Transient 3D groundwater and temperature model of the North German Basin below the State of Brandenburg (1953-2014)

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1. Licence

2. Citation

When using the data please cite:

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Table of contents

3. Abstract

The dataset is the basis for describing a 6-decade-long evolution of groundwater dynamics and thermal field in the North German Basin beneath the Federal State of Brandenburg (NE Germany), covering the period between 1953 and 2014 with monthly increments. It was produced by one-way coupling of a near-surface distributed hydrologic model to a 3D basin-scale thermohydraulic groundwater model with the goal of investigating feedbacks between climate-driven forcing (in terms of time- and space-varying recharge and temperature), basin-scale geology, and topographic gradients. Modeled pressure and temperature distributions are validated against published groundwater level and temperature time series from observation wells. The novelty of our approach stems from the integration of basin-scale flow modeling principles (thermo-hydraulic coupling, capturing heterogeneity of an entire sedimentary fill) with modeling tools typically applied in catchment hydrology (transient hydrometeorological forcing, utilizing the true depth of the water table as the boundary condition, rather than assuming the water table is a subdued replica of topography). To our knowledge, this is the first model of this kind, at least in the selected geographic area. Our results indicate the depth extent of the groundwater system subjected to nonlinear interactions between local geological variability and climate conditions.

4. Data Description

4.1. Project coordinate system

PROJCS["DHDN_3_Degree_Gauss_Zone_4",

GEOGCS["GCS_Deutsches_Hauptdreiecksnetz",

DATUM["D_Deutsches_Hauptdreiecksnetz",

SPHEROID["Bessel_1841",6377397.155,299.1528128]],

PRIMEM["Greenwich",0.0],

UNIT["Degree",0.0174532925199433]],

PROJECTION["Gauss_Kruger"],

PARAMETER["False_Easting",4500000.0],

PARAMETER["False_Northing",0.0],

PARAMETER["Central_Meridian",12.0],PARAMETER["Scale_Factor",1.0],

PARAMETER["Latitude_Of_Origin",0.0],

UNIT["Meter",1.0],

AUTHORITY["EPSG",31468]]

Model extent in project coordinates (meters):

	5930000	
4450000		4700000
	5720000	

Model Extent in Lat/Lon (EPSG:4326 WGS 84):

	53.4636308°	
11.2766714°		15.010188°
	51.6121916°	

4.2. Data sources

The table below lists data sources used for the model building and the analysis.

Input data for the hydrological model mHM mostly comes from DeutcherWetterdienst Climate Data Center. Full inputs and outputs for the German-wide hydrological model mHM is available upon request. This data publication contains the subset of the output required to run the coupled surface water – groundwater model for Brandenburg.

Data content	Author	Usage rights	Reference	Data Description	Data link
Structural model	Noack, V., et al. (2013)	Published data	Noack V, Scheck-Wenderoth M, Cacace M, Schneider M. Influence of fluid flow on the regional thermal field: results from 3D numerical modelling for the area of Brandenburg (North German Basin). Environmental earth sciences. 2013;70(8):3523-44.		https://doi.org/10.1007/s12665-013-2438-4
Digital elevation model (DEM)	The Federal Agency for Cartography and Geodesy (BKG) and GeoBasis-DE	Data Licence Germany – Attribution – Version 2.0	GeoBasis-DE / BKG (2023): Digitales Geländemodell Gitterweite 200 m (DGM200)	https://sg.geodatenzentrum.de/web_public/gdz/dokumentation/deu/dgm200.pdf	https://gdz.bkg.bund.de/index.php/default/digitales-gelandemodell-gitterweite-200-m-dgm200.html
River network	Landesamt für Umwelt Brandenburg	Data Licence Germany – Attribution – Version 2.0	LfU Brandenburg (2023): Gewässernetz des Landes Brandenburg	https://lbv.brandenburg.de/download/Schifffahrt/binnenschifffahrt_erlass_erhaltung_und_n.pdf	https://geoportal.brandenburg.de/detailansichtdienst/render?url=https://geoportal.brandenburg.de/gs-json/xml?fileid=B9D461F1-99A1-4C10-97B4-9C36C0BD40B9
Groundwater level monitoring data (Brandenburg)	Landesamt für Umwelt Brandenburg	Data Licence Germany – Attribution – Version 2.0	LfU Brandenburg (2023): Auskunftsplattform Wasser (APW)	https://geoportal.brandenburg.de/detailansichtdienst/render?view=gdibb&url=https%3A%2F%2Fgeoportal.brandenburg.de%2Fgs-json%2Fxml%3Ffileid%3DE09AE237-7061-4AD3-AE5A-9D010CF2D231	https://apw.brandenburg.de/
Groundwater table maps (Brandenburg)	Landesamt für Umwelt Brandenburg	Data Licence Germany – Attribution – Version 2.0	LfU Brandenburg (2023): Hydroisohypsen und Messwerte des oberen genutzten Grundwasserleiters im Land Brandenburg - Datenserie	https://geoportal.brandenburg.de/detailansichtdienst/render?url=https%3A%2F%2Fgeoportal.brandenburg.de%2Fgs-json%2Fxml%3Ffileid%3D2435B954-BA43-4598-B6E1-06AA36F2BAB7	https://apw.brandenburg.de/
Groundwater level data (Berlin)	Senatsverwaltung für Mobilität, Verkehr, Klimaschutz und Umwelt	Data Licence Germany – Attribution – Version 2.0	Das Wasserportal Berlin: Gewässerkundliche Messdaten	https://wasserportal.berlin.de/download/wasserportal_berlin_getting_data.pdf	https://wasserportal.berlin.de/
Shallow groundwater temperature monitoring data (Berlin)	Senatsverwaltung für Mobilität, Verkehr, Klimaschutz und Umwelt	Data Licence Germany – Attribution – Version 2.0	Das Wasserportal Berlin: Gewässerkundliche Messdaten	https://wasserportal.berlin.de/download/wasserportal_berlin_getting_data.pdf	https://wasserportal.berlin.de/

Shallow groundwater temperature maps (Berlin)	Senatsverwaltung für Stadtentwicklung, Bauen und Wohnen Berlin	Published data	SenSBW (Berlin Senate Department for Urban Development, Building and Housing) (ed.) Year: 2020 Berlin Environmental Atlas, Berlin.		https://www.berlin.de/umweltatlas/en/water/groundwater-temperature/
Shallow groundwater temperature monitoring data (Brandenburg)	Landesamt für Umwelt Brandenburg	Data Licence Germany – Attribution – Version 2.0	unpublished data		personal communication (Abt.W 1, Referat W15 – Altlasten, Bodenschutz, Grundwassergüte)
Surface temperature grids	Deutscher Wetterdienst	https://opendata.dwd.de/climate_environment/CDC/Terms_of_use.pdf	DWD Climate Data Center (CDC): Grids of monthly averaged daily air temperature (2m) over Germany, version v1.0.	DESCRIPTION_gridsgermany_monthly_air_temperature_mean_en.pdf (dwd.de)	https://opendata.dwd.de/climate_environment/CDC/grids_germany/monthly/air_temperature_mean/
Thermal model	Noack, V., et al. (2013)	Published data	Noack V, Scheck-Wenderoth M, Cacace M, Schneider M. Influence of fluid flow on the regional thermal field: results from 3D numerical modelling for the area of Brandenburg (North German Basin). Environmental earth sciences. 2013;70(8):3523-44.		https://doi.org/10.1007/s12665-013-2438-4
Deep temperature calibration data	Förster, A. (2001)	Published data	Förster A. Analysis of borehole temperature data in the Northeast German Basin: continuous logs versus bottom-hole temperatures. Petroleum Geoscience. 2001;7(3):241-54.		https://doi.org/10.1144/petgeo.7.3.241

5. Workflow

5.1. Hydrological modeling

Hydrological fluxes are simulated via the mesoscale Hydrological Model (mHM) (Samaniego et al., 2010), a spatially distributed hydrologic modeling tool that is available for download at https://git.ufz.de/mhm/mhm and https://doi.org/10.5281/zenodo.1069202 (Sanmaniego et al., 2023).

We make use of the results from a Germany-wide realization of mHM to derive time- and space-varying water fluxes (groundwater recharge (or percolation) and baseflow (or Qb), which we translate into boundary conditions at the top of our groundwater model.

The output of the mHM model is a NETCDF file consisting of monthly 5 km x 5 km grids as used in Rakovec et al. (2016) and Samaniego et al. (2019), covering the period 1953–2014.

5.2. Structural modeling: building a 3D-dimensional mesh.

1. Structural grids for mesh generation are taken from an earlier 3D structural model of the subsurface beneath Brandenburg (Noack et al., 2013). The model was built by integrating a set of depth structure maps and exploration wells and was further constrained against potential field data (Scheck and Bayer, 1999, Maystrenko, 2010, Stackebrandt, 2010).

2. A conversion of ASCII grid surfaces to a 3D Exodus mesh is conducted using ASCII2EXODUS tool available at https://git.gfz-potsdam.de/moose/ascii2exodus

    GEOMETRY: The lateral resolution of the FEM mesh has been kept the same as the original grid data (1 km x 1 km). The lowermost stratigraphic boundary is Sedimentary Rotliegend (Base Zechstein). Top of the mesh is a DEM surface. The base of the mesh is a constant level: -6000m a.s.l. plane.

    REFINEMENT: each modeled stratigraphic unit has been vertically subdivided into four computational layers, while a higher resolution has been applied to the Quaternary unit, which was refined by a factor of 10.

    BOUNDARY: we limited the spatial extent of the original model within the administrative boundaries of the state of Brandenburg in order to ensure the consistency of groundwater monitoring data, being collected and stewarded by the countries' administrative bodies independently. Note that the southern limit of the original 3D model does not cover the southernmost part of Brandenburg.

    GRID DIMENSION 250x210

    CHECK_MESH: YES (0.1 m)

3. The resulting 3D Exodus mesh covers an area of 28800 km^2, extends down to 6000 m below sea level, consists of 1.59 million nodes, and contains 12 stratigraphic units from pre-Permian to Quaternary:

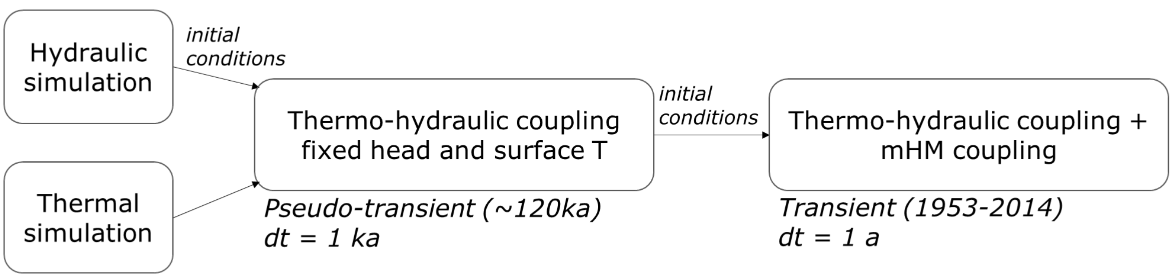
Block ID	Unit
0	Quaternary
1	Tertiary, post-Rupelian
2	Rupelian
3	Tertiary, pre-Rupelian
4	Upper Cretaceous
5	Lower Cretaceous
6	Jurassic
7	Keuper
8	Muschelkalk
9	Buntsandstein
10	Zechstein
11	Pre-Salt

5.3. Groundwater modeling: prepare boundary conditions files.

We prepared several Python Jupiter notebooks to export data from NETCDF files (mHM output format) to text files with the file formatting and units required by GOLEM. The notebooks are available at https://git.gfz-potsdam.de/tsypin/brandenburg-groundwater.

5.4. Groundwater modeling: setting up thermo-hydraulic simulations

1. All simulations were conducted with GOLEM, a Finite Element Method (FEM) modelling platform for thermal-hydraulic-mechanical and non-reactive chemical processes in fully-saturated porous media (Cacace and Jacquey, 2017), available for download at https://git.gfz-potsdam.de/moose/golem/
2. Rock and fluid properties are assigned in accordance with Table 1 in Tsypin, Mikhail; Cacace, Mauro; Guse, Björn; Güntner, Andreas; Scheck-Wenderoth, Magdalena (2024): Modeling the influence of climate on groundwater flow and heat regime in Brandenburg (Germany), Frontiers in Water.
3. Steady-state conditions were derived by solving separately for the hydraulic and the thermal cases. These uncoupled steady-state simulations have been used as initial conditions to run a coupled pseudo-transient simulation, the results of which have been later imposed to initialize the pore pressure and the temperature in the final transient simulation.
4.



5. For the steady-state runs, we assume hydrostatic conditions with respect to a spatially variable hydraulic loading at the surface as given by a fixed hydraulic head. The initial distribution of hydraulic heads for the Quaternary unit across the study area is based on ~100 groundwater level measurements taken in 1953 together with a trend from hydroisohypses map as of 1999 (Landesamt für Umwelt Brandenburg, 2023). The resulting hydraulic head grid has been converted into a pressure boundary condition as follows:

$$P = -(Z - h) * \rho g + P_0$$

where P is the assigned pressure at the top boundary, P_0 is 1 bar (pressure at the water table), Z is ground elevation, h is the hydraulic head.

To better approximate the shallow groundwater dynamics, we additionally integrate the 15 longest rivers in Brandenburg as a nodeset to which we assign a Type I (Dirichlet) pressure boundary condition with a constant value of 1 bar, thereby forcing the groundwater level to match the model top at these locations.

We close the side edges of the 3D model, therefore assuming that no significant lateral flow or heat transport occurs into or out of the domain. This assumption particularly applies for the shallowest aquifer, for which the Oder river in the east, the Elbe river in the west, and watershed divides in the north and south act as natural hydraulic no-flow boundaries.

A Type I temperature boundary condition is assigned along the top surface as derived from grids of monthly averaged daily air temperature 2 m above the ground from the German Weather Service (DeutscheWetterDienst - Climate Data Center, 2021) and averaged over a period of 1951-1953.

Along the base of the model, we assign no flow and a Type I temperature boundary conditions. Given the extremely low permeability at a depth of -6000 m, flow through this boundary can indeed be considered negligible. The basal temperatures have been extracted from a lithosphere-scale thermal conductive model of Brandenburg, which has been additionally validated against temperature measurements from deep exploration wells (Noack et al., 2012).

6. In the next step, we use the results from the uncoupled thermal and hydraulic runs as initial conditions for a pseudo-transient coupled thermo-hydraulic simulation, that is, a transient simulation, which has been run till reaching equilibrium conditions. For this run we impose the same set of boundary conditions as described above. We set a constant timestep of 1000 years and considered steady state conditions if the maximum change in temperature and pressure per simulation step drops to values lower than 0.1°C or 10 kPa, respectively. Steady-state conditions were achieved after approximately 120 thousand years.
7. In the final simulation step, we take the output of the pseudo transient coupled simulation as initial conditions for the transient thermo-hydraulic simulation to quantify the influence of time-varying climate-driven surface forcing conditions over the period from 1953 to 2014, with a timestep of one month. This period was chosen due to availability of all input data required to compute recharge in a hydrological model. As a caveat, the onset of the transient simulation coincides with increasing groundwater abstraction due to population growth and mining activities in Brandenburg.

   The temperature boundary conditions imposed along the top surface have been derived from a spatial interpolation of the monitored monthly air temperature time series (DeutscheWetterDienst - Climate Data Center, 2021).

   We apply the net recharge flux, which is the difference between recharge and baseflow fluxes in an mHM cell at any given time, as a Type II (Neumann) pressure boundary condition, where positive net flux indicates that recharge outweighs baseflow, and vice versa. Major rivers in the study area are integrated into the model with a constant pressure (1 bar).

5.5. Output data processing

1. GOLEM output mesh with attributes is available in EXODUS II format. It can be opened with ParaView (Ayachit, 2015), an open source 3D visualization toolkit (https://www.paraview.org/download/). After installation the *.e file can be opened via File->Open and will be available in the pipeline browser. The file then has to be loaded by selecting the desired blocks, interfaces and properties in the properties panel and afterwards clicking on apply. Included elemental attributes are Darcy flux (v) and permeability (k). Included nodal attributes are the pore pressure (pore_pressure), the temperature (temperature), and the outflow residual. It also contains the object Id and global element Id (Frick, 2021).
2. The file contains 744 monthly time steps, from January 1953 to December 2014. The default Paraview time format is months since the start of the simulation. The calendar time in years can be displayed using Annotate Time Filter (Shift=1953, Scale=0.08333). For all of these time steps, extractions of all parameters at different places in space can be carried out, the most common of which would be cross-sections and depth slices, which can be accessed via the slice tool (Filters->Search-Slice). Note that these will linearly interpolate the values from the node or element information. For further processing and extraction, the user is advised to either look at the Paraview guide (https://docs.paraview.org/en/latest/) or contact the corresponding author (Frick, 2021).
3. We prepared several Python Jupiter notebooks to extract data from EXODUS files as maps or well probes, and plot them against measured values for validation. The notebooks are available at https://git.gfz-potsdam.de/tsypin/brandenburg-groundwater.

6. File description

The uploaded dataset comprises of source fluxes from the hydrological model, input files and scripts required to run the groundwater model, output files from the transient thermo-hydraulic simulations, references to validation data, and workflows for data pre-conditioning and post-processing. The data is organized as separate archived folders (*.gz format) for the model inputs and outputs.

6.1. File inventory

File	**File structure**	**Description**
\input\steady\ic_H_upbc.i	MOOSE Hierarchical Input Text	GOLEM input file for calculating the hydraulic steady state field
\input\steady\ic_T_lubc.i	MOOSE Hierarchical Input Text	GOLEM input file for calculating the thermal steady state field
\input\steady\master_lubc_steady_river_head.i	MOOSE Hierarchical Input Text	GOLEM input file for calculating the initial thermo-hydraulic field for the transient simulation
\input\steady\BC\P_golem_1999_DEM.csv	X [m] - Y [m] - Pressure [MPa]	Grid of mean water table for steady state upper pressure BC assignment
\input\steady\BC\steady_tavg1951-1953.csv	X [m] - Y [m] - Temperature [°C]	Grid of mean surface temperature for 1951-1553 for steady state upper temperature BC assignment
\input\steady\BC\temp_z6000_brb_modwrupel.csv	X [m] - Y [m] - Temperature [°C]	Grid of temperature at -6000 m for lower temperature BC assignment
\input\steady\mesh\brb_refine_x4_all.e	Block ID - Point ID - X [m] - Y [m] - Z [m]	Exodus file of the structural model containing 12 blocks, and top/bottom boundaries
\input\steady\prop\postrupelian_permeability.csv	X [m] - Y [m] - Permeability [m^2]	Grid of permeability for Tertiary Post Rupelian unit
\input\steady\prop\rupelian_permeability.csv	X [m] - Y [m] - Permeability [m^2]	Grid of permeability for Rupelian unit
\input\steady\tops\mesh_top_river_region.txt	X [m] - Y [m] - Z [m]	Coordinates of river nodes for River BC assignment
\input\transient\master_transient.i	MOOSE Hierarchical Input Text	GOLEM input file for the transient thermohydraulic simulation
\input\transient\BC\temp_z6000_brb_modwrupel.csv	X [m] - Y [m] - Temperature [°C]	Grid of temperature at -6000 m for lower temperature BC assignment
\input\transient\BC\urbc_trans_schedule_in_months.csv	time [month] - BC file path	Schedule file for transient recharge BC
\input\transient\BC\utbc_trans_schedule_in_months.csv	time [month] - BC file path	Schedule file for transient surface temperature BC
\input\transient\BC\urbc\rechargeYYYY-MM-DD.csv	X [m] - Y [m] - Net Recharge [m/month]	Grids of average monthly net recharge flux (from 1954-01 to 2014-12, with monthly increments)
\input\transient\BC\utbc\tavgYYYY-MM-DD.csv	X [m] - Y [m] - Temperature [°C]	Grids of average surface monthly temperature (from 1954-01 to 2014-12, with monthly increments)
\input\transient\prop\postrupelian_permeability.csv	X [m] - Y [m] - Permeability [m^2]	Grid of permeability for Tertiary Post Rupelian unit
\input\transient\prop\rupelian_permeability.csv	X [m] - Y [m] - Permeability [m^2]	Grid of permeability for Rupelian unit
\input\transient\tops\mesh_top_river_region.txt	X [m] - Y [m] - Z [m]	Grid of temperature at -6000 m for lower temperature BC assignment
\output\rivers_recharge_baseflow_Kf1e-5_exo.e	Timestep [month] - Block ID - Point ID - X [m] - Y [m] - Z [m] - Temperature [°C] - Pressure [MPa] - Flux [m/d]	Exodus file of the transient simulation results containing pressure, temperature and darcy flux for 12 blocks

7. References

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