

Development of the AquiferSim Model of Cumulative Effect on Groundwater of Nitrate Discharge from Heterogeneous Land Use over Large Regions

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EXTENDED ABSTRACT

Regional-scale prediction of the effects of nitrate discharge from land use on the quality of the underlying groundwater requires two major model components: (1) a climate-driven model of agricultural land use that predicts nitrate discharge at the bottom of the plant root zone, for locations over horizontal space; and (2) a groundwater transport model, which predicts nitrate concentration at horizontal and vertical locations within the aquifer as well as the nitrate discharge to surface-water bodies. AquiferSim is a recently-developed groundwater transport model, for which the inputs of recharge and nitrate from the land surface are received from a GIS user interface that accesses the root zone nitrate discharge model.

The AquiferSim groundwater transport model is designed to address two particular requirements. The first is that model run times should allow for real-time examination of land use scenarios and assessment of uncertainty. The second is that dimensions of computational cells should allow for realistic transport dispersion in both horizontal and vertical dimensions, as well as allowing improved accuracy of flowpaths to surface-water bodies. These latter requirements imply very large numbers of computational cells for regional-scale studies, with associated costs in model run time. These issues are addressed in the AquiferSim

model by: assuming steady-state groundwater flow and transport; solving 2D horizontal groundwater flow on $\sim 10^6$ computational cells with a fast, full-multi-grid solver; and then solving flow and transport on vertical sections of $\sim 10^4$ cells along selected groundwater flowpaths, with a successive-over-relaxation solver. The software was developed entirely in Microsoft Visual C# on the .NET framework. This enables the AquiferSim engine to run on modern Windows PCs and on Linux and clustered environments using the MONO platform.

Computational time performance of the AquiferSim engine enables the horizontal 2D steady-flow groundwater problem and pathline tracking to be solved in about 5 s for a region occupying one third of the 1025 x 1025 computational grid. Solution for groundwater flow, nitrate transport, and groundwater age on the $\sim 10^4$ cells of one vertical slice requires up to 20 s.

Implementation of AquiferSim within a regional council for environmental planning purposes is the next phase of development. The major issues are likely to be: quantifying the predictive uncertainty caused by inadequate description of aquifer recharge and properties; and software design for interrogation of AquiferSim output to meet yet unspecified requirements for end-user information.

1. INTRODUCTION

Contamination of groundwater by nitrate leached from agricultural land use is a problem in many countries of the world because of the effects on drinking water quality and on the ecology of surface waters. This issue has been formally reported in New Zealand for more than 30 years but has become more important as increasing intensification of agriculture appears to conflict with public expectations for health and environmental quality. The research described in the present paper is part of the multi-agency programme, IRAP (Integrated Research for Aquifer Protection), which is directed to management of the impact of agricultural land use on groundwater underlying the relatively flat alluvial plains of New Zealand. The primary stakeholders in this issue are the regional councils, responsible to the public for environmental management, and the landowners themselves. Modelling tools provided from the IRAP Programme are intended to be operated, initially, by the regional councils but in a format that is transparent to all parties in the public forum.

Bidwell et al. (2005) describe the initial concept for the model architecture of these tools as:

- A GIS to manage spatial data that is required by the models, including land use, soil, and aquifer characteristics
- An agricultural land use simulation model (FarmSim) that generates soil drainage and associated nitrate concentration at farm scale (Good and Bright, 2005)
- A groundwater model (AquiferSim) that integrates the effects of nitrate-contaminated recharge at farm scale, and provides information about the resulting horizontal and vertical distribution of effects in the aquifer
- An end-user interface for the user to define *what-if* catchment-scale scenarios, and to view model outputs.

The common platform for these components is the Microsoft .NET 2.0 framework, with appropriate interfaces to GIS for data and information transfer. The present paper describes the rationale and computational development of the regional-scale groundwater transport model AquiferSim.

2. MODEL REQUIREMENTS

The AquiferSim groundwater transport model is intended for application at regional scale, a few thousand square kilometres, for prediction of the effects of nitrate discharge from land use that can

be specified at one-hectare scale. The horizontal transport distances in the underlying groundwater are up to 50 km, and the associated longitudinal dispersivities are therefore likely to be up to a few hundred metres. For effective use of the computational grid as a contributor to simulation of dispersive transport the desirable mesh size is ~ 100 m, which is similar to the scale of land use description. The result is that the 2D horizontal representation of groundwater transport requires ~ 10^6 computational cells.

The vertical dimension imposes two quite stringent requirements on the computational mesh in order to achieve the full 3D description. Firstly, the dispersivity scale is likely to be only a few metres. This component of dispersion is important because concentration contrasts from adjacent land uses are compressed into a few metres of aquifer depth, given the typical 100:1 ratio of horizontal to vertical aquifer dimensions. Secondly, the description of groundwater flowpath contribution to surface waters depends significantly on the resolution of the vertical dimension. This requires ~ 100 horizontal model layers for the 100 – 500 m thickness of the large alluvial aquifers in New Zealand.

The result of the above requirements for the computational grid indicates a 3D groundwater transport model with ~ 10^8 cells. This number exceeds the limits for conventional finite-difference and finite-element groundwater models that simulate transient water flow and solute transport. Even with appropriately arranged software and computing structure, the forward run time of the model would be excessively long.

This assessment is based on another important requirement, which is the need to be able to quantify predictive uncertainty in applications of AquiferSim. The alluvial aquifers are highly heterogeneous, and the contribution of river recharge is known to be significant but is very difficult to measure in the field. Therefore, aquifer properties and river recharge will be treated as parameters, usually as sets of larger dimension than the number of available data. The methods for analysing the predictive uncertainty of such underdetermined models, as described by Moore and Doherty (2005), require many model runs. Therefore, fast forward run time is desirable for practicable assessment of predictive uncertainty.

3. ADOPTED MODEL PRINCIPLES

The current version of AquiferSim is based on the following principles, as a compromise between process realism and model run time as required for

a reasonable response time for end users simulating landuse change scenarios and for uncertainty analysis:

1. The model simulates steady-state flow and transport. This enables use of fast solvers. A measure for time-based contamination effects is obtained from model simulation of groundwater age.
2. The 2D horizontal flow problem is solved separately and then used to find groundwater flow paths. The transmissivity field is assumed to be heterogeneous but isotropic.
3. The vertical 2D flow and transport problem is solved within the curved slice along the flow path passing through a selected location. Automatic selection of multiple locations enables more of the full 3D picture.
4. Hydraulic conductivity in the vertical 2D slice is heterogeneous and anisotropic (horizontal and vertical components). Porosity is heterogeneous.
5. Dispersion in the vertical 2D slice is determined by the effect of the horizontal and vertical computational cell dimensions and the respective water flux components. Transverse horizontal dispersion is not simulated.

4. COMPUTATIONAL METHODS

4.1. Selection of solvers

Our decision to adopt steady-state flow and transport means that the numerical solutions are expressed as boundary value problems. We were guided by the recommendations of Press et al. (2002) to use a linear full multigrid (FMG) approach for the large ($\sim 10^6$) 2D horizontal flow problem and successive over-relaxation (SOR) for the smaller ($\sim 10^4$) 2D vertical flow and transport problem. Software development for these methods involved following the principles described by Press et al. (2002) but constructing algorithms that are problem specific.

4.2. 2D horizontal groundwater flow

The objective is to obtain the solution piezometric surface from input data (via GIS) about groundwater recharge (including head dependent river/drain flows) and transmissivity at each node, and boundary conditions (specified head, specified flux). A block-centred, finite difference description was used for the numerical code.

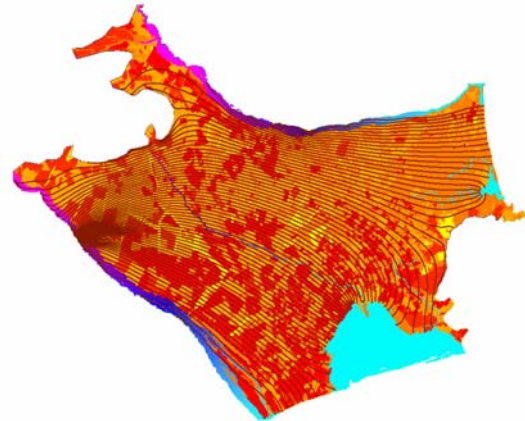


Figure 1. Example of groundwater pathlines, overlying land use, for one realisation of the transmissivity and recharge pattern for Central Canterbury.

The FMG solver requires a hierarchy of square solution grids with dimensions of $2^n + 1$ so that each successively coarser grid has double the mesh dimensions of the previous finer grid. We selected our finest grid as 1025×1025 ($n = 10$), which is equivalent to a $102.4 \text{ km} \times 102.4 \text{ km}$ square land area for 100 m mesh size. These dimensions were sufficient for the Central Canterbury regional study, and much larger regions could be accommodated by use of an appropriate mesh size. The coarsest grid of 33×33 ($n = 5$) is solved by the SOR method during each sweep of the FMG algorithm up and down the six solution grids. Most of the software work was related to interpolation between grids for irregularly-shaped boundary conditions, rivers, springs and aquifer properties.

4.3. 2D horizontal flow path

Our approach to determining 2D horizontal groundwater flow paths (Figure 1) could be simplified in comparison to established methods (e.g., Kinzelbach et al., 1992) because only direction, not velocity, was required. For any selected starting point within the flow field, the up- and down-gradient flow paths were determined from the x and y components of piezometric gradient within each mesh element. Logical tests were included to handle valleys or ridges between adjacent elements due to solution noise.

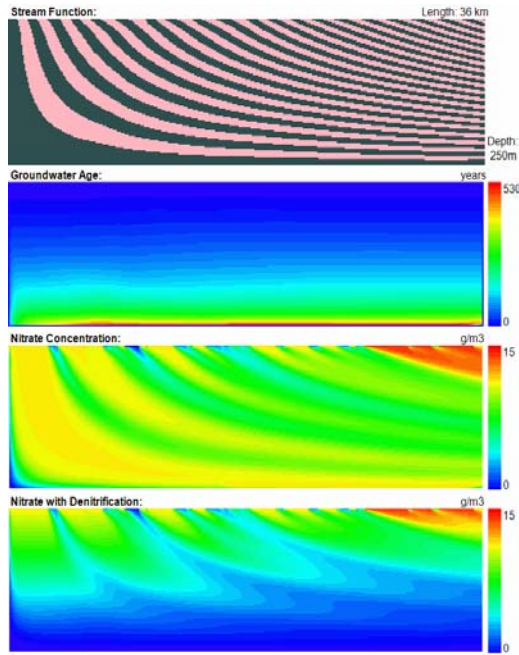


Figure 2. Example of output from the vertical slice solver, showing groundwater flow (streamfunction), age, and nitrate concentration .

Termination conditions were specified for boundaries and discharge sinks to surface waters and pumped abstraction.

4.4. 2D vertical groundwater flow

Groundwater flow within the curved vertical slice defined by a selected flow path is obtained as the block-centred, finite difference solution of streamfunction. This approach is restricted to steady flow and handling of sources or sinks within the flow field requires special boundary “cuts”. This raises a question about how to handle pumped abstraction. In AquiferSim, the options are to include shallow wells as part of the land surface recharge input or to apply pumped discharge to the bottom boundary of the vertical slice.

The SOR solver is used to obtain the streamfunction field, which describes groundwater flow (Figure 2, top). The upper (land surface) boundary is set by interpolation of the GIS recharge layer along the horizontal flow path. The remainder of the boundary is specified by no-flow conditions, pumped abstractions assigned to the bottom of the aquifer, and discharges to surface waters. The resulting values of streamfunction on the slice boundary represent the line integration of recharge (positive) and discharge (negative) in (say) a clockwise direction.

4.5. Nitrate transport and transformation, and groundwater age

Nitrate transport, nitrate transformation, and groundwater age within a vertical slice (Figure 2) are obtained by the mixing cell (finite volume) method applied to each mesh element. Water fluxes are computed from the streamfunction solution at the bounding nodes. Resident volume is determined from cell dimensions and input values of porosity.

AquiferSim includes only first-order decay as a transformation process. The decay rate may vary spatially and is applied to the resident volume of each cell as a term in the concentration flux balance equation. This decay process is based on time as determined by the steady-state water flux distribution.

Groundwater age is obtained by the method of Goode (1996), in which age is treated as a solute with zero-order growth and concentration initially zero at the land surface. This age “concentration” increases within each cell according to a “decay” rate of +1 applied to the resident volume term.

The SOR solver is used for nitrate transport, transformation and groundwater age. Nitrate concentration for the inflow boundary is interpolated from the GIS along the groundwater flowpath as recharge flux-weighted values. The vertical slice solutions for nitrate concentration can be interrogated for discharge concentration contributing to surface waters.

5. SOFTWARE IMPLEMENTATION

5.1. Software Design

AquiferSim itself is designed as a stand-alone computational engine. This enables the engine to be controlled from a graphical user interfaces such as a GIS or by batch-processing interfaces such as those used in uncertainty analysis. AquiferSim was developed entirely in Microsoft Visual C# on the .NET 2.0 framework. This enables the engine to run on modern Windows PCs and on Linux and clustered environments utilising the MONO platform (Mono Project, 2007).

The cell data are stored in a two-dimensional array, with an object-oriented structure that allows for the numerous types of cells and their relationship to the mathematical solvers. These types allow for inactive cells within the grid as well as compute, boundary and river cells. Boundary cells can be either fixed, general head or no-flow in nature. This structure is used to

generate the computational grids that are required by the various solvers.

5.2. Engine Implementation

The computational engine comprises three main components: *AquiferSimData*, contains the data structure described in Section 5.1; *AquiferSimMaths* contains all the various mathematical solvers listed in Section 4.1; and *AquiferSimEngine* controls the loading of data, the execution of the solvers and the production of output. These components are built as a COM component that can be called directly from any external application e.g. a DOS based batch-processing application or an ArcGIS based user interface.

The various solvers are highly customised adaptations of existing numerical methods. They were developed to take advantage of the inbuilt mathematical functions and generic collection classes provided within the .NET 2.0 framework.

5.3. GIS Interface Implementation

AquiferSim requires considerable input data. For our pilot study area all of these data were stored in ArcGIS. All of the data were represented in ESRI GRID format files. Reading of these files required incorporation of the Geospatial Data Acquisition Library (Open Source Geospatial Foundation, 2007) into the application. The *AquiferSim* .NET GDAL wrapper was developed to use GDAL to import data into *AquiferSim* and to convert into the internal coordinate system used by the model. Our pilot implementation used ArcGIS for user interaction and data storage. However, this could have been another GIS system or one of the specific groundwater modelling and data visualisation packages that are available.

6. COMPUTATIONAL PERFORMANCE

The initial test problem for the pilot study region of Central Canterbury required ~230,000 computational cells for the 2D horizontal description, within the 1025 x 1025 solver grid. Solution of the piezometric surface and plotting of 70 groundwater flow paths takes about 5 s. Each vertical slice represents a flow path up to 50 km length (at 100 m resolution) and a specified aquifer thickness of 250 m (divided into 100 layers), resulting in up to 50,000 cells. Total solution time for streamfunction, nitrate concentration, and groundwater age is about 20 s on a modern standard office Windows PC. These processing times are for the *AquiferSim* engine, excluding GIS processing and data transfer.

7. IMPLEMENTATION ISSUES

AquiferSim provides a capacity for input data about land use, nitrate discharge, and aquifer properties that far exceeds existing knowledge for alluvial aquifers in New Zealand. The 2300 km² Central Canterbury region has been designated as the pilot study area. In this region, only three boreholes exist which have penetrated the estimated 200 – 500 m thickness of the aquifer. The pattern of hydraulic conductivity and porosity is highly heterogeneous and poorly quantified in the large alluvial fans that have evolved over several glacial periods.

Our approach is to provide *AquiferSim* as a fast model that can process input data in the context of scenarios or as output values from a full examination of predictive uncertainty. In order to obtain some measure of uncertainty in aquifer transmissivity and recharge patterns, Environment Canterbury (regional council) is constructing a MODFLOW groundwater flow model of the 7,800 km² Canterbury Plains at 1 km x 1 km mesh scale. This model has a large number of parameters to represent patterns of river recharge and aquifer transmissivity. This underdetermined model is calibrated by means of regularisation with the pilot-point method (Doherty, 2003) and use of PEST software (Watermark Numerical Computing, 2007).

The uncertainty of information about aquifer thickness, porosity, and vertical variation in hydraulic conductivity is still to be addressed. These properties have very significant influence on the spatial distribution of nitrate concentration in the aquifer.

The output data formats for *AquiferSim* will also be determined during the forthcoming implementation phase. The model architecture currently allows for interrogation of vertical slices across multiple pathlines to provide values for horizontal maps at selected depths or even to generate a database for 3D viewing. However, the decisions about what is required for regional council purposes will only emerge as staff become engaged with using the model.

8. DISCUSSION AND CONCLUSIONS

AquiferSim is a single-purpose, regional-scale model of nitrate transport in groundwater. In order to meet requirements for processing speed, minimal uncontrolled numerical dispersion, and 3D simulation, some compromises on process description have been necessary. Groundwater flow and transport are steady state, but predictions

of groundwater age enable some assessment of transport times for contamination effects at specific locations.

Realistic simulation of longitudinal and vertical transport dispersion is achieved by controlling computational mesh size. However, horizontal transverse dispersion is ignored in the current model. This could be considered to be a serious omission if there is strong contrast in nitrate discharge from adjacent land uses, but the associated contrast in the vertical direction is usually two orders of magnitude greater because discharge streamlines from the horizontal scale of land use are compressed into the aquifer thickness. Therefore, the AquiferSim model is not expected to be a good predictor of point source contamination effects at local scale, in comparison with existing groundwater transport models

The effect on predictions of process approximations within the AquiferSim model are dwarfed by the effects of uncertainties in the input data. These uncertainties in land use, recharge, and aquifer properties will be addressed within a formal statistical framework of model prediction uncertainty. The large numbers of model executions required for this approach was one of the strong drivers for a model with a forward run time that is very fast in comparison to the use of existing multi-purpose groundwater software.

Verification of model predictions is a difficult issue because AquiferSim is a steady-state model and the available nitrate data represent samples in space and time of dynamic groundwater transport in response to a poorly recorded history of land use and nitrate discharge. However, initial predictions from prototype model runs indicate spatial patterns of nitrate concentration with depth below groundwater table that are consistent with observations.

At the present stage of development, the computational performance of AquiferSim has reached expectations as a fast processor of large amounts of input data. The more immediate issue for the implementation phase is to manage the end-user requirements for model output to serve the planning and management of nitrate discharge in the region.

9. REFERENCES

Bidwell, V.J., L.R. Lilburne and J.M. Good (2005), Strategy for developing GIS-based tools for management of the effects on

groundwater of nitrate leaching from agricultural land use. In Zerger, A. and Argent, R.M. (eds) *MODSIM 2005 International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand, December 2005.* pp. 1354-1360. ISBN 0-9758400-2-9.

Doherty, J. (2003), Ground water calibration using pilot points and regularization. *Ground Water*, 41(2), 170-177.

Good, J. & J. Bright (2005), An object-oriented software framework for the farm-scale simulation of nitrate leaching from agricultural land uses - IRAP FarmSim. In Zerger, A. and Argent, R.M. (eds) *MODSIM 2005 International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand, December 2005,* pp. 662-668. ISBN: 0-9758400-2-9.

Goode, D.J. (1996), Direct simulation of groundwater age. *Water Resources Research*, 32(2), 289-296.

Kinzelbach, W., M. Marburger and W-H. Chiang (1992), Determination of groundwater catchment areas in two and three spatial dimensions, *Journal of Hydrology*, 134, 221-246.

Mono Project, (2007), Main Page – Mono, http://www.mono-project.com/Main_Page Last accessed July 26 2007.

Moore, C. and J. Doherty (2005), Role of the calibration process in reducing model predictive error. *Water resources Research*, 41, W05020, doi:10.1029/2004WR003501.

Open Source Geospatial Foundation, (2007), GDAL – Geospatial Data Acquisition Library, <http://www.gdal.org/> Last Accessed July 26, 2007.

Press, W.H., S.A. Teukolsky, W.T. Vetterling and B.P. Flannery (2002), Numerical Recipes in C++: the art of scientific computing (2nd ed.), Cambridge, 1032p, UK.

Watermark Numerical Computing (2007), PEST <http://www.sspa.com/pest/> Last Accessed July 26, 2007.