magnitude and distribution of the background concentration and pollutant (added seawater) load. Changes in

Fig. 8 Simulated TDS concentration contours after year 23 (2013) in layer 1. Fresh water lenses are shown with yellow and green

conductivity affect the groundwater velocity, causing redistribution of solute concentration. In general, the higher the conductivity, the faster is the movement of the solute. The longitudinal dispersivity was increased to 1.0 m (from 0.2 m), and the transverse dispersivity was taken as one-tenth of the longitudinal dispersivity. Significant changes in total dissolved solids concentration were noticed due to increase in dispersivity. This shows that the dispersion together with the advection is the predominant mode of solute migration.

3.5.1 Aquifer Properties

Transient groundwater models need to be able to calculate changes in groundwater storage to simulate changes in heads and flows over time. The storage parameters, derived from model Fig. 9 Simulated TDS concentration contours after year 23 (2013) in layer 1. Shaded colour shows TDS with values less than 1500 mg/L. Pink shading shows low concentrations. Green shading shows high concentrations. Red lines represent contaminant sources (oil and or sea water lakes)

calibration, are tabulated in Table [2](#page-14-0). The specific storage is the storativity divided by the saturated thickness of the layer. The specific yield expresses the volume of water that is released per unit of water table drop per unit surface area.

The effective porosity of the aquifers was assumed to be 0.29, which is higher than the estimated specific yield, as some water is retained by the aquifer matrix against the force of gravity. The effective porosity of the semi-permeable layers was set to the value of 0.15.

The simulated concentration profiles for total dissolved solids over the past 23 years (from 1991, at time zero, to 2013) at selected monitoring bores P-10, P-17, P-18 and P-19 are shown on Fig. [7](#page-15-0). The simulated total dissolved solids time series have similar trends with the observed total dissolved solids time series, but do not match data at all times; however, they are considered to reasonably represent the overall trend.

Effort was made to obtain a better match by modifying the magnitude and distribution of the background concentration and pollutant (added seawater) load. Changes in conductivity affect the groundwater velocity, causing redistribution of solute concentration. In general, the higher the conductivity, the faster is the movement of the solute. The longitudinal dispersivity was increased to 1.0 m (from 0.2 m). Transverse dispersivity was taken one-tenth of the longitudinal dispersivity. Significant changes in total dissolved solids concentration were noticed due to increase in dispersivity. This shows that the dispersion together with the advection is the predominant mode of solute migration.

4 Results and Analysis

Figures [8](#page-17-0), [9](#page-18-0), 10, and 11 show the spatial distribution of total dissolved solids (TDS) 23 years after the source was added. The predictions and estimates of the plume extent should be viewed as approximate only, but are based on the best estimates of hydraulic and transport

Fig. 11 Simulated TDS concentration contours after year 23 (2013) in Umm Al-Aish in layer 1. Shaded colour shows TDS with values less than 1500 mg/L. Pink shading shows low concentrations. Green shading shows high concentrations. Red lines represent contaminant sources (oil and/or sea water lakes)

Fig. 12 Predicted distributions of TDS concentration in 73 Years (2063) from the start of the pollution event in layer 1. Shaded colour shows TDS values less than 1500 mg/L. Pink shading shows low concentrations. Green shading shows high concentrations. Red lines show contamination source areas. Fresh water lenses are shown as purple outline (Under Source Removal Scenario)

parameters. Prior to 1991, the salinity of the groundwater in the vicinity of the central portion of both fresh water lenses was <1000 mg/L as total dissolved solids. The computed total dissolved solids plumes originating from the sources of contamination appear to be moving towards the fresh lenses by the end of the 23 year simulation. The predicted total dissolved solids plume migration is a distance of 300 m from the source regions after 23 years, with an average groundwater velocity of 40 m/year (using present day calibrations). In absence of heavy groundwater pumping in the Al-Raudhatain basin, there is a relatively slow migration of the total dissolved solids plume towards the fresh water lenses in this area (Fig. [8\)](#page-17-0). It is assumed that total dissolved solids migration will be the precursor for the total petroleum hydrocarbon migration in the mass transport modelling (e.g., Rao et al. [2011\)](#page-23-0).

The results of the salinity transport model suggest that although the fresh water – saline interface, as defined by the 1500 mg/L contour, has moved towards the centre of the lens, in some

areas up-gradient of the fresh water recharge, the extent of the fresh water lens has actually increased slightly in the down-gradient areas. The fresh water body of Al-Raudhatain has moved 40 m, following the flow direction, relative to the 40 m depression line (Fig. [10\)](#page-19-0). For Umm A-Aish the fresh water lens has not moved much in relation to the 35 m depression level (Fig. [11](#page-19-0)).

After 23 years and with respect to the total area of the fresh water body at Al-Raudhatain (55.2 km^2), the areal extent of the total dissolved solids plume is estimated to be 15 km^2 for the 1500 mg/L contour. This equates to total dissolved solids impacting 27% of the fresh water body. The wet and dry lakes located at the Al-Raudhatain fresh water lens are 2.38 and 0.07 km², respectively.

After 23 years, and with respect to the total area of the fresh water body at Umm Al-Aish (37 km^2) , the areal extent of the total dissolved solids plumes is estimated to be 11 km² for the 1500 mg/L contour. This equates to total dissolved solids impacting 29% of the fresh water body. The wet and dry lakes located at the Umm Al-Aish fresh water lens are 1.71 and 0.46 km^2 , respectively.

The total dissolved solids concentrations (Fig. [10\)](#page-19-0) decreased to 4500 mg/L from approximately 7800 mg/L, after 50 years (total period of 73 years). Under the scenarios assumed, there are large masses of salts stored in the soil profile that will leach over time to the water table.

Simulated total dissolved solids concentration contours at 73 years after the spill (year 2063) are shown in Fig. [12](#page-20-0), with the simulated time series for total dissolved solids concentrations in the aquifers since the source was added shown in Fig. [5.](#page-13-0)

The predicted total dissolved solids concentration simulation (Fig. [12](#page-20-0)) provides a worstcase scenario of the likely extent of contaminant movement in groundwater in the two fresh water fields. Further data, from drilling sampling and other testing and experimentation should help clarify these assumptions and assist in updating the modelling.

5 Conclusions

A three-dimensional numerical computer model was constructed using the MODFLOW-SURFACT numerical code. The use of these codes helped to overcome the limitations of earlier models of the fresh water lenses. These models were able to combine both fresh water lenses in one modelling domain simulating the vadose zone together with the saturated zone. The interactions between these two fresh water lenses could also be simulated. The time-variant salinity transport model was calibrated simultaneously with the transient groundwater flow system and this included variably saturated flow and transport. This was done prior to proceeding to simulate contaminant (hydrocarbon) transport as the hydraulic gradients and flow directions (and storage volume) are significant controls on contaminant migration. The model simulated the period from 1991 onwards, at which point a large volume of saline water was injected to simulate the seawater used to extinguish oil fires, along with a pulse of contaminant, assumed to enter the groundwater system at this time. The model grid was refined to better address the saline transport issues. These simulations would require a more refined and more regular grid than the flow simulation. The salinity transport model was set up to run from March 1991 to July 2013 for historical matching, simultaneously with the transient flow model. The purpose was to allow 50 to 100 years of predictive remediation simulation time from the end of 2013.

The results of the salinity transport model suggest that although the fresh water – saline interface, as defined by the 1500 mg/L contour, has moved towards the centre of the lens in some areas up-gradient of the fresh water recharge, the extent of the fresh water lens has actually increased slightly in the down-gradient areas. The fresh water body of Al-Raudhatain has moved 40 m, following the flow direction, relative to the 40 m depression line. For Umm A-Aish, the fresh water lens has not moved much in relation to the 35 m depression level.

After 23 years, and with respect to the total area of the fresh water body at Al-Raudhatain (55.2 km^2), the areal extent of the total dissolved solids plume is estimated to be 15 km^2 for the 1500 mg/L contour. This equates to total dissolved solids impacting 27% of the fresh water body. The wet and dry lakes located at the Al-Raudhatain fresh water lens are 2.38 and 0.07 km², respectively.

After 23 years, and with respect to the total area of the fresh water body at Umm Al-Aish (37 km^2) , the areal extent of the total dissolved solids plumes is estimated to be 11 km² for the 1500 mg/L contour. This equates to total dissolved solids impacting 29% of the fresh water body. The wet and dry lakes located at the Umm Al-Aish fresh water lens are 1.71 and 0.46 km², respectively. These results indicate that after 23 years, the areal extent of the injected sea water salinity plume impacts approximately 26 $km²$ of the fresh water aquifers. There has been little experience in the world to make a comparison with such an extensive impact; it seems that oil spill during the Gulf war in 1991 was the biggest in human kind history.

The total dissolved solids concentrations decreased to 4500 mg/L from approximately 7800 mg/L, after 50 years (total period of 73 years). Under the scenarios assumed, there are large masses of salts stored in the soil profile that will leach over time to the water table. This indicates that the ecological and economic impacts and the full impact of the Gulf war, which began on August 2, 1990 when Iraq invaded Kuwait, probably will not be realized in the near future. The predicted total dissolved solids concentration simulation provides a worst-case scenario of the likely extent of contaminant movement in groundwater in the two fresh water fields. The environment in a war always seems to be one victim, and the scenario was no different in the case of the Gulf war crisis from 1990 to early 1991. What can be determined is that Kuwait suffered severe losses not only to its oil industry, but also to its ecological system. Further data, from drilling sampling and other testing and experimentation should help clarify these assumptions and assist in updating the modelling.

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