

## Characterizing a heterogeneous hydrogeological system using groundwater flow and geochemical modelling

### Utilisation d'un modèle couplé géochimie/ d'écoulements souterrains pour caractériser un système hydrologique hétérogène

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#### ABSTRACT

Characterization of heterogeneous hydrogeological systems plays an important role in groundwater protection and remediation of contaminated sites. However, sparse field observations and/or lack of relevant *in situ* test results hinder regional characterization process. In such cases, advanced modelling techniques can improve characterization of such complex hydrogeological systems. A sequential approach using groundwater flow modelling with nonlinear inverse calibration, advective transport and geochemical modelling and isotope study to characterize heterogeneous systems has been developed in this case study. It was used to better understand the regional hydrogeology and groundwater system of the Triassic Sherwood Sandstone aquifer underlying the Belfast area, Northern Ireland. Based on the inversely calibrated flow model and advective transport modelling by particle tracking, geochemical interpretation of groundwater quality data and isotopic and geochemical inverse modelling at well-distributed spatial locations in the sandstone were carried out to verify the flow pathways and residence times and to identify the geochemical evolution in this heterogeneous hydrogeological system. These approaches provide multiple lines of evidence for characterization of the heterogeneous aquifer system. The flowpaths and residence times from the flow and advective transport modelling agreed well with the geochemical modelling and isotopic radiocarbon dating. This demonstrates the importance of incorporating both flow and geochemical analysis techniques in a hydrogeological study.

#### RÉSUMÉ

La caractérisation des systèmes hydrogéologiques hétérogènes joue un rôle important dans la protection des eaux souterraines et la réhabilitation des sites contaminés. Cependant, la distribution sporadique des observations de terrains et/ou la rareté des résultats d'essai *in-situ* valables limitent la portée d'une caractérisation régionale. Dans de tels cas, les techniques de modélisation avancée peuvent améliorer la caractérisation de systèmes hydrogéologiques complexes. Une approche séquentielle a été développée dans ce cas d'étude : elle utilise un modèle d'écoulement souterrain avec un calage inverse non-linéaire, la modélisation du transport géochimique par advection et un suivi isotopique pour caractériser des systèmes hétérogènes. Cette approche a été employée pour mieux comprendre l'hydrogéologie régionale et l'organisation des écoulements souterrains de la couche aquifère triasique des grès de Sherwood sous la région de Belfast en Irlande du Nord. Basée sur un modèle d'écoulement étalonné par inversion et un transport advectif modélisant la propagation de particules, l'interprétation géochimique des données de qualité des eaux souterraines et la modélisation inverse isotopique et géochimique, selon des stations distribuées de manière appropriée dans le grès ont été exécutées pour vérifier les cheminements et les temps de séjour et pour identifier l'évolution géochimique dans ce système hydrogéologique hétérogène. Ces approches suggèrent de multiples voies pour la caractérisation de ce système hydrogéologique hétérogène. Les cheminements et les temps de séjour issus de la modélisation des écoulements et des transferts par advection sont en bon accord avec le modèle géochimique et les datations isotopiques au radiocarbonate. Ceci montre l'importance d'intégrer l'écoulement et les techniques d'analyse géochimique dans une étude hydrogéologique.

*Keywords:* Characterization, hydrogeology, heterogeneity, inverse modelling, geochemistry.

#### 1 Introduction

Characterization of heterogeneous hydrogeological systems is an important step in regional groundwater management and contaminated site remediation. Successful modelling can result in an improved understanding and conceptualization of the

hydrogeological systems. Numerical groundwater modelling has provided a valuable tool to understand regional hydrogeology at various spatial and temporal scales through simulation of groundwater flow and transport systems.

System characterization using *in situ* pumping tests and tracer tests are widely used in small-scale studies of site-specific

hydrogeology and groundwater systems. However, it is always difficult to characterize hydrogeological systems with large-scale study area and limited resources. Data scarcity is a major problem in most cases. Some non-intrusive geophysical techniques, as reviewed by Hubbard and Rubin (2000), can be used to estimate hydrogeological parameters but need dense geophysical sampling and proper interpretation. In this context, numerical models become powerful and practical modelling tools for complicated regional hydrogeological simulations under various conditions (Anderson and Woessner, 1992; Bredehoeft and Hall, 1995). There are good arguments for using numerical models to test both conceptual models and system behaviour and to assist/guide in planning further data collection (e.g. Carter *et al.*, 1994). Geochemistry and isotopic techniques also have been used to identify and characterize regional groundwater systems (Barbecot *et al.*, 2000; Elliot *et al.*, 2001). Therefore, a methodology was developed in the characterization of the regional hydrogeology and groundwater systems in the Triassic Sherwood Sandstone aquifer systems in the Lagan and Enler Valleys, Northern Ireland incorporating both numerical flow modelling and geochemical modelling. The integration between these approaches and the case study are outlined in this paper.

Forward groundwater flow modelling, inverse parameter optimization, advective transport modelling and geochemical/isotopic study have been carried out for both the porous sediments and the fractured bedrock aquifer at a regional scale. Groundwater flow model of the heterogeneous systems was calibrated by inverse method to achieve the best fits between the modelled and observed groundwater heads. Based on this calibrated flow model, further particle tracking modelling of advective transport was carried out. Geochemical sampling and interpretation of the analysis results were carried forward to gain a more reliable knowledge of the groundwater geochemical evolution and residence times in the aquifer. Thus, the characteristics of the heterogeneous systems obtained from the groundwater flow modelling results were verified by geochemical study, inverse geochemical modelling and isotope dating. This study highlights the importance of incorporating groundwater flow and geochemistry in the characterization of heterogeneous hydrogeological systems using numerical modelling.

## 2 Methodology

Sound estimates of aquifer properties and processes (e.g. recharge), good understanding of system boundaries, and a reasonable conceptualization of subsurface structures and details are crucial for an accurate and reliable numerical simulation of the system. These elements can be better achieved by both physical and geochemical investigations and collaboration of the two aspects, which are traditionally pursued independently. Inverse numerical modelling can provide more efficient parameter calibrations than traditional manual calibration and facilitate assessment of prediction reliability (Poeter and Hill, 1997) by considering *a priori* information and analysing statistically the output data; it therefore can provide insights

into the functioning of the physical system. If the advective transport obtained from the inverse flow calibration results, are incorporated with geochemical interpretation, inverse modelling and isotopic/hydrogeochemical study of the aquifer system, improved characterization and understanding of complex systems can be achieved. Therefore, multiple lines of evidence from groundwater advective transport, geochemical modelling and isotopic study were combined to provide a more robust characterization of the heterogeneous system. A sequential approach of inverse flow calibration, advective transport, geochemical modelling was developed to characterize the heterogeneous hydrogeological systems in the Belfast area, Northern Ireland.

### 2.1 Inverse modelling and advective transport

Nonlinear inverse model implemented is a weighted least square method based on Gauss–Marquardt–Levenberg optimization scheme, from the program PEST98 (Watermark Computing, 1998). Detailed background on the optimized calibration and system uncertainty was described by Yang *et al.* (2000).

The basic idea of the inverse approach is to optimize the adjustable parameters to minimize an objective function, e.g.  $\min F(\text{parameters}) = \text{Weight}_{\text{obs}} J [H_{\text{obs}} - H_{\text{mod}}]$ , through making comparison between the observed and modelled heads ( $H_{\text{obs}}$  and  $H_{\text{mod}}$ ) with certain transformation ( $J$ ) and considering factors that may affect quality of the observation data. A set of initial model parameters, with upper and lower bounds for an appropriate searching space, is usually used to start the optimization. The parameters are optimized until the objective function or fit between model-generated value and observed one, is reduced to a minimum in the weighted least square sense (Yang *et al.*, 2000).

The inverse calibrated flow model was used then to model the advective transport of groundwater in the regional Belfast area, Northern Ireland. Groundwater flow directions and residence times of the sandstone aquifer were estimated using the particle tracking technique. These results present information of the aquifers system yielded from the inverse-calibrated flow model; they may be further validated using other sources of information.

### 2.2 Geochemical modelling

In order to verify the inverse groundwater flow calibration and prediction results, further groundwater sampling and geochemical analysis were carried out along with  $\delta^{13}\text{C}$  analysis and radiocarbon dating. Geochemical evolution and flow paths in the aquifer were characterized with inverse geochemical modelling (Plummer *et al.*, 1994). The hydrogeochemical evolution in this sandstone aquifer is dominated by carbonate mineral dissolution and congruent dissolution of calcite, dolomite and gypsum, which may lead to the precipitation of calcite through dedolomitization (Hounslow, 1995). This allows delineation of flowpaths through the aquifer using Mg/Ca ratios, as dedolomitization leads to an increase of the Mg/Ca ratio along the flow directions. However, due to the multiple sources and sinks for these elements,

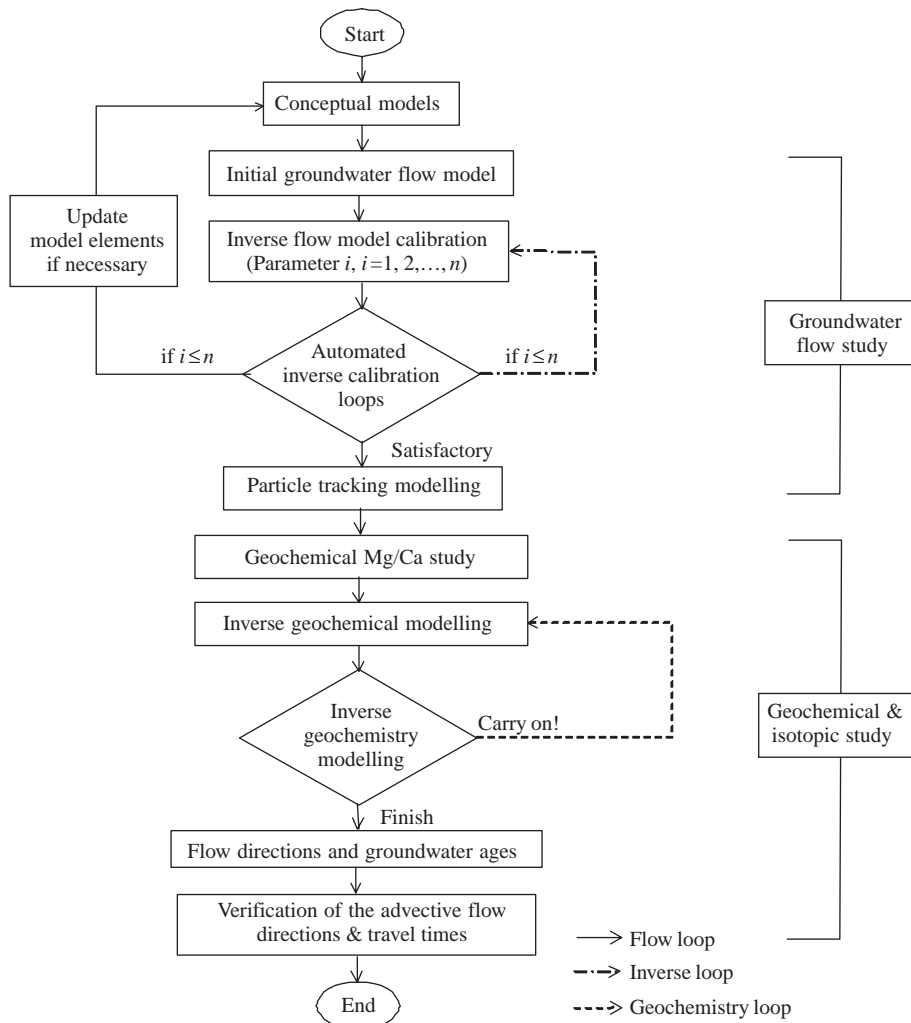


Figure 1 Schematic flow chart showing the research methodology.

$\delta^{13}\text{C}$  was used as a further constraint on delineating the flow-path directions (Cronin *et al.*, 2000). The flowpaths obtained from the flow model and Mg/Ca ratios were further checked by inverse geochemical modelling and groundwater evolution interpretation. Residence time for the sandstone aquifer was further verified by radiocarbon ages.

### 2.3 Procedure

An outline of the procedure is shown in Fig. 1. A preliminary numerical flow model was built based on an initial conceptualization of the aquifer systems. The inverse flow model then was calibrated for  $i$  parameters until the optimal results were reached. The conceptual model was adjusted sequentially after optimization in each step if necessary. Advective transport modelling for flow path identification and transit residence time estimation was carried out with this inversely calibrated flow model. The geochemical calculation of Mg/Ca ratios was then used to verify the flow paths obtained from the flow modelling. Finally, geochemical inverse modelling was used to evaluate groundwater evolution along the flowpaths from the main recharge source (a typical chalk spring water) to the sampled well chemistry. The resulting model possibilities then were further constrained using the  $\delta^{13}\text{C}$  values. Thus, altogether three iterative loops were

linked and/or embedded in the characterization procedure. After this system characterization with inverse optimization and geochemical verification, the more reliable forward flow model is ready for further predictive modelling and thorough analysis of groundwater evolution.

## 3 The case description

### 3.1 Regional setting

The study area is located in the Lagan and Enler Valleys, Northern Ireland. The River Lagan, a major river with an average flow of  $8\text{ m}^3/\text{s}$ , extends to the southwest of Belfast and the Enler is a small river in the east (Fig. 2). The Lagan is flanked by large hills to the west and north that reach 480 mAOD. The Enler Valley is fairly flat except for an imposing dolerite hill near Newtownards. The average rainfall is 950 mm per annum and evapotranspiration 400 mm (Yang *et al.*, 2000). The regional geology is shown in Fig. 2. The Permo-Triassic strata dip shallowly at about  $14^\circ$  to the NW. Tertiary dykes intrude into the bedrock sandstone aquifer and the boundary lithologies. The heterogeneous geology is further complicated by numerous faults parallel and perpendicular to the axis of the valley.

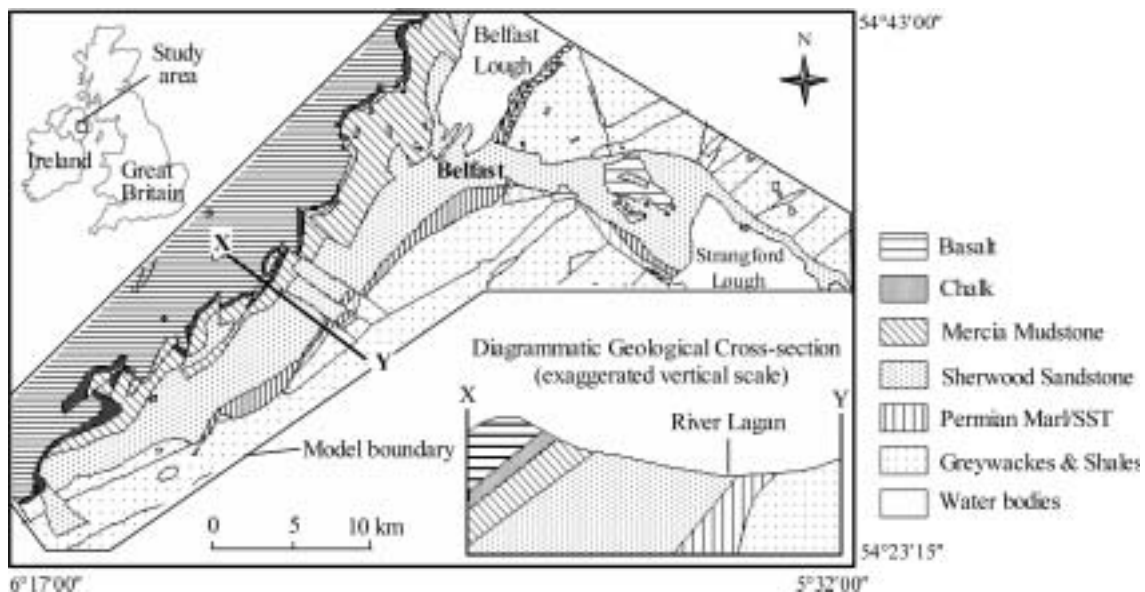


Figure 2 Geology of the study area and the regional conceptual model (after Yang *et al.*, 2000).

The Triassic Sherwood Sandstone is Northern Ireland's most important aquifer, although other formations such as sand and gravel drift is also important for local water supply source. The groundwater in the Sherwood Sandstone flows towards the valleys from both sides of the typical glacier U-shape valley then to the sea. The aquifer receives limited recharge from precipitation along the valley centres where the drift is up to 35 m thick but significant recharge is from overlying formations along the northwest side of the Lagan Valley (Bennett, 1976). Additional limited recharge through the till may occur along preferential pathways, such as filtration along till discontinuities and sandy patches (Robins, 1996).

### 3.2 Conceptualization and forward flow model

The sandstone is the main aquifer of the study area. Six solid geology layers were represented in the regional conceptual model: the Ordovician and Silurian Greywackes; Permian Marl; Triassic

Sandstone; Mercia Mudstone and Sandstone; Chalk and Tertiary Basalt (Fig. 2). Considering variation of the heterogeneous aperture and fracture development in depth, two layers of solid geology (50–120 m thick) were conceptualized to represent the permeability–depth profile of the sandstone. The drift was also characterized to investigate the role of the Quaternary sediments and their relationship to the underlying solid geology. Three layers were modelled: the alluvium and sand/gravel (few metres thick), and subglacial till (up to 35 m thick).

A regional numerical groundwater flow model was built using MODFLOW based on this conceptual model. Meteorological and hydrological, monitoring and pump test results were analysed and integrated into the model (Yang *et al.*, 2000). The model domain was chosen to cover the sandstone outcrop and expanded out to include the majority of the strata so as to reduce the boundary effect that may be posed on the groundwater flow system. A constant head of 0 m was placed at the coastal boundaries. An effective recharge of 30 mm was initially taken for the valleys and

Table 1 Model-estimated parameter values of  $K$  and comparison to the data obtained in previous hydrogeological studies

No.	Geological layer	Modelled $K$		$K$ from previous studies (m/s)	Data sources/comments
		(m/day)	(m/s)		
1	Alluvium	7.71	$8 \times 10^{-5}$	$5 \times 10^{-6}$	Test [1]
2	Sand/Gravel	49.82	$5 \times 10^{-4}$	$10^{-5} \sim 10^{-3}$	Tests and [1]
3	Till	4.32	$4 \times 10^{-5}$	$10^{-11} \sim 4 \times 10^{-5}$	[2]; [3]
4	Basalt	10.24	$1 \times 10^{-4}$	$10^{-5}$	Test [1]; over-estimated
5	Chalk	35.44	$4 \times 10^{-4}$	$7 \times 10^{-5}$	Test [1]
6	Greywackes	0.016	$1 \times 10^{-7}$	$1.2 \times 10^{-7}$	[1]
7	Permian Sandstone	0.22	$2 \times 10^{-6}$	$10^{-6} \sim 10^{-4}$	[2]; [1]
8	Permian Marl	0.16	$1 \times 10^{-6}$	$\sim 10^{-9}$	[2]
9	Mercia Mudstone	2.33	$2 \times 10^{-5}$	$\sim 10^{-9}$	[2]; over-estimated
10	Sandstone (upper layer)	0.03~4.5	$10^{-7} \sim 10^{-5}$	$10^{-7} \sim 6.6 \times 10^{-5}$	Pumping test; [1]
11	Sandstone (lower layer)	0.02~0.8	$10^{-7} \sim 10^{-6}$		

[1] Robins (1996); [2] Kalin and Roberts (1997); [3] McConville (1999).

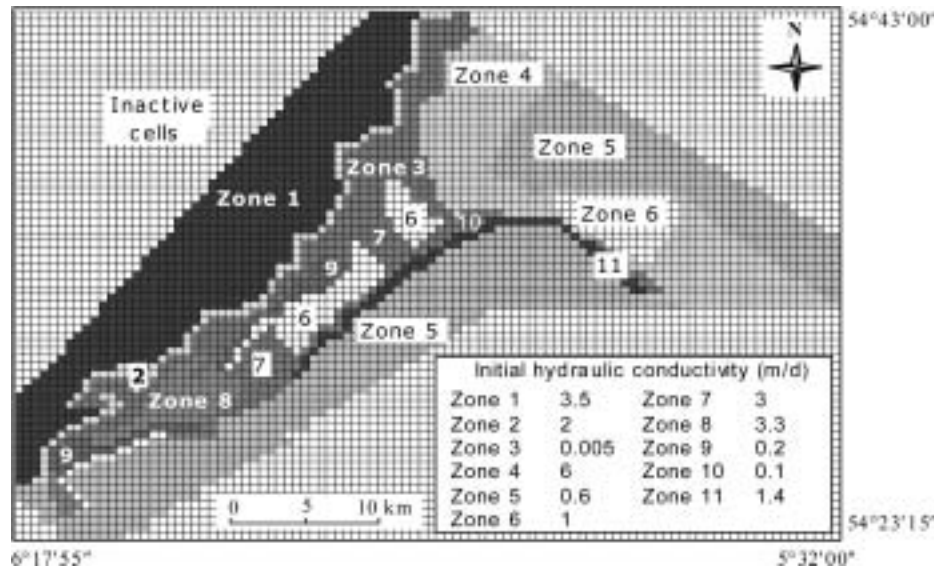


Figure 3 Model grids and hydraulic conductivity zones of the shallow sandstone layer.

urban areas (Hartley, 1935). A higher value of 150–300 mm was used for further calibration on areas where the till cover is thin or preferential flows exist. River cells with conductance values from 2000 to 3400 m<sup>2</sup>/day were calculated according to previous study results and assigned in the model. Aquifer property values were taken from various pumping test results and previous reports carried out on the study area (e.g. Robins, 1996; Kalin and Roberts, 1997). For example, a typical  $K$  value of the Sherwood Sandstone obtained from the pumping test in Queens University campus borehole was  $2.56 \times 10^{-6}$  m/s, see Table 1. The geological structures and intrusion dykes were taken into account when assigning permeability values (Figs 2 and 3). Regular finite difference grids of 500 m<sup>2</sup> were used for the model (Fig. 3).

Seasonal variations in the groundwater head were examined. Comparing to the large modelling area and great variation of topography, the ranges over decades were relatively low, 1–2 m, at most observation sites except some wells near boundaries of the sandstone aquifer. Therefore, a steady-state flow model was chosen for the system characterization.

### 3.3 Inverse calibrations

The regional groundwater system was calibrated through non-linear inverse numerical modelling. Three major issues were calibrated for: heterogeneous distribution of hydraulic conductivities ( $K$ ); lateral flows into/out of the aquifer and spatial recharge loading. Due to scarcity of field pumping tests in the regional modelling area,  $K$  was more important than other factors as far as the system characterization concerned. Data of groundwater head from 22 boreholes were used based on the means of 1971–1975 observations in the modelling area.

Hydraulic parameters of aquifer are important in modelling a groundwater system.  $K$  was calibrated by the inverse modelling based on the forward flow model. Zonation of the hydraulic conductivity was determined on the basis of the geology, structure, land use, topography and hydrology (Fig. 3). The optimal

objective function was achieved after five inverse iterations. The optimized  $K$  results are shown in Table 1. Sensitivity analysis of  $K$  shows that the inverse calibration of the regional model was sensitive to the  $K$  values of the sand/gravel, till and Sherwood Sandstone in the middle part of the Lagan Valley, and then to the basalt and greywackes (Yang *et al.*, 2000). Parameters with higher sensitivity are more significant in the model performance with respect to all observations in the model.

To identify the boundary condition of the groundwater model at spatial (location) and quantitative (rate) scales, several inverse scenarios were investigated. The in/out flows were identified along the boundaries between the sandstone aquifers and the greywackes to the eastern parts and the basalt to the west of the Lagan Valley. Wells were assigned to represent the lateral flows along the boundaries and the lateral flow rates and their spatial locations were identified. The overall optimization shows that the model was sensitive only to the inflows in the lower layers along the greywackes boundaries, and not to that in the Quaternary drift. This may imply groundwater from the greywacke fractures interacts laterally with the sandstone but little water flows into the drift (Fig. 4a). The low-permeability clay till prevents groundwater from moving into the sand/gravel aquifers. The lateral inflow to the sandstone from the greywackes in the northwestern area was optimized as 2.11 m<sup>3</sup>/day/m of boundary. The model was not sensitive to the western boundary, suggesting that the lateral inflow recharge along these boundaries is insignificant in comparison with the sandstone aquifer totals. This is identical to the regional conceptual hydrogeology (Fig. 4b): the mudstone conformably overlying the sandstone forms an aquitard in the regional sense and prevents groundwater from penetrating it. The groundwater then comes out as springs and flows to the sandstone as surface recharge. This agrees with the characterization of recharge by Bennett (1976).

The spatial distribution of the recharge was characterized after calibration of the  $K$  and boundary inflow. Eleven recharge zones were assigned taking into consideration the land use,

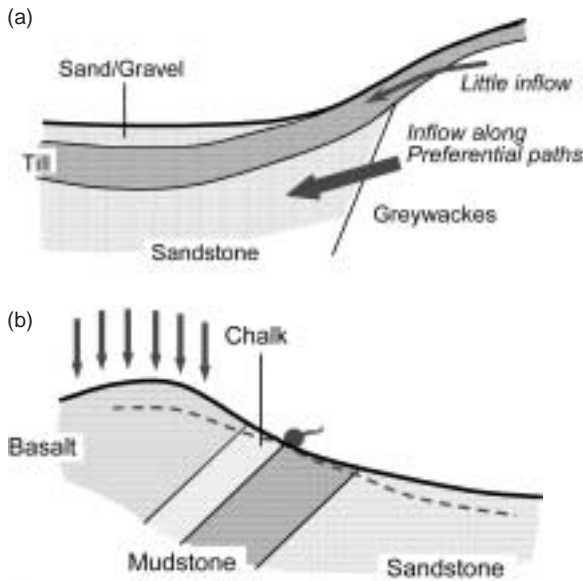


Figure 4 Diagrammatic presentation of the boundaries in the (a) north-east and (b) west.

geology and topography in the modelling area. The calibrated recharge is 420 mm/annum around the dyke in the Enler area and along the chalk where springs are located, reflecting influence of structures and strata. Most of the effective recharge comes out in the springs at the basalt/chalk escarpment to the west of the Lagan Valley (Bennett, 1976). It is only 10 mm/annum in the southern area where the till may be thick. The value of some cells where the faults cross the boundary between the chalk and sandstone reaches as high as 970 mm/annum. This demonstrates that this system is highly heterogeneous and most recharge occurs along some preferential flow paths. There is little recharge in less permeable areas such as the basalt, greywackes and area of urban development. The contour of the calibrated groundwater heads, measured points and their location of the sandstone aquifer are shown in Fig. 5.

#### 4 Advective transport

Advective transport modelling was carried out based on this inversely calibrated flow model to identify flowpaths and estimate groundwater residence times in the valleys. There was no continuous flow path in the sandstone that travelled from up-gradient to down-gradient in the Lagan Valley. Most particles originated from up-gradient were intercepted by rivers indicating discharge of groundwater to surface water to form river baseflow along flowpaths. However, some particles in the middle and lower sections of the valley reached the sea at Belfast and Strangford Loughs. Flow paths orthogonal to the equipotential lines of groundwater under this steady state flow condition, delineate the movement routes of individual water particles in the valleys. Some typical groundwater pathlines are shown in Fig. 6 (broken-curve arrows).

The maximum modelled groundwater residence time in the sandstone is 7000 years in the southwest area of the Lagan Valley. Transit times are 2000–4000 years to the west of Belfast Lough. Groundwater is relatively younger in the middle of the Lagan Valley (around Lisburn) and the Enler Valley, 300–2000 years; two locations near Lisburn and Newtownards are less than 200 years. Looking at the travel times of the groundwater particles across the mudstone in the west of the Lagan Valley, they are mostly about 6000–12000 years. This compares well to the analysis of the conceptual model regarding characteristics of the west boundary.

#### 5 Geochemical modelling

Groundwater sampling was carried out at 40 wells throughout the study area and analysed for all major and minor ions, along with  $\delta^{13}\text{C}$  and  $^{14}\text{C}$  radiocarbon dating at selected wells (Cronin *et al.*, 2000). As with other Triassic Sandstone aquifers in the UK, the groundwater geochemical evolution is dominated by carbonate mineral dissolution and dedolomitization. The approach using Mg/Ca ratios and  $\delta^{13}\text{C}$  to delineate the flowpaths was applied

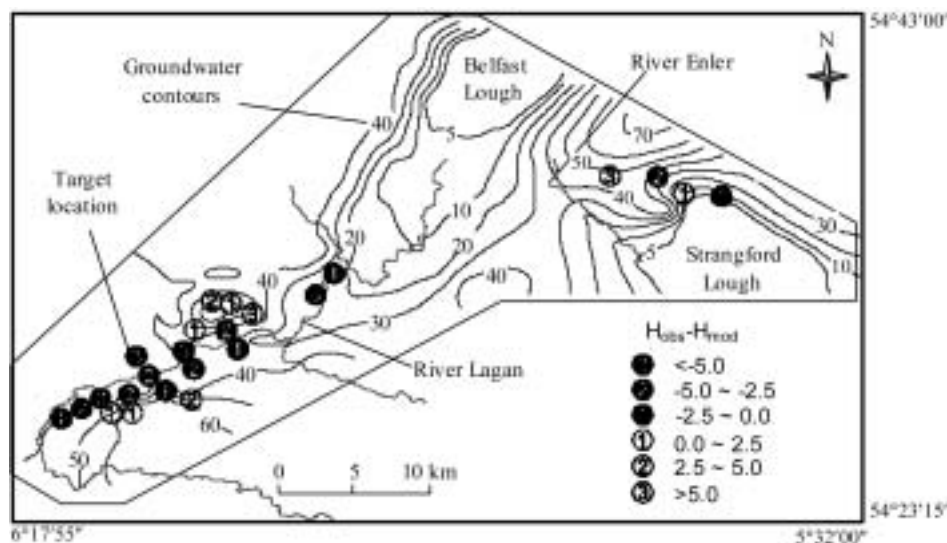


Figure 5 Inverse-calibrated hydraulic results of the regional groundwater flow model.

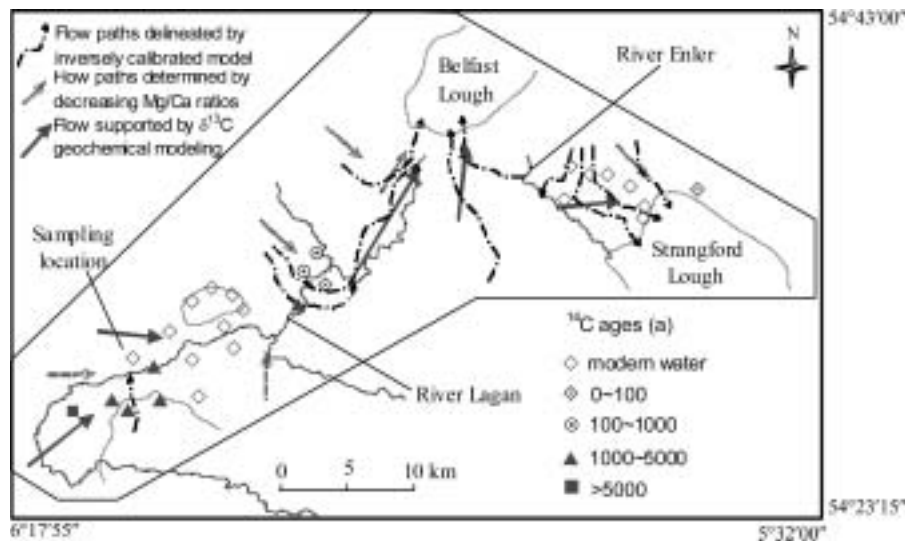


Figure 6 Regional groundwater advective transport and geochemical modelling results with brief hydraulic contour background.

in this case study. The consequence of dedolomitization is an increase of Mg/Ca ratio in the direction of flowpaths. The flowpaths obtained by this method are shown in Fig. 6 (dotted-line arrows). They generally match the particle tracking results of the advective transport modelling well.

Based on the flowpaths from the advective transport of flow model verified by the Mg/Ca ratio, further geochemical inverse modelling was carried out using NETPATH (Plummer *et al.*, 1994), an interactive geochemical modelling code for NET geochemical reactions along a flow PATH. The distribution of chemical species in the aqueous solution was calculated and then was linked to main mass-balance/isotope balance model. Such a model is based on the conservation of mass and electrons during geochemical evolution of groundwater whilst considering the redox state of the chemical elements and/or isotopes. Isotopic calculation with  $^{13}\text{C}$  is independent of the process of speciation modelling and mass balance calculation and is therefore a valuable tool to verify results from other calculations in the Lagan Valley. Identification of the geochemical reactions, dissolution (D), precipitation (P) and other processes, was made by examining the relationship between the ionic species concentrations in order to interpret the groundwater evolution.

Groundwater flow modelling showed the primary recharge source was the chalk springs to the west of the Lagan Valley. The geochemical inverse modelling used a spring water as the source water term, assuming an initial  $^{14}\text{C}$  activity of 90 percent modern carbon (pmc) composition (Barnes, 1998). The chosen phases for the geochemical modelling were calcite (D or P), dolomite (P), gypsum (P), halite (P), carbon dioxide (D) and ion exchange ( $\text{Na}^+$  for  $\text{Ca}^{2+}$ ). The model was run by constraining the elements C, Ca, Mg and Na (Cl and S were not chosen due to the possibility of their addition from anthropogenic sources). A mean  $\delta^{13}\text{C}_{\text{TDIC}}$  value of  $-3.1\text{‰}$  was used for the sandstone matrix along with a  $\delta^{13}\text{C}$  value soil gas carbon dioxide of  $-26.1\text{‰}$  (Smith *et al.*, 1976; Cronin, 2000).

Geochemical inverse modelling of  $\delta^{13}\text{C}$  using the NETPATH model indicates a partly closed water evolution by decreased  $\text{pCO}_2$  values downgradient in the study area (Cronin *et al.*,

2000). Geochemical evolution along the flowpaths through the sandstone aquifer was constrained by  $\delta^{13}\text{C}$  values within the range of  $+2\text{‰}$  (cf. Kimblin, 1995), representing the uncertainty in soil  $\text{CO}_2$   $\delta^{13}\text{C}$  values. Once a plausible geochemical evolution model was identified, radiocarbon dates were evaluated by the model correcting for all the sources and sinks of carbon along the flow paths. Most, not all, of the flowpaths from the advective transport and Mg/Ca ratios were supported by radiocarbon ages (solid-line arrows in Fig. 6). The corrected ages allowed a plot of residence times within the aquifer to be made (Fig. 6).

## 6 Discussion

The overall inverse flow calibration shows a good match. However, some of the calibrated results may not be representative due to the lack of observations or other uncertainty in the modelling. The model-estimated  $K$  values of the Quaternary are elevated with respect to field data and this may indicate an exaggeration phenomenon to the Quaternary due to the scale effects (i.e. thickness).  $K$  value of the sandstone is characterized by a general decrease from shallow layers to depth.  $K$  is relatively greater, horizontally, in the north and middle of the study area, which features the high heterogeneity of the aquifer as a result of geological structures. The Mercia Mudstone and basalt were also much over-estimated, as there was no observation control in these areas and possibly “ill-posed” data ranges (Yang *et al.*, 2000). It may be a good practice to introduce “soft data” in such areas according to existing knowledge, spatial extrapolation or other methods (e.g. Poeter and McKenna, 1995); otherwise the calibrated value could be too large or too small because of insensitivity of the model to the parameters. The boundary flow calibration and sensitivity analysis reveal the hydraulic interactions between the sandstone and the surrounding strata. Highly heterogeneous recharge mechanisms exist in the groundwater system. The advective transport modelling provided pathlines of groundwater particles in the valley and produced overall residence times in the sandstone. Some

flow paths with irregular transport route may indicate preferential flow paths (Fig. 6). The groundwater flow paths from particle tracking matched well with the geochemical modelling results.

The geochemical modelling result suggests a groundwater evolution with an available source of carbon dioxide in the Sherwood Sandstone aquifer. CO<sub>2</sub> gas needs to be included in the model in order to match the computed  $\delta^{13}\text{C}$  to the depleted values observed in the field. This is surprising as the aquifer in the Lagan Valley is thought as effectively confined by the glacial till. Such an “open” nature indicated by the geochemical modelling may be confirmed by the larger recharge estimated in the inverse modelling of groundwater flow along preferential paths. An alternative CO<sub>2</sub> source may be oxidized organics in a closed groundwater system, involving a reaction of “C<sub>organic</sub> + O<sub>2</sub> → CO<sub>2</sub>”. No dissolved organic carbon (DOC) was carried out in this study, however, the DOC in the similar UK aquifers is very little, 0.1–4 mg/l (Cronin, 2000). Geochemical modelling with correction of radiocarbon dating provides more accurate residence times, which was used to further verify the groundwater flow modelling output. Actually, the radiocarbon dating results matched the residence times obtained from advective transport well, see illustration in Fig. 6. This is very good geochemical evidence to confirm the results from the inversely calibrated flow model. This groundwater system has a long turnover time, both advective transport modelling and radiocarbon dating indicates some relatively old water, e.g. over 5000 years in the south of the Lagan Valley (Fig. 6). However, modern water components occur where the local recharge was induced by well abstractions, or short circuiting of the well (e.g. in the Enler area to the east of Belfast).

## 7 Conclusions

Regional numerical modelling is useful to characterize regional flow and better understand aquifer systems. Flow modelling with nonlinear inverse calibration, advective transport, geochemical and isotopic inverse modelling were incorporated to better characterize the heterogeneous hydrogeological systems. The methodology was illustrated by using a case study in a Triassic Sherwood Sandstone aquifer in the Belfast area, Northern Ireland.

Hydrogeological parameters were optimized with a nonlinear inverse model; then flow paths and residence times were further investigated and verified by using geochemical Mg/Ca ratio study, geochemical inverse modelling and isotopic studies. The hydraulic conductivity was estimated as 49 m/day for the sand/gravel and 0.02–4.5 m/day for the sandstone in this area. The lateral inflow was estimated as 2 m<sup>3</sup>/day/m of boundary in the northeast area. The recharge was mainly from the areas where preferential paths exist. The flowpaths from flow modelling were well confirmed by the geochemical and isotopic study. The residence times and flowpaths from the inversely calibrated flow model and geochemical analysis were supported by isotopic radiocarbon dating. Geochemical modelling, coupled with radiocarbon dating, produced residence times over 5000 years

old, especially in the southern half of the Lagan Valley. This matched advective transport modelling result well. The flow modelling with inverse parameter optimization, when incorporated with geochemical inverse modelling, proved to be a better way to understand regional hydrogeology. It is useful to apply geochemical and isotope modelling to incorporate groundwater flow modelling in regional hydrogeology study.

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