Validation of simulated flow direction and hydraulic gradients with hydraulic head observations using open source GIS

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Calibrated Steady-State Groundwater Flow Model

Validation

Horizontal flow directions and hydraulic gradients

Vertical hydraulic gradient

Variability of flow direction and hydraulic gradient in time

Discussion

Conclusions and recommendations
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It is recommended to check hydraulic gradients and flow directions predicted by a groundwater flow model that is calibrated solely with hydraulic head observations. It has been demonstrated in literature that substantial errors can be made when the model is not calibrated on these state variables.

Calibrated Steady-State Groundwater Flow Model | Validation

- Horizontal flow directions and hydraulic gradients
- Vertical hydraulic gradient
- Variability of flow direction and hydraulic gradient in time

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Therefore, we performed a validation of a groundwater flow model, representing part of the Neogene aquifer (60 km²) in Belgium. This model was developed and calibrated solely on groundwater head measurements in the framework of the environmental impact assessment of the near surface repository for low- and intermediate-level short-lived waste in Belgium.

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Horizontal flow directions, horizontal and vertical gradients for the entire area of the groundwater model were estimated from measurements at shallow monitoring wells within the groundwater flow model domain, and compared to the flow directions and gradients predicted by the model.

Calibrated Steady-State Groundwater Flow Model → Validation

Horizontal flow directions and hydraulic gradients → Vertical hydraulic gradient

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Besides model validation on average hydraulic heads, the variability of flow direction and hydraulic gradients in time was checked, by using the actually measured monthly time series, to verify the applicability of the steady-state modelling approach.
Horizontal flow directions and hydraulic gradients were estimated from measurements at shallow monitoring wells within the groundwater flow model domain, and compared to the flow directions and vertical gradients predicted by the model.

Calibrated Steady-State Groundwater Flow Model

Updated groundwater flow model following intensive site characterization campaign (Gedeon et al., 2011)
Calibrated on groundwater head measurements

Calibrated Steady-State Groundwater Flow Model

Measured versus simulated groundwater levels in the groundwater flow model. Dashed lines represent ± 0.5 m from the full zero residual line. The error bars are calculated as the measurement ± σ (Gedeon et al., 2011)

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- For a groundwater flow model that is calibrated with hydraulic head observations, it is recommended to check gradients and flow directions, as the model is not calibrated on these state variables (e.g. Ruskauff & Rumbaugh 1996).

- Horizontal flow directions and gradients for the entire groundwater flow model area were estimated at shallow monitoring wells used for calibration of the groundwater flow model and compared to the flow directions and gradients calculated from the simulated equivalents (model predictions). A few additional wells within the groundwater flow model area were used as well (Rogiers et al. 2014b).
Validation of simulated flow direction

- For obtaining horizontal flow directions and gradients, **triangulation** of groundwater levels was done for combinations of three neighbouring hydraulic head observations/model predictions in the same hydrogeological layer.

- Comparison of the flow directions and flow gradients obtained from measurements and simulations gives an indication on the **model performance**.

- The calculations were done for the **three sandy hydrogeological units** used in the model: Mol Upper, Mol Lower and Diest Sands.
Validation of simulated flow direction and hydraulic gradients with hydraulic head observations using open source GIS.

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Horizontal flow directions, horizontal and vertical gradients for the entire area of the groundwater flow model were estimated from measurements at shallow monitoring wells within the groundwater flow model domain, and compared to the flow directions and vertical gradients predicted by the model.

Triangulation was done using SAGA GIS (http://www.saga-gis.org):
- System for Automated Geoscientific Analyses
- Modular architecture
- Graphical user interface
- Comprehensive set of free modules
  - Importing and exporting several data formats
  - Data manipulation and analysis of vector and raster data
  - (Geo)statistical analysis

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Updated groundwater flow model following intensive site characterization campaign (Gedeon et al., 2012)

Triangulation procedure in SAGA GIS

1. Load **shape file** with **data points** (observed/simulated heads)
2. **Convert** point shape file to **TIN** (module TIN – Tools: Shapes to TIN)
3. Calculate **gradients** from observed and simulated heads based on the values of each triangle’s points (module TIN Tools: Gradient)
   - Output: azimuth + decline
4. Create **centroids** for each triangle (module Shapes – Polygons: Polygon Centroids)
5. **Add coordinates** to each polygon centroids (module Shapes – Points: Add coordinates to points)
6. **Export** gradient file (SHP format)
- Visualization of results was done using QGIS (http://www.qgis.org)

- User friendly and open source GIS

- Tool for making, editing, visualizing, analyzing and publishing geo-spatial information

- Operates under Windows, Mac, Linux, BSD and Android

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Visualization of gradient (azimuth + decline) in QGIS

1. **Import** gradient file
2. Open **Layer Properties** – Advanced
3. Fill in appropriate variables for **rotation field** (azimuth) and field for **size scaling** (decline or transformed values for decline; in our case we used a sqrt transformation to have a gradual slope change)
Results: flow directions and horizontal gradients

Overview of calculated flow directions and horizontal gradients from measured and simulated average groundwater heads for the Mol Lower stratigraphical layer in the groundwater flow model.
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Results: flow directions and horizontal gradients

Updated groundwater flow model following intensive site characterization campaign (Gedeon et al., 2012)

Detailed flow directions and horizontal gradients from measured and simulated heads close to the future waste disposal site.
Results: flow directions and horizontal gradients

- In general, over the whole model domain, deviations between flow directions derived from measured heads and flow directions derived from calculated heads are small. In most cases, they are less than 10 degrees.

Detailed flow directions and horizontal gradients from measured and simulated heads close to the future waste disposal site.
Results: flow directions and horizontal gradients

- Although **large deviations** are present, they are mostly related to a **small triangle size**, and not so much to the gradient size.

![Mean gradient versus absolute difference in flow direction angle for Mol Upper, Mol Lower and Diest hydrogeological layer.](image1)

![Area of triangle versus absolute difference in flow direction angle for Mol Upper, Mol Lower and Diest hydrogeological layer. The triangle size is inversely related to the difference in flow direction angle.](image2)

**Discussion**  **Conclusions and recommendations**
Results: flow directions and horizontal gradients

- From the plot of the cumulative distribution of absolute difference in flow direction angle, it is shown that for most analyzed flow directions (about 88 percent), the absolute difference in flow direction angle for measured and simulated heads stays below 45 degrees. For about 80% of the analyzed flow directions, the difference stays below 20 degrees.

Cumulative distribution of absolute difference in flow direction angle. For Mol Upper and Mol Lower, in about 87% of the cases, and for Diest in about 62% of the cases, the absolute difference between measured and computed angle is less than 45 degrees.
Validation of simulated flow direction and hydraulic gradients with hydraulic head observations using open source GIS

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- The vertical gradient over a hydrogeological layer is defined as $\frac{\Delta H}{\Delta x}$, where $\Delta x$ is the thickness of the hydrogeological layer and $\Delta H$ is the head difference.

- The vertical gradients are calculated from observed and simulated groundwater heads in the different aquifers. Vertical gradients are calculated for the upper aquifer (aquifer above the Kasterlee Clay), across the Kasterlee Clay and for the lower aquifer (aquifer below the Kasterlee Clay).

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Results: vertical gradient across Kasterlee Clay from simulated and average observed groundwater heads.
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Results: vertical gradient across Kasterlee Clay

Vertical gradient across the Kasterlee Clay from simulated and average observed groundwater heads near the waste disposal site.
Results: vertical gradient across Kasterlee Clay

- In most cases, the directions from simulated and observed gradients coincide over the whole model domain. This is especially the case near the waste disposal site, where vertical gradients from simulated and observed values coincide well.

- Only at site R24a-R24b, the directions from simulated and observed gradients are opposing. This site is situated between the Kleine Nete River (area of upward flow) and the infiltration area (downward flow), and is mostly dominated by horizontal flow. Consequently, the heads above and below the Kasterlee Clay are similar here, which is reflected in the relatively small gradients (0.01 and -0.01 for the gradients calculated from observed and simulated heads respectively).
- As the steady-state groundwater model was calibrated on temporal-averaged hydraulic heads, the primary analysis concerned the average hydraulic heads.

- Besides model validation on average hydraulic heads, the variability of flow direction and hydraulic gradients in time were checked, by using the actually measured monthly time series, to verify the applicability of the steady-state modelling approach.

- The variability was checked by calculating the flow direction, the horizontal and vertical gradients for the months January, April, July and October for the years 2007 and 2009, representing respectively a recent wet and a recent dry year, as can be seen from the piezometric measurements (Labat, 2011).
Results: variability in flow direction

Flow directions (angle in degrees) calculated from observed heads for 4 different months for the year 2007 and 2009. The flow directions derived from averaged observations is also given.

- The variability in the flow direction for the different TIN ID's for 4 time periods for the years 2007 and 2009 is shown. For most TIN ID's, the variability in the flow direction over the different time periods is small to moderate: for about 70% of the locations for the years 2007 and 2009, the range in flow direction is less than 45 degrees.

- However, for the year 2007, the variability in flow direction for TIN ID's 1, 3, 10 and 14, and for the year 2009, for TIN ID's 22, 24, 27, 31, 33, 34, 38, 40 and 42 is rather large (> 45 degrees). The main reason for the large deviations is a small triangle size in combination with a small horizontal gradient size.
Validation of simulated flow direction and hydraulic head

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- Updated groundwater flow model following intensive site characterization campaign (Gedeon et al., 2012)

- The variability in time of the gradient across the Kasterlee Clay is limited.

Results: variability in vertical gradient

Time dependent gradient across the Kasterlee Clay (2009).

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Discussion

- The basic assessment of flow directions and hydraulic gradients using hydraulic head observations has shown that in general the errors with respect to gradient and direction in the model are reasonable. Large errors do occur however. Mostly these large errors are attributed to TIN elements with a very small area which make gradients and directions sensitive to small measurement errors. In some other cases, errors are linked to the presence of very small horizontal gradients which also involves large uncertainties on directions. The latter is often due to the existence of a large vertical flow component, compared to the horizontal flow, and therefore larger errors are found for instance at the interfluvium for the Mol Lower hydrogeological layer.

- The relative importance of different TIN triangles was not accounted for. Triangles with a small area, or elongated triangles might be considered less important, or could even be removed from the TIN. Moreover, triangles intersecting important surface water features might not provide an estimate of the true flow direction and/or hydraulic gradient, but only give an indication on the relative differences between the three hydraulic head observations/predictions.

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- When groundwater flow direction varies in time, it promotes the dispersion of solutes (Goode and Konikow, 1990). Hence, **when variations in time are considerable, transient modelling should be performed for making accurate estimates on solute behaviour.** In terms of **maximum expected concentrations** however, **neglecting variations in time is likely to give conservative results** (Gedeon and Mallants, 2009). The results from this work show that most of the temporal flow direction variations are restricted to less than 45 degrees.
Conclusions and recommendations

- The flow directions and vertical gradients calculated from observations were compared to the same variables calculated from the groundwater model results.

- For the flow directions, we can conclude that, generally speaking, the model flow directions coincide well with the flow directions calculated from observations. Large deviations are however present at a few locations. These locations always show very low horizontal gradients (which systematically occur at the interfluves), large fluctuations at piezometer locations due to groundwater extraction, or they result from a less representative TIN triangle (small area, intersection of surface water bodies, …).

- In areas where these high uncertainties on horizontal flow directions exist, and if horizontal flow is not negligible compared to vertical flow, it is recommended to check the direction with other methods as well (e.g. radioactive tracer tests (Drost et al., 1986); within-well tracer tests (Guthrie, 1986); direction-sensitive flow meters (Masciopinto and Palmiotta, 2014; Guaraglia et al., 2009); geophysical techniques (White, 1994)).
Conclusions and recommendations

- The calculated vertical gradients from simulations are generally in good agreement with the vertical gradients from observations. Near the waste disposal site, only one site has (small) opposing gradients from observed and simulated groundwater heads. For the gradients across the upper aquifer and across the Kasterlee Clay, average and maximum absolute gradient differences are rather small, in the order of 0.02.

- This was a basic assessment of flow directions and gradients, and hence it can be used to identify potential areas of interest, were more detailed investigations with more direct estimates or measurements of mainly flow directions would be recommended (see e.g., Rogiers et al, 2014a).

- Checking flow directions and gradients for different months in a wet (2007) and dry (2009) year, showed that variability exists in time. Especially for the flow direction, we recommend checking the influence of transient groundwater flow simulation on solute transport. Neglecting the transient behaviour, as has been done by Gedeon et al. (2011) would most likely lead to conservative estimates in terms of solute concentrations, not in terms of solute spreading.
References
