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HMSE: A tool for coupling MODFLOW and HYDRUS-1D computer programs

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ABSTRACT

A new software HMSE has been developed to facilitate external coupling between two well-known programs for surface flow modeling: MODFLOW-2005 (saturated zone flow) and HYDRUS-1D (unsaturated zone flow). Two coupling schemes have been implemented. In the first case the groundwater recharge flux is calculated by HYDRUS-1D assuming a fixed water table position and then passed to MODFLOW input files. In the second case the water table position in HYDRUS-1D is updated periodically using the solution from MODFLOW. HMSE can be deployed in 3 modes: local, Docker and Kubernetes cluster. A web-based interface is provided to configure and run the simulation in all three cases. The software is applied to simulate groundwater table fluctuations observed in a shallow aquifer during three years.

Code metadata

Current code version	1.0.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-23-00705
Code Ocean compute capsule	
Legal Code License	MIT License
Code versioning system used	Git
Software code languages, tools, and services used	Python, Javascript, Kubernetes, Airflow, MinIO
Compilation requirements, operating environments & dependencies	Python >= 3.8, Airflow >= 2.3.0
If available Link to developer documentation/manual	https://github.com/WaterlinePL/HMSE-frontend#readme
Support email for questions	adam.szymkiewicz@pg.edu.pl balis@agh.edu.pl mat.pawlowicz1@gmail.com

1. Motivation and significance

Numerical models are increasingly used for groundwater management. They allow us to understand better the past, present, and future conditions of groundwater systems, find optimal management scenarios, implement protection measures for wellheads and aquifers, and evaluate the impact of climate and land use change on groundwater resources. Water in the subsurface occurs in two distinct zones: the unsaturated zone (or vadose zone) between the ground surface and groundwater table and the saturated zone (groundwater zone) below the groundwater table. In the unsaturated zone the pores of soils and rocks are filled partly with water and partly with air, while in the saturated zone the pores are completely filled with water. From the computational point of view, the simulation of flow in the vadose zone is much more challenging than in the saturated zone, because the governing equations are highly nonlinear and require a significant number of parameters which are often difficult to obtain.

Groundwater is extracted from aquifers, highly permeable geological formations in the saturated zone. However, the quantity and quality of water in aquifers critically depends on the processes occurring in the unsaturated zone. Groundwater is replenished mainly by water from

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precipitation which seeps through the unsaturated zone and ultimately arrives at the groundwater table as recharge. The recharge amount is strongly affected by climatic conditions, the permeability of soils in the unsaturated zone, the type of plants and the depth of groundwater table. Recharge determines the amount of groundwater that can be sustainably extracted from aquifers and understanding its spatial and temporal variability is crucial for efficient groundwater management. If the groundwater table is shallow, water can be taken up by capillary action and lost due to evapotranspiration (combined action of evaporation and uptake by plants). Thus, accurate representation of vadose zone processes can significantly improve groundwater modeling.

A number of integrated hydrological models have been developed that consider both unsaturated and saturated zones as a 3D continuum (e.g. PAR-FLOW [1], CATHY [2], Hydro-Geo-Sphere [3], FEFLOW [4], HYDRUS (2D/3D) [5]). However, their use in routine groundwater management applications is still limited, because of their high demand for input data, computer resources, and user expertise. Groundwater models used in management practice are commonly developed using the MODFLOW family of programs [6,7], which simulate 3D water flow in the saturated zone. MODFLOW can be extended by coupling with 1D vadose zone models, describing water flow in representative soil profiles associated with selected parts of the groundwater model domain. This is justified as the flow in the vadose zone occurs mostly in the vertical direction. This approach has several advantages: (i) it is more efficient computationally than a full 3D saturated/unsaturated model (1D simulations of the vadose zone can be easily parallelized); (ii) it allows for representing a variety of vadose zone processes relevant to groundwater flow in realistic, physically-based manner (1D models were shown to be useful in representing spatial and temporal variability of recharge and predicting the effects of land use and climate change (e.g. [8])); (iii) vadose zone modeling can be applied only to selected parts of the groundwater model domain. The UZF package [9] included in MODFLOW simulates 1D gravity-driven flow in the vadose zone using the kinematic wave approach. While it is very efficient computationally, the kinematic wave model neglects capillary-driven flow, which can be important in some situations (e.g. upward flow caused by root water uptake). The Richards equation provides a more comprehensive vadose zone flow model, which considers both gravity and capillary forces. State-of-the art simulators based on the Richards equation are available, including HYDRUS-1D [10] and SWAP [11] and have been coupled to MODFLOW programs [12–14]. The coupling of HYDRUS-1D and MODFLOW was initially done for MODFLOW-2000 and later applied to MODFLOW-2005 [15–17]. It was also extended to solute transport modeling with MT3DMS [18]. However, the previous versions were coupled on the code level, i.e. parts of the computer code of HYDRUS-1D were merged into MODFLOW (both are written in Fortran) and a new standalone computer application was created. One disadvantage of such an approach is that it cannot be used with standard input files of HYDRUS-1D and MODFLOW and creating application-specific input files is awkward. Moreover, any modification or update of standard MODFLOW or HYDRUS-1D codes must be ported manually into the merged code.

In this work we developed a new coupling approach for HYDRUS-1D and MODFLOW-2005: HYDRUS-MODFLOW Synergy Engine (HMSE). We use external coupling via an independent application, which allows the user to prepare MODFLOW and HYDRUS-1D models independently, using the graphical user interfaces available for both programs. The application modifies input files to pass information between HYDRUS-1D and MODFLOW, but each of these two programs is called externally as an executable file.

2. Software description

The HMSE comes in 3 deployments: desktop application (standalone webserver), docker container (standalone webserver) and Kubernetes cluster (microservice architecture). A part of HMSE code is based on existing open-source Python libraries for handling MODFLOW models (FloPy, [19]) and HYDRUS-1D (PHydrus, https://github.com/phydrus/phydrus). The following sections briefly describe the details of the software. More detailed benchmark of the software on a simple model can be found in the Supplementary material.

2.1. Software architecture

The logical architecture of the software is shown in Fig. 1 . The yellow and purple blocks describe system elements present in all the deployments. The dashed boxes indicate components which differentiate among application versions. The orange blocks describe components used in desktop deployment, the blue ones are used by Docker version and the gray ones are used by Kubernetes deployment. Users interact with a Web User Interface, a web application powered by a Python WSGI HTTP Server. The interface allows for setting up projects where users can define recharge zones, upload HYDRUS-1D and MODFLOW models, set various configuration parameters, run the simulations, and download the results.

The project's configuration is handled by the Project configuration module, which facilitates the setup of hydrological simulations. The projects' storage depends on the type of deployment. In a desktop deployment, this module interfaces with the local file system. In Docker deployment, it uses container volumes mapped to the host file system. Finally, in a Kubernetes cluster deployment, it communicates with an S3-compatible object storage (e.g., MinIO) through its API.

The Scheduling component supervises hydrological simulations, orchestrates actions and invokes simulations using third-party programs (HYDRUS-1D and MODFLOW-2005). Both the desktop deployment and the Docker version create Python supervisor threads for this purpose. By contrast, the Kubernetes cluster version leverages the Airflow scheduler for running the simulation pipeline as a set of Kubernetes Jobs in a cluster of machines.

Finally, the Workflow environment is where all the simulations occur. In the desktop version, the simulations are performed on copies of project files within the local file system by creating OS processes to run simulations. The Docker deployment operates similarly, but using a shared volume and the Docker-in-Docker technique to run the simulation steps as containers. On the other hand, the Kubernetes deployment runs the HYDRUS models in parallel using Pods in a dedicated namespace. Consequently, a distributed file system is needed to share data between the simulation steps. This can be achieved, for example, through an NFS Persistent Volume (PV) provided by the cluster. The simulation pipeline first retrieves the simulation data files from an S3 storage and places them in a working directory on the shared file system. Then the simulation steps are executed as Kubernetes Jobs (Pods). Finally, the results are uploaded back to S3.

2.2. Software functionalities

The coupling between MODFLOW and HYDRUS-1D models is implemented in HMSE along the lines described in [12,13]. A conceptual scheme is shown in Fig. 2. The area of the MODFLOW model is divided into several recharge zones, and HYDRUS-1D models are assigned to all or selected zones. Each HYDRUS-1D model represents a typical soil profile, land cover, depth to groundwater and weather conditions in the considered zone. MODFLOW model then represents transient groundwater flow, the simulation of which is divided into several user-defined stress periods, representing variations in boundary conditions, groundwater extractions etc. The main information obtained from HYDRUS-1D and passed to MODFLOW is groundwater recharge in each stress period. HMSE offers two coupling modes. In the simple coupling mode the groundwater table position is assumed constant in time and corresponding to the bottom of each HYDRUS-1D profile. First, simulations for all HYDRUS profiles are performed for the entire considered time period. Then, the average recharge rate corresponding

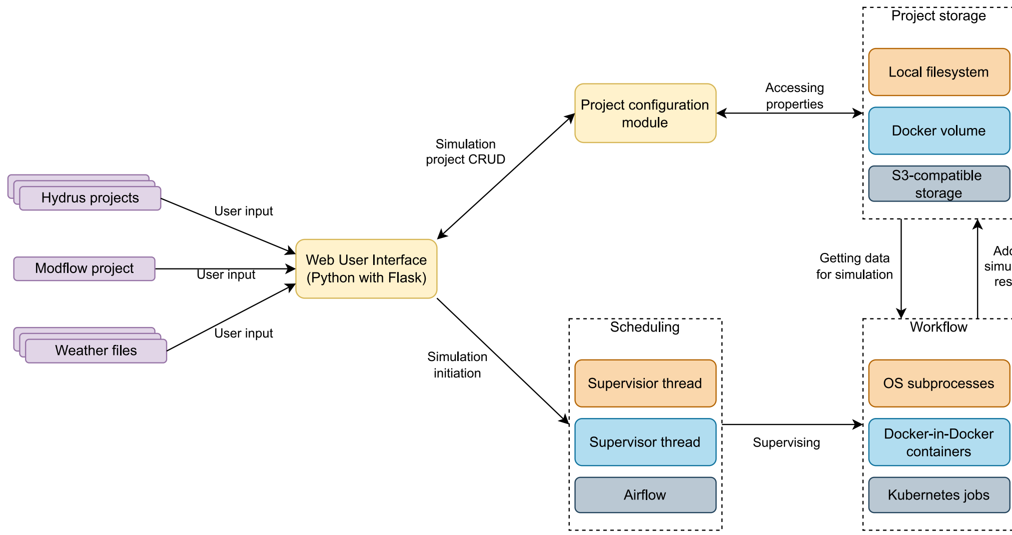

Fig. 1. Logical architecture of HMSE. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

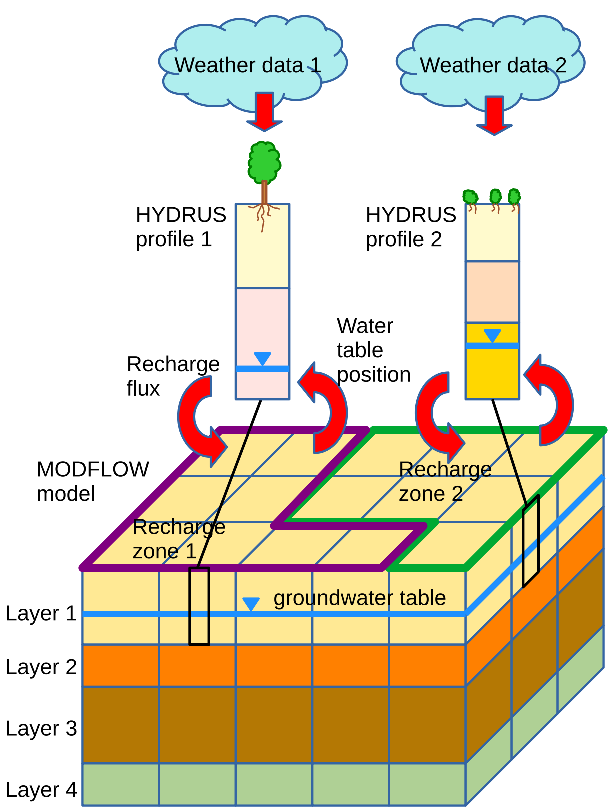

Fig. 2. Conceptual scheme of coupling between HYDRUS-1D and MODFLOW implemented in HMSE.

to each zone in each stress period is calculated by HMSE and written to the MODFLOW RCH file, which provides recharge rates for the groundwater flow simulation. In the second stage, the MODFLOW simulation is carried out.

The second coupling mode includes feedback from MODFLOW to HYDRUS-1D, to update the position of the water table in HYDRUS-1D profiles after each stress period in the MODFLOW simulation. To achieve this, the MODFLOW model is split into a number of models corresponding to subsequent stress periods of the main simulation. For each stress period the HYDRUS-1D simulations are performed first, then the recharge data is passed to the RCH file and a MODFLOW simulation is run for a single stress period. Based on the MODFLOW results, the average depth to the water table is calculated for each recharge zone and the corresponding HYDRUS profile is updated. The algorithm for updating water pressure distribution in the soil profile allows for avoiding spurious oscillations in the recharge flux due to discontinuities in the water table position between subsequent stress periods. It is described in detail in [16].

HMSE runs using the default web browser on a given machine. In the Configure tab the user has to specify paths to MODFLOW-2005 and HYDRUS-1D executables, which must be independently installed on the computer. Work in HMSE is organized into projects. Each project contains a single MODFLOW-2005 model (the user must upload all model files as a single *.zip archive). A number of models developed in HYDRUS-1D for various parts of the MODFLOW model domain can be added by the user (each HYDRUS model is uploaded as a single *.zip archive containing all input text files). Additionally, at least one file with weather data must be added. The weather file is in CSV format and contains daily precipitation, maximum and minimum temperature, relative humidity, wind speed, solar radiation, as well as the latitude, longitude and elevation of the weather station. The user assigns a weather file to each HYDRUS profile and a HYDRUS model to one or more recharge zones in the MODFLOW model. It should be noted that weather data are typically provided in HYDRUS-1D input files atmosph.in and meteo.in. In HMSE these files are overwritten with data from the weather files provided by the user as a separate input. The main purpose of such solution was to facilitate the use of different weather data sets and different simulation periods with the same HYDRUS-1D profiles. Weather data can be changed without the need for the user to update manually the HYDRUS profiles, which is useful especially in long-term simulations. Potential evapotranspiration is calculated internally by HYDRUS-1D, based on the weather data and other parameters specified by the user in the definition of soil profile (such as leaf area index LAI or crop height). In the future we plan to support more input options for weather data, including user-defined potential evapotranspiration.

HMSE offers two ways to define recharge zones in the MODFLOW model. The first method is based on the analysis of the existing RCH file in the model provided by the user. Various recharge zones are typically defined in existing groundwater models, based on geological, hydrological, and other factors. The cells in a single zone are assigned the same value of a recharge flux in a given stress period in the RCH file. HMSE parses the RCH file of the original MODFLOW model and divides the model domain into several recharge zones. In the

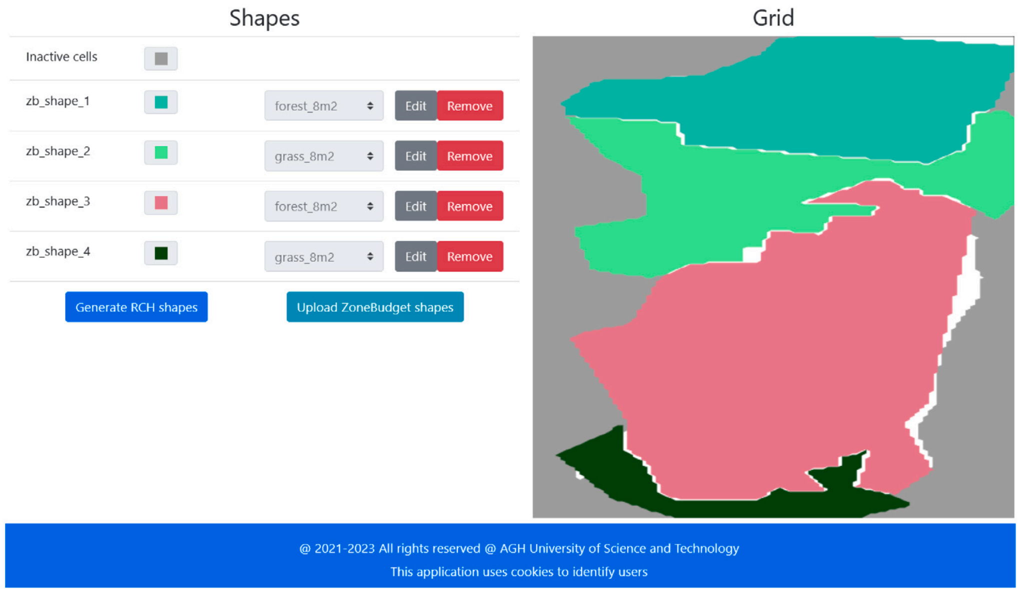

Fig. 3. HMSE interface screenshot showing the assignment of recharge zones.

second method the recharge zones correspond to the zones defined with the ZONEBUDGET [20] tool, which is often used as a post-processor to MODFLOW. In this case HMSE reads the text file defining ZONEBUDGET zones, which must be provided by the user together with other MODFLOW files in the *.zip archive. The preprocessing functionalities of HMSE are limited to handling the recharge zones and weather data. The MODFLOW and HYDRUS-1D models must be prepared independently by the user using other available tools, such as GMS,[1] ModelMuse [21], or FloPy [19] (for MODFLOW-2005) and the HYDRUS-1D GUI[2] or PHydrus library[3] (for HYDRUS-1D). For running the HYDRUS models under HMSE we recommend to use the HYDRUS-1D versions available in the GitHub repository for Windows and Linux systems, which are based on the open-source version of HYDRUS-1D,[4] with some minor changes to improve stability and ensure compatibility with the most recent version of HYDRUS-1D (v. 4.17). Currently HMSE is only compatible with MODFLOW-2005 models, however work is in progress to extend coupling to MODFLOW 6.

Once the recharge zones are defined, the uploaded HYDRUS-1D models can be assigned to one or more zones, Fig. 3. The user also defines the starting date of the simulation period, which is used to extract weather data from the external file. It is also possible to define a warm-up period. In the warm-up period HYDRUS-1D models are run with the corresponding weather data. The water pressure distribution at the end of the warm-up period is then used as a realistic initial condition for HYDRUS simulations in the time period of interest.

3. Illustrative example

HMSE *(desktop version)* has been applied to model a shallow aquifer on an outwash plain in northern Poland, as studied in [22]. The aquifer has horizontal extent of about 2 km^2 and is enclosed by four lakes in the west, the south and the east and a partially wet depression in the north (Fig. 4). The MODFLOW model consisted of gridblocks (cells) with horizontal dimensions of 10 by 10 m arranged in four layers (74 770 cells in total). Each layer was assigned a uniform and isotropic hydraulic conductivity k. From top to bottom the layers were: (1) outwash sand and gravel (upper aquifer, k = 25 m/d), (2) glacial till (k = 0.05 m/d), (3) outwash sand (lower aquifer, k = 10 m/d), (4) silt and glacial till (k = 0.01 m/d). Water flow between the surface water (lakes) and the aquifers (layers (1) and (3)) was represented with a third-type boundary condition (General Head Boundary). In the aquitard layers (2) and (4) a no-flow condition was imposed at lake boundaries. The northern boundary was perpendicular to groundwater head contours, so it was assigned a no-flow (second-type) condition.

Two recharge zones with different plant cover (pine forest and grassland) were distinguished (Fig. 4). The two corresponding soil profiles were taken from [22] and are denoted here as P1 and P3, consistent with that study. Each profile had two sandy layers (Sand I and II) separated by a layer of sandy loam. The hydraulic characteristics of each soil material were described with the van Genuchten–Mualem model [24]. An atmospheric boundary condition with no water ponding option (instantaneous runoff) was specified on the soil surface based on daily weather data measured on-site. Potential evapotranspiration (PET) was calculated using the Penman–Monteith equation [25] with a leaf area index (LAI) equal to 3.0 in the pine forest and 2.0 in the grassland. The vegetation height was set to 30 cm (it is not possible to specify realistic values for forests with the current implementation of PET calculation, nevertheless, the resulting PET estimates were reasonable for both land covers). Root water uptake was estimated using the Feddes macroscopic model [26] with a root zone depth of 1.5 m for the forest and 0.5 m for the grass cover. The reader is referred to [22] for a detailed soil characterization and parameters. Simulations were performed for a 3-year period (15 April 2017–14 April 2020), with a 3-year warm-up simulation carried out to determine initial flow conditions. HYDRUS-1D used automatically adjusted time step with a maximum of 1 day. MODFLOW simulation was divided into 36 monthly stress periods.

Simulations were carried out using the two coupling methods described above. In the first scenario (one-way coupling) profiles were 6.60 m (forest), and 7.05 m (grassland) deep and the bottom boundary condition was assumed to be a constant pressure head equal to zero (water table level). In the second scenario (two-way coupling), the profiles were extended to 8 m, and the water pressure head at the bottom was updated according to the results obtained from MODFLOW.

The recharge fluxes obtained using the two coupling methods are shown in Fig. 5. The one-way coupling results in a smoother evolution

[1] https://www.aquaveo.com/software/gms-groundwater-modeling-system-introduction
[2] https://www.pc-progress.com/en/Default.aspx?hydrus-1d
[3] https://github.com/phydrus/phydrus)
[4] https://www.pc-progress.com/en/Default.aspx?H1D-description#k8

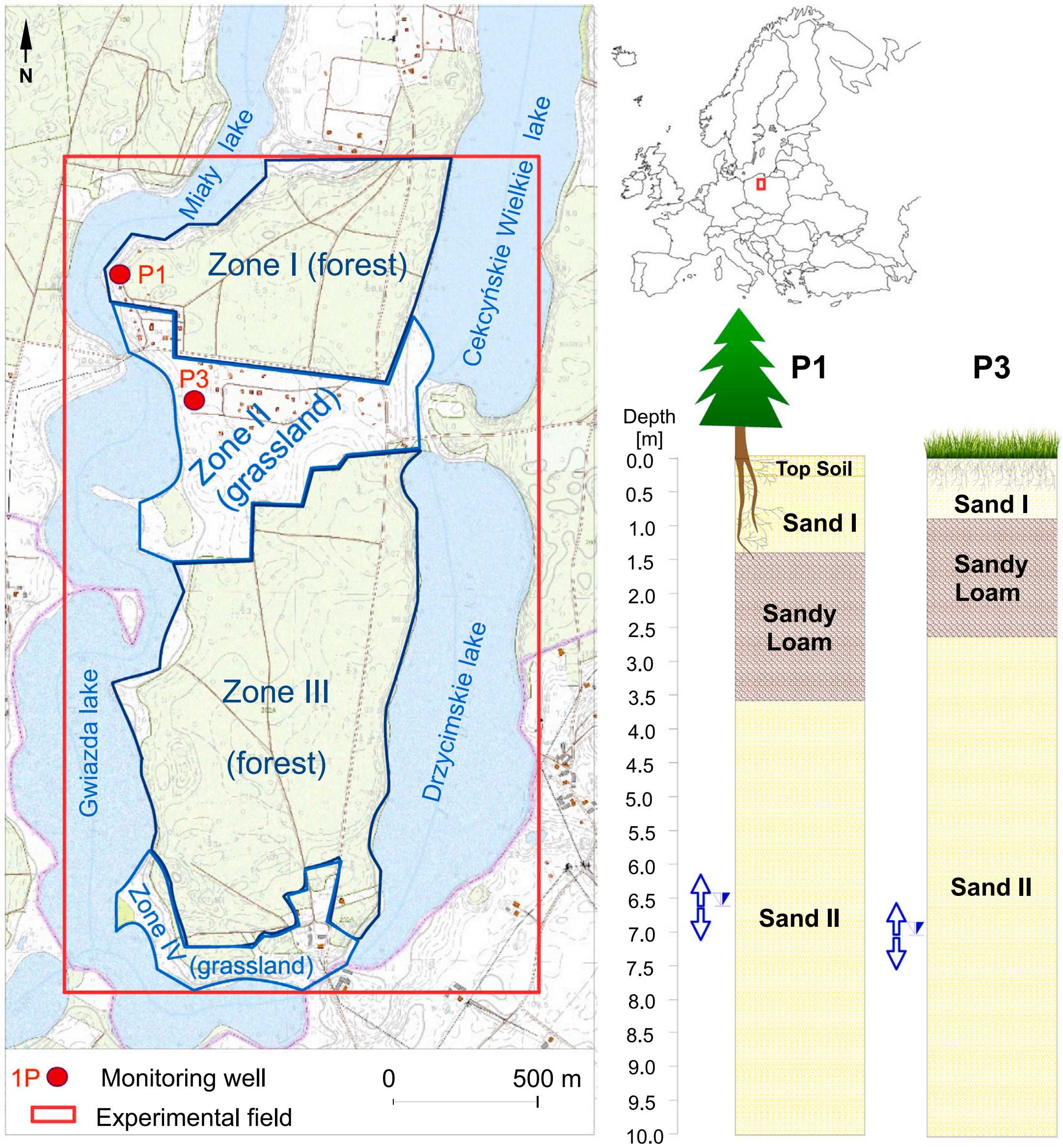

Fig. 4. Model area and characteristic soil profiles.
Source: Modified from [23].

of recharge in time, while two-way coupling leads to more fluctuations due to the changes in the position of the water table between MODFLOW stress periods. Negative recharge values appear in two-way coupling, indicating upward water movement due to capillary uptake.

The simulated water table elevation was compared to field measurements carried out in P1 and P3 [22] (Fig. 6). The trends and magnitude of water table movement in simulations show reasonable similarity to the observations, even though the agreement is less than perfect. The differences are larger for the grassland than for the forest. Also, the one-way coupling seems to give the results more aligned with observations than the two-way coupling, especially during the dry period, when the simulation overestimates the magnitude and speed of the water table drawdown. This might be attributed to several reasons, such as variability in aquifer parameters, extrapolating data from single soil profiles to larger areas and comparing point measurements of the groundwater table to area averages obtained from MODFLOW. The fit could possibly be improved by recalibrating the coupled model. However, such a task is beyond the scope of our study.

4. Impact

The current version of HMSE allows for extending existing groundwater models developed with MODFLOW-2005 by coupling them with HYDRUS-1D models simulating hydrological processes in representative vadose zone profiles. Both HYDRUS-1D and MODFLOW-2005 are mature, state-of-the-art computer programs validated on thousands of case studies and supported by large user communities. Our application brings synergy effects of more comprehensive hydrological modeling based on the combined use of these two programs. Including detailed description of vadose zone processes can be especially helpful in: (i) improved understanding of time and space variability of groundwater recharge, (ii) establishing protection zones for groundwater intakes and aquifers, (iii) evaluation of the impact of climate and land use change on groundwater resources, (iv) assessing vulnerability of aquifers to pollution originating from the ground surface, (v) evaluation of managed aquifer recharge (MAR) schemes, which are often based on artificial infiltration of water from the surface via the vadose zone to aquifers. Future work will focus on the implementation of coupling for solute transport and integration with MODFLOW 6

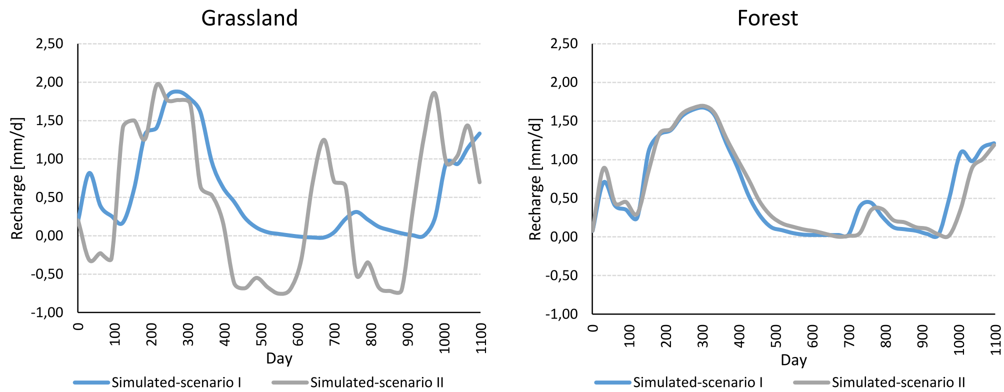

Fig. 5. Groundwater recharge flux calculated by HYDRUS.

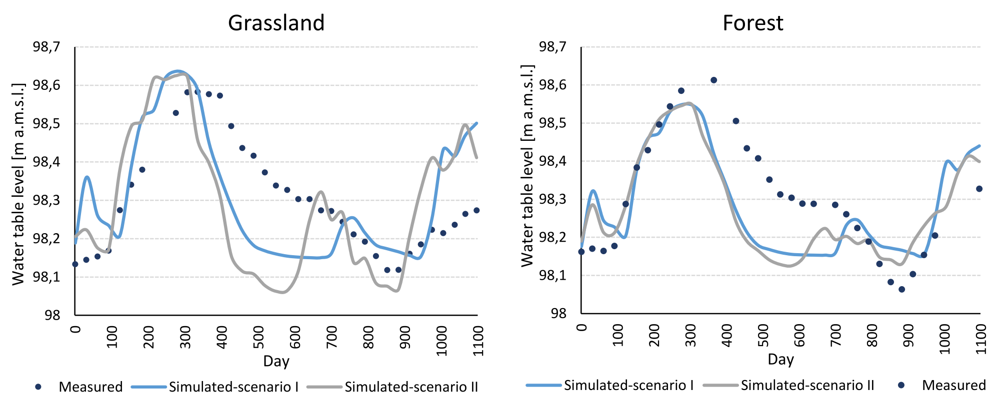

Fig. 6. Observed and simulated groundwater table elevation.

5. Conclusions

A new application has been developed that enables to couple MODFLOW-2005 groundwater models with HYDRUS-1D vadose zone models in a user-friendly way. The application allows two coupling modes and two methods to delineate recharge zones in MODFLOW models. Preliminary validation has been performed on a 3-year series of observations in a shallow sandy aquifer and showed satisfactory performance of the new computer tool.

CRediT authorship contribution statement

Mateusz Pawlowicz: Writing – review & editing, Writing – original draft, Software. **Bartosz Balis:** Writing – review & editing, Writing – original draft, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Adam Szymkiewicz:** Writing – review & editing, Writing – original draft, Supervision, Resources, Methodology, Investigation, Conceptualization. **Jirka Šimůnek:** Software, Conceptualization. **Anna Gumuła-Kawęcka:** Writing – review & editing, Writing – original draft, Visualization, Validation, Resources, Investigation, Conceptualization. **Beata Jaworska-Szulc:** Writing – review & editing, Writing – original draft, Validation, Resources, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2024.101680.

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