

## **Calibration of the Oro Moraine multi-aquifer system: role of geology and objective function**

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**Abstract** Calibration results obtained using different objective functions and geology-based zonation alternatives are compared as part of developing a numerical model of the Oro Moraine multi-aquifer system. The numerical model combines a simplified unsaturated zone representation with a high conductivity layer atop the domain to accommodate the complex recharge mechanism characterizing heterogeneous aquifers. The calibration objective functions specify the least squares fit of the model to point head values as well as baseflow and runoff measurements. Streamflow data are found to be very important for constraining model-predicted fluxes; a calibration based on static water level data alone completely misrepresents observed streamflows. A model zonation based on constraints from the geological history of the study area results in a good overall fit to the calibration data.

### **INTRODUCTION**

A numerical model of the Oro Moraine multi-aquifer system in central Ontario (Fig. 1) was developed by Beckers (1998), making use of the methodology described in Martin & Frind (1998) for the earlier Waterloo Moraine study. An important objective of the Oro Moraine study is to determine the potential impact of urbanization on groundwater fluxes to the ecologically significant Minesing Swamp. The correct simulation of the water mass balance for this system is therefore of particular concern.

This paper describes the inverse method used in calibrating the Oro Moraine model and illustrates the important role of geological information and stream gauge measurements in the model calibration. The calibration of this complex three-dimensional (3-D) model is a challenge because of data limitations. The quality of the geological logs which are used in generating the hydraulic conductivity distribution, is at best moderate, and water level data used in the calibration are sparse and noisy.

### **METHODOLOGY AND BACKGROUND INFORMATION**

The adopted inverse method, implemented in the three-dimensional WATFLOW finite element code (Molson *et al.*, 1995), uses a minimization algorithm as described in Neuman (1980). The inverse problem is solved using a Fletcher-Reeves conjugate gradient algorithm combined with a Gauss-Newton iterative search to determine the step size in log conductivity. The adjoint method is used as an efficient means to

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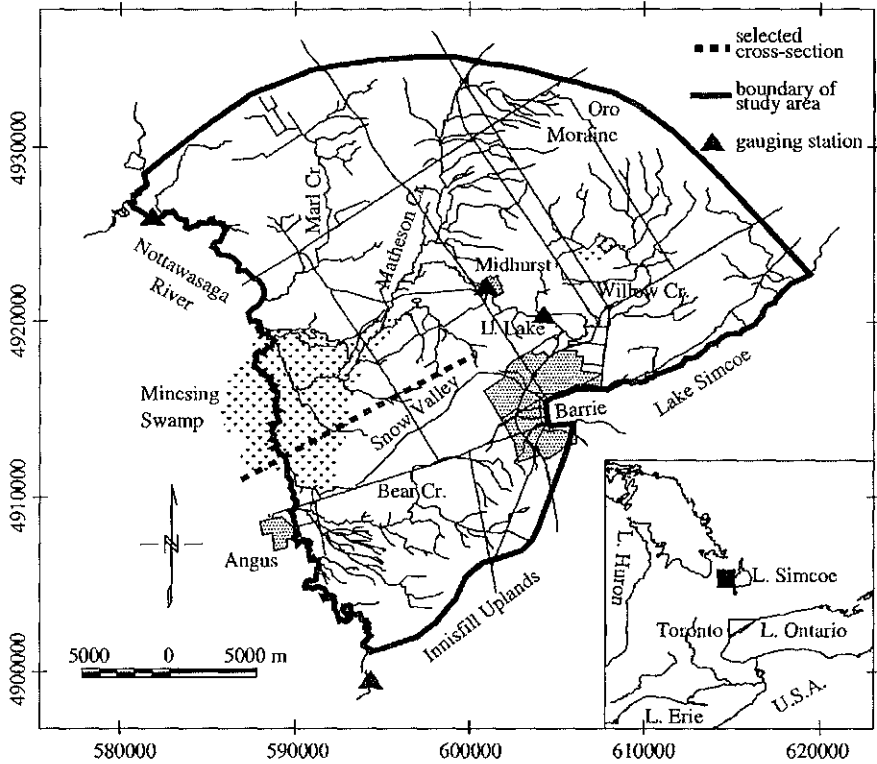


Fig. 1 Map of the study area. The black square in the insert indicates the location of this area in central Ontario.

calculate sensitivity coefficients of the calibration measure(s) with respect to log conductivity. A widely used performance measure is the weighted least squares residual  $J_h$  between model predicted ( $h$ ) and observed ( $h^*$ ) point hydraulic heads:

$$J_h = \sum_i c_i [h_i - h_i^*]^2 \quad (1)$$

In equation (1) the  $c_i$  represent the calibration weights. These weights are calculated from the measurement error in the head data, which is estimated to be 5 m, mainly as a result of the poorly constrained borehole elevations. A total of  $N = 392$  water level measurements are used in the model calibration.

The WATFLOW code was enhanced for the Waterloo Moraine study to include a simplified unsaturated zone representation suitable for regional-scale modelling (Beckers & Frind, 2000a). This pseudo-unsaturated model was coupled to a high conductivity recharge spreading layer (RSL) atop the domain to accommodate the complex recharge mechanism characterizing heterogeneous aquifer systems. The RSL laterally transfers water that cannot infiltrate over low conductivity units, either to more pervious regions where it can infiltrate more easily, or to surface water bodies. An important advantage of this model formulation is that runoff does not need to be *a priori* accounted for in determining groundwater infiltration. Instead, specified fluxes at the land surface are entirely determined by measured values of precipitation and

evapotranspiration while groundwater infiltration, which depends strongly on near-surface soil properties, is an integral part of the flow solution. Runoff and baseflow contributions to long-term streamflow generation are calculated and can be compared to data from gauging stations during model calibration. Water courses are entered in the numerical model as Dirichlet boundaries. Fluxes to these boundaries are calculated from the partitioned matrix equations in the standard fashion. An objective function ( $J_f$ ) is specified that minimizes the difference between the observed ( $F^*$ ) and model-predicted fluxes:

$$J_f = \sum_{s=1}^{NS} c(s) \left[ \sum_{i=1}^{NB} \sum_{j=1}^{NC(i)} A_{i,j} h_j - F^*(s) \right]^2 \quad (2)$$

where the first sum is over the  $NS$  stream segments for which stream gauge measurements are available, the second sum is over the  $NB$  mesh nodes that are used to represent a particular stream segment in the numerical model,  $NC$  is the number of nodes connected to a certain Dirichlet node  $i$ , and  $A$  is the coefficient matrix with the conductance terms. The model-predicted fluxes are split into contributions from the domain and RSL for comparison with measured baseflow and runoff quantities (Beckers, 1998). The calibration weights are based on the error in the streamflow data. This error is estimated to be 20% of the measured values. The four gauging stations that are located in the study area (Fig. 1) were used to determine the streamflow accumulation along the corresponding stream segments (Beckers & Frind, 2000b).

A penalty criterion minimizing the difference between the prior (non-calibrated) and posterior (calibrated) log conductivities is often used to stabilise the solution of the inverse problem, and improve its plausibility (e.g. Neuman, 1980). However, when the prior conductivity field is derived from indirect information, such a criterion does not necessarily make sense and it has not yet been included in the present calibration algorithm.

The complex hydrogeology of the Oro Moraine multi-aquifer system and the development of a conceptual hydrostratigraphic model of the study area are detailed in Beckers & Frind (2000b). The geometry of the aquifers and confining units was defined through a cross-sectional interpretation of borehole geological logs (Fig. 2). Hydraulic conductivity is spatially distributed within the individual hydrostratigraphic units, making use of kriging. The model parameterization therefore combines a zonation with a geostatistical approach (see for example Figs 12–14 in Martin & Frind, 1998).

The calibration algorithm was designed to handle a zonation and/or geostatistical parameterization: average conductivities within user-specified hydrogeological units (e.g. individual aquifers and aquitards) can be optimized in an entirely zonation-based approach. Log conductivities are thus updated uniformly within a zone. Pilot points (e.g. de Marsily, 1984) can be used as an alternative means to achieve local conductivity updates within individual hydrostratigraphic units. The pilot-point method will be detailed in a forthcoming paper that illustrates the impact of various conductivity parameterization options for the Waterloo Moraine model (Martin & Frind, 1998) on calibration results and on inferred capture zones for the Waterloo Region's municipal wells. For the Oro Moraine investigation, a zonation-based approach has been chosen because the differences in the geological history of the uplands (Oro

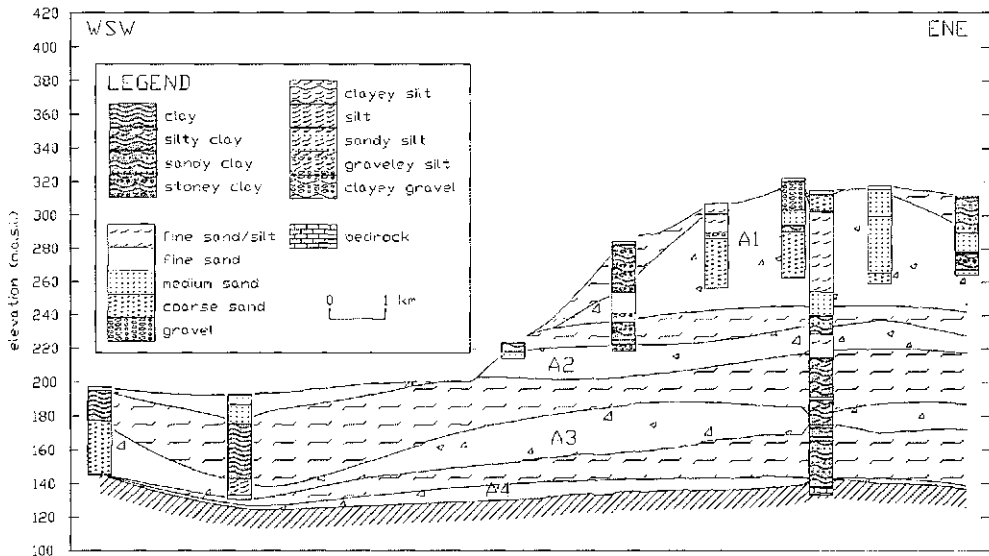


Fig. 2 Selected cross-section. Refer to Fig. 1 for location.

Moraine, Innisfill Uplands and Snow Valley, Fig. 1) and lowlands (Minesing Swamp and stream valleys) provide a good basis for defining distinct hydrogeological units. In this approach, the lithologic descriptions are used to define areas of high and low conductivity within each zone through kriging, while the average conductivity of these zones is optimized to account for any bias introduced as a result of using indirect information to constrain this conductivity distribution.

## RESULTS

Based on the hydrostratigraphic interpretation, several zonation alternatives were considered in the model calibration. Beckers (1998) found that best results are obtained when the lowermost two aquifers (A3 and A4 in Fig. 2) are grouped into a single zone separated by discontinuous pockets of aquitard 4 (the resulting unit is known as the Alliston aquifer complex), and when the uppermost aquifer (A1) is separated into three zones comprising the distinct Oro Moraine, Ski Valley and Innisfill Uplands (Fig. 1). Table 1 compares calibration results for this zonation and different objective functions. This comparison is based on the value of the performance measures (equations (1) and (2)) and on the difference between the initial ( $Y^*$ ) and final calibrated ( $Y$ ) log conductivities as expressed by:

$$J_Y = 1/NZ \sum_{i=1}^{NZ} [Y_i - Y_i^*]^2 \quad (3)$$

where  $NZ$  is the number of hydrostratigraphic units (zones) in the multi-aquifer system.

The two different calibration objectives (O1–O2) lead to relatively small variations in the match to the point water levels but result in order-of-magnitude changes in  $J_f$ .

**Table 1** Initial and calibrated log conductivity values ( $m\ s^{-1}$ ) for two performance measures (O1–O2) together with corresponding values for  $J_Y$ ,  $J_h$ , and  $J_f$ .

	Initial	$J_h$ (O1)	$J_h + J_f$ (O2)
Aquitard 1	-7.50	-5.49	-4.68
Oro Moraine	-4.15	-3.96	-3.90
Ski Valley	-4.12	-5.09	-5.05
Innisfill Uplands	-3.96	-5.40	-5.11
Aquitard 2	-7.89	-7.22	-7.62
Aquifer 2	-4.34	-5.18	-4.68
Aquitard 3	-8.17	-5.14	-5.24
Alliston	-5.88	-6.37	-6.64
$J_Y$		2.21	2.42
$J_h$	$0.47 \times 10^6$	$0.18 \times 10^4$	$0.25 \times 10^4$
$J_f$	$0.67 \times 10^4$	$0.22 \times 10^3$	$0.47 \times 10^1$

When only point water level measurements are considered (O1), the discharge data are poorly simulated ( $J_f = 0.22 \times 10^3$ ). This suggests that groundwater flow patterns are poorly predicted by the calibrated model. Although this seems an obvious limitation of using static water level data alone, the use of flow measurements in groundwater model calibration has not been investigated thoroughly, and the full importance of using flow measurements in addition to hydraulic heads is rarely recognized (e.g. Hill *et al.*, 1998). The streamflow data are simulated much better when these measurements are included in the model calibration (O2,  $J_f = 0.47 \times 10^1$ ). However, the data from the four gauging stations put limited constraints on the system water mass balance. Although the observed streamflow accumulation for the Nottawasaga River provides information on the overall water mass balance, fluxes to individual tributary streams that contribute to this accumulation remain largely unknown. Additional gauging stations located in these tributary creeks are therefore crucial for further constraining the water mass balance of the Oro Moraine system.

The results shown in Table 1 are under-calibrated with respect to the water levels, whereas for performance measure O2 the few streamflow measurements are already well matched. Large conductivity perturbations ( $J_Y = 2.42$ ) are required to achieve this result. To improve the calibration, several zonation alternatives were considered based on the different geological history of the uplands and valley areas. The final calibration, detailed in Beckers & Frind (2000b), is based on a total of 32 zones for the subsurface and eight zones for the RSL. This RSL zonation was used previously for a surface hydrological model of the Nottawasaga River basin (NVCA, 1988). The preferred zonation results in an improved match of the model to both water level data ( $J_h = 0.14 \times 10^4$ ) and streamflow measurements ( $J_f = 0.26 \times 10^1$ ), while average modifications to the prior log conductivity field are considerably reduced ( $J_Y = 1.29$ ) compared to the earlier scenarios (Table 1), increasing the plausibility of the solution.

For the preferred zonation, observed baseflow and runoff quantities are well matched within the 20% measurement error (Table 2). The model fit to the water level measurements for each aquifer is detailed in Table 3 in terms of the standard deviation  $\sigma$ , the average error or bias,  $\text{avg}(\epsilon)$ , and the average absolute value of error  $\text{avg}|\epsilon|$ , where  $\epsilon = h - h^*$ . Although the overall trend in the water level measurements is well matched (evident from the small bias), considerable residual scatter does remain. Some of this scatter can be explained by uncertainty in the elevation of the measurement points

**Table 2** Assessment of streamflow calibration.

Stream segment	Baseflow ( $\text{m}^3 \text{s}^{-1}$ ):		Runoff ( $\text{m}^3 \text{s}^{-1}$ ):	
	Observed	Simulated	Observed	Simulated
Nottawasaga River	1.89	1.68 (-11%)	4.61	5.51 (+20%)
Willow Creek (Little-Lake-Midhurst)	0.08	0.07 (-13%)	0.81	0.86 (+6%)
Willow Creek headwaters	0.03	0.03 (+0%)	0.26	0.22 (-15%)

**Table 3** Assessment of water level calibration.

Aquifer	$\sigma$ (m)	avg( $\epsilon$ ) (m)	avg  $\epsilon$   (m)	$N$
A1	9.7	-4.0	7.5	76
A2	7.9	-1.2	6.5	154
A3	8.8	1.3	6.9	134
A4	15.0	-3.3	10.0	28
Total	9.2	-1.0	7.1	392

(borehole elevations and observed head values). Uncertainty in the water level elevations was taken to be 5 m, the contour interval of the topographic maps used to estimate the borehole elevations. In some instances actual errors may be considerably larger. This source of error can only be eliminated by accurately surveying all borehole elevations using an efficient technique such as GPS.

## CONCLUSIONS

The incorporation of automated calibration in the existing methodology for modelling glacial aquifers has been a major advance in better simulating these systems. Automated calibration enables the user to objectively compare alternative modelling scenarios for complex systems, as illustrated by the above examples. The Oro Moraine model was calibrated to point water level measurements and streamflow data from four gauging stations. The streamflow measurements were found to be very important for constraining model-predicted fluxes, as a calibration based on static water level data alone misrepresents observed baseflow and runoff quantities. A zonation of the model based on constraints from the geological history of the study area was found to be an effective means of refining the model calibration. The final calibrated model approximates the available water level, baseflow, and runoff data with reasonable accuracy.

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