Investigating an OpenMI coupling of FEFLOW and MIKE SHE

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ABSTRACT: Effective environmental management requires integrated modelling not only of catchment processes but their interactions. The motivation of this study was to combine the strengths of FEFLOW and MIKE SHE to improve our ability to solve complex problems in water resources and environmental management. This is achieved by coupling the two models using OpenMI technology. OpenMI is a standard which allows different modelling tools to exchange data dynamically during the simulation. One advantage of such a coupling is that the comprehensive surface and unsaturated zone processes in MIKE SHE can be combined with the advanced subsurface modelling in FEFLOW. This represents a very challenging coupling problem as both models are individually quite complex; FEFLOW is based on the finite-element method and can handle quadrilateral or unstructured triangular meshes, while the finitedifference based MIKE SHE employs a regular (Cartesian) grid. The proposed coupling requires exchange of data between one-dimensional, two-dimensional and three-dimensional fields. This paper briefly describes how the coupling of these two models is achieved. Systematic tests of the coupled modelling tools have been carried out in order to verify the coupling of different components of FEFLOW and MIKE SHE. Selected cases involving different combinations of processes within the coupling such as river flows, unsaturated flows, drainage and extractions are examined against existing analytical and numerical solutions. A number of interesting potential new applications emerge by combining the strengths of both models. These results demonstrate how the coupled model can address such new problems, including high-resolution modelling of groundwater within a large-scale catchment, and coupling of overland and unsaturated flow processes with seawater intrusion in coastal aquifers which can in turn be used to examine the impacts of climate change.

INTRODUCTION

Proper understanding of water cycle in nature is needed for the effective management of water resources. Numerous studies have been carried out to analyse individual components of the cycle and modelling tools have been developed to achieve this. Traditionally different hydrological processes such as surface water and groundwater have been managed and modelled separately in part due to the complexity of the real hydrological systems and limitations in computational resources. However in reality not only are the details of each process important but also the mutual interactions between the different processes are often crucial to our understanding of the water cycle. Surface water and groundwater interactions affect a number of water management issues such as conjunctive water use for water supply and irrigation, the transformation of nutrients, wetland dynamics and ecology, flooding behaviour, bio-geochemical conditions in riparian areas, stream temperature, etc. Groundwater resources often have a complex dependency with adjacent water courses, wetlands and stream networks. Groundwater is on the other hand is an important factor in freshwater wetlands and in controlling low flows and maintaining environmental flows. The interactions between groundwater bodies, groundwater dependent terrestrial ecosystems and surface water bodies play a central role in the requirements of the EU Water Framework. Therefore, a more comprehensive and holistic modelling approach is required to solve many of today's complex water management problems. For example, assessing the impact of climate change or land use change on sustainability of a coastal aquifer system may require integrated modelling of the surface water resources, the aquifer and their interaction.

There are a growing number of surface water-groundwater models. However each model has its own strengths and weaknesses, for example there are relatively few that include river management capabilities (Valerio et al., 2010). The motivation of this study is to combine the strengths of two comprehensive water resources models, MIKE SHE and FEFLOW to address more complex environmental problems. In this study, we aim to achieve this by coupling MIKE SHE and FEFLOW using OpenMI technology. Linking existing models provides a cost-effective and powerful method for expanding integrated modelling capabilities. This paper demonstrates how this approach is being used to enhance the process modelling capabilities of both tools. There are however a number of important challenges in successfully integrating different process descriptions using different models. These include matching the temporal and spatial scales of the different processes, modelling subgrid processes, ensuring fast, accurate and stable numerical solutions and properly accounting for the effects of coupling between the processes.

MIKE SHE is a fully distributed, process-based hydrological model and includes process models for evapotranspiration, overland flow, unsaturated flow, groundwater flow, and channel flow and their interactions including solute transport (Abbott et al 1986a&b; Refsgaard and Storm, 1995). Each of these processes is described by its governing equation or by a simpler conceptual representation and a user can tailor the model structure by choosing processes to be included and the solving methods (Butts et al, 2004). MIKE SHE is a comprehensive catchment modelling framework with applications ranging from aquifer management and remediation to wetland management, flooding and flood forecasting (Graham and Butts, 2006; Butts & Graham, 2008). MIKE SHE is dynamically coupled to MIKE 11, which is a one-dimensional surface water model that simulates fully dynamic channel flows and is therefore able to represent river processes and river management (Butts et al., 2004; Thompson et al., 2004). While the process-based approach allows different model structures to be applied within the same modelling framework, in the original concept the different flow processes are described by the governing partial differential equations and these are then solved by discrete numerical approximations in space and time using finite differences.

FEFLOW is an advanced subsurface water modelling system for modelling fluid flow and transport of dissolved constituents and/or heat transport processes in the subsurface including density dependent flow (Diersch and Kolditz 1998, Kolditz et al., 1998, Diersch, 2001; Trefry and Muffels 2007; DHI-WASY 2010) FEFLOW is a highly flexible finite element model for subsurface flow and transport and more recently interactions with river systems (Monninkhoff and Li, 2009). The advantage of the finite element approach is the flexibility to represent complex geologies with a high spatial resolution, including sloping layers and anisotropy and the ability to precisely represent features like rivers, fractures, tunnels and well locations. One of the other key strengths of FEFLOW is the number of advanced descriptions of subsurface processes such as variably saturated and density dependent flow, saltwater intrusion, multi species chemistry and transport and heat transport. Applications of FEFLOW include: regional groundwater management, saltwater intrusion, seepage through dams and levees, mine water management, groundwater management in construction and tunnelling projects, land use and climate change scenarios, groundwater remediation and natural attenuation, geothermal energy and groundwater-surface water interactions.

The main reasons for coupling MIKE SHE and FEFLOW are

- the powerful subsurface modelling capabilities of FEFLOW, especially grid refinement, three dimensional unsaturated flow and variable density flow including saltwater intrusion would be available in MIKE SHE
- the surface process capabilities in MIKE SHE particularly the ability to calculate dynamically recharge to groundwater directly from precipitation and potential evapotranspiration and subsequently determine both groundwater flow and river discharge,. would be available in FEFLOW

The exchange of data needed to couple FEFLOW and MIKE SHE is performed using the OpenMI protocol. The Open Modelling Interface and Environment (OpenMI) is a set of standardized interfaces and classes that have been developed by the OpenMI Association (www.openmi.org), and partly funded by EU through the 5th framework project, HarmonIT, and the LIFE Programme, OpenMI-LIFE.

OpenMI allows models to communicate at run-time, across differences in time step, spatial resolution, and discretization. OpenMI was developed and designed in an attempt to provide a widely accepted unified method to simplify linking of hydrology-related models, both legacy codes and new ones, (Gregersen et al., 2005, 2007). It is based on direct links between the models at run-time, not using files for data exchange. To achieve a dynamic coupling between MIKE SHE and FEFLOW, both models were made OpenMI compliant by developing the appropriate interfaces. These interfaces allow for run-time and times step control to an outside entity and provide access to internal state variables and parameters.

In this study we briefly describe the approach used in coupling MIKE SHE and FEFLOW using OpenMI. This represents quite a challenging coupling problem as it contains both one-dimensional, two dimensional and three-dimensional elements. In addition, the coupling must match the block-centred finite difference solutions from MIKE SHE with the variable mesh finite element solutions from FEFLOW. The performance of this coupled model is then demonstrated and evaluated against both analytical and numerical solutions for a number of verification cases involving both surface water and groundwater components. From the resulting coupled hydrological model, a number of interesting potential new applications emerge that combine the strengths of both models.

COUPLING METHODOLOGY

In this study, the groundwater system is modelled by FEFLOW and surface water and unsaturated zone is modelled by MIKE SHE. While FEFLOW has the option to represent the unsaturated zone using the three-dimensional Richards equation, in many cases the unsaturated flow is predominantly vertical. Therefore the one-dimensional solution used in MIKE SHE is often sufficient and expected to save computation time particularly for large-scale catchment modelling. MIKE SHE also has detailed descriptions of the evapotranspiration and recharge processes.

The two models exchange recharge to the top of the groundwater system and groundwater head in each computational layer of aquifer. MIKE SHE calculates the recharge entering the aquifer which is passed to FEFLOW as a source term. MIKE SHE calculates the exchange flows between the aquifer and the river, based on the differences in head between the river and groundwater in MIKE SHE. These exchange flows are also passed to FEFLOW as a source term. FEFLOW performs the calculation of the groundwater flows and heads in each of the computational layers, and the levels are passed to MIKE SHE. The calculations in MIKE SHE are based on the ground water heads of the last time step in FEFLOW; hence these exchange calculations are based on an explicit/"old" value and may require careful choice of time step. While in simple cases it is possible to carry out this exchange for a single groundwater computational layer, in more general cases the entire three-dimensional groundwater head field calculated by FEFLOW must be passed to MIKE SHE. This is the case for example if the river is connected to several computational layers in the groundwater zone and is the approach used in this study. To implement this we have assumed that the MIKE SHE model must contain computational layers in its groundwater component that are identical to the layers in FEFLOW: This means more generally that the models need to be specifically set up for coupling.

The MIKE SHE model and the FEFLOW model differ in both their spatial discretization and in their time stepping strategy. The computational mesh in MIKE SHE is always a block-centred, finite difference grid that is uniform in the horizontal plane, while the FEFLOW mesh can use either quadrilateral or triangular elements with variable element size. In order to exchange data between the two models, both temporal and spatial interpolations are required. For the temporal interpolation, time buffering adaptors are applied. These buffers store exchange values for a number of time steps for one model, in order to perform proper temporal interpolation at the times required by the other model. This temporal interpolation process is illustrated in Figure 1. In this study the OpenMI coupling is configured so that FEFLOW is the trigger. Timestep t_i is the latest FEFLOW timestep and t_i is the latest MIKE SHE timestep. (1) When FEFLOW is the trigger, it requests recharge values from MIKE SHE to simulate t_{i+1} . (2) MIKE SHE advances the simulation to provide the recharge value at this timestep. To simulate the next timestep t_{i+1} MIKE SHE needs head elevations from FEFLOW at this time. (3) For the explicit coupling used here FEFLOW passes the latest hydraulic head at t_i to MIKE SHE. (4) MIKE SHE uses this extrapolated hydraulic head to simulate t_{i+1} . MIKE SHE continues to simulate using this value until it reaches or exceeds the FEFLOW timestep t_{i+1} . (5) In the simple examples presented here, then once the MIKE SHE simulation has advanced sufficiently, the recharge at t_{i+1} for FEFLOW is calculated as a time-weighted average of two simulated values around this time. In more general cases this can be modified to estimate the accumulated recharge. (6) The interpolated recharge is provided to FEFLOW and FEFLOW simulates t_{i+1} .

Similarly spatial adaptors are applied that interpolate values between the block centred finite difference grid and the unstructured finite element mesh. The spatial interpolations are performed on a layer-by-layer basis. This assumes that the computational layers in the saturated zone of the two models match exactly, both in terms of the number of layers and depth of each layer. The actual interpolation is then carried out in two steps. In the first step, the head values at the nodes of the finite element mesh in FEFLOW are interpolated to the centroid of each finite element prism. In the second step a two-dimensional interpolation is then used to map these values onto the centroid of the finite difference grid of MIKE SHE. Further details concerning data exchange and the spatial and temporal adaptors can be found in the OpenMI technical documentation (OpenMI 2007a, b).



Figure 1: Time adaptor in OpenMI coupling of FEFLOW and MIKE SHE (see explanation in the text)

VERIFICATION STUDY

A series of test cases have been analysed to verify the coupled modelling tool. The tests were designed to test the transient behaviour of the coupling, matching of the finite difference and finite element meshes, particular components of the coupling as well as model performance and accuracy.

Transient stream depletion (Hunt, 1999)

Hunt (1999) presented an analytical solution for the transient drawdown due to constant pumping in an infinite uniform aquifer containing a stream that acts as a constant head boundary. Figure 2 shows the problem considered by Hunt together with the geometry and boundary conditions used in the numerical modelling. This problem can be modelled using either MIKE SHE or FEFLOW or the coupled MIKE SHE-FEFLOW model. This provides a verification of the transient behaviour of the coupling and interaction between groundwater and the river model. The model parameters used are presented in Table 1. The numerical model domain of 1000 m by 1000 m is sufficiently large that the boundary conditions don't affect the flow for the time scales considered. The aquifer is represented as a single computational layer.



Figure 2: Schematic of the stream depletion problem considered by Hunt (1999)

Shortest distance from the stream to the pumping well	95 m
Pumping rate	3.17 x 10 ⁻⁴ m ³ /s
Thickness of the aquifer	10 m
Transmissibility of the aquifer	0.001 m ² /s
Storage coefficient of the aquifer	0.2
Stream bed leakage coefficient	1 x 10 ⁻⁵ m/s
Initial hydraulic head	10 m
Recharge	0 m ³ /s

Table 1: Model parameters for the stream depletion verification case

The river has symmetric trapezoidal cross-sections as shown in Figure 2 which are 10 m wide at the elevation of the levees (11 m) and 5 m wide at the riverbed level (9.5 m). The initial water depth and boundary water depth are fixed as 0.5m. The MIKE SHE setup used 10 m by 10 m grid (10000 grid cells). In order to investigate the impact of FEFLOW spatial resolution, two triangular meshes were generated for FEFLOW; a fine mesh (29944 elements) and a coarse mesh (3263 elements).



Figure 3: (a) Comparison of the analytical drawdown by Hunt and the simulated drawdown by MIKE SHE and the MIKE SHE- FEFLOW coupled model. The results are obtained at a point along the line through the pumping well perpendicular to the river, 50 m away from the well. (b) The simulated leakage from the river to the aquifer in the numerical simulations.



Figure 4: Comparison of the analytical drawdown by Hunt (1999) and the simulated drawdown in MIKE SHE and MIKE SHE- FEFLOW coupled model, perpendicular to the river and through the well after 23 days of pumping.

The simulated drawdown of groundwater and the analytical solution are compared in Figure 3(a). This shows the transient behaviour during the first 23 days after the onset of pumping for a well located directly between the pumping well and the river, 50 m from the well. The corresponding leakage, for the numerical models, from the river to the aquifer is shown in Figure 3(b). Figure 4 shows the analytical drawdown and the simulated drawdown after 23 days along the cross-section through the well perpendicular to the river. This figure compares the analytical solution with the results obtained using MIKE SHE and with simulations using the coupling of FEFLOW and MIKE SHE. The simulated results match the analytical solution very well in all cases. The same accuracy could be achieved using the coarse mesh by using grid refinement around the well and the stream. This illustrates one of the powerful features of FEFLOW's finite element formulation. At the same time detail describing drawdown near the well can be obtained, Figure 4.

Transient stream depletion with unsaturated flow

The stream depletion model set-up was then modified to verify the coupled model when including unsaturated flow and multiple layers, Figure 5. The geometry is similar but not identical to the first case and the pumping rate is increased to 0.003 m^3 /s. A single soil type is used in the unsaturated zone. The soil properties are shown in Figure 6 and correspond to a fine sand. Initially, the rainfall and recharge is zero, then after 13 days a constant rainfall of 2.4 mm/day is applied over the next 5 days.



Figure 5 Modified stream depletion model including unsaturated flow and multiple layers.





In this case only numerical solutions are available, so this was first simulated using just MIKE SHE. These results are then compared with the coupled MIKE SHE- FEFLOW model in Figure 7. The comparison shows the results obtained from MIKE SHE (solid lines) with the coupled model (lines and symbols). Once again there is good agreement between the two models and the pressure distribution in the different layers is captured. Nevertheless there are some small differences in both the head elevations and timing close to the well. The simulated heads that are plotted for the coupled model are the FEFLOW model results interpolated to the MIKE SHE cell centres for each day. It should be noted that close to the well the gradients are quite large and the MIKE SHE grid resolution (10 m) is comparable to the distance to the 10 m well. This is the likely explanation for these small discrepancies.



Figure 7 Comparison of the head elevation in different layers simulated by MIKE SHE and the MIKE SHE- FEFLOW coupled model. The results are obtained at a point along the line through the pumping well, perpendicular to the river, (a) 50 m from the well and (b) 10m from the well.

DISCUSSION AND CONCLUSIONS

In this paper we develop and demonstrate a dynamic coupling of MIKE SHE and FEFLOW as an integrated modelling approach. This is achieved using the open modelling interface tools in OpenMI. The motivation for this study was to develop an integrated hydrological modelling tool that enhances the capabilities of both models. Firstly the powerful subsurface modelling capabilities of FEFLOW, especially grid refinement, three dimensional unsaturated flow and variable density flow including saltwater intrusion are made available to MIKE SHE. Conversely, the surface process capabilities in MIKE SHE particularly the ability to calculate dynamically recharge to groundwater directly from precipitation and potential evapotranspiration and subsequently to simulate groundwater–river exchanges are available to FEFLOW.

The coupling developed here represents a challenging application of OpenMI technology. This coupling not only contains one-dimensional, two dimensional and three-dimensional elements but the coupling must also match the block-centred finite difference solutions from MIKE SHE with the variable mesh finite element solutions from FEFLOW. The exchange of data in both space and time exploits built-in tools available within the OpenMI framework. The initial results shown here verify the ability of the coupling between FEFLOW and MIKE SHE to represent dynamically the interactions between the river and groundwater systems in a few well-defined cases. The results also highlight the ability of the flexible finite element to effectively represent complex geometries and boundary conditions. Complementary investigations for lake-groundwater interaction have also been successfully carried out.

This new coupled tool provides the capability to address more complex integrated modelling problems which was one of the key motivations for developing OpenMI. We are currently verifying coupling with transient recharge and investigating the use of this tool to examine problems related to saltwater intrusion. Here we can take full advantage of such a coupling by combining, the ability of MIKE SHE to represent spatial and temporal variations in recharge with the ability to represent variable density subsurface flow in FEFLOW. This will allow us not only to investigate more complex saltwater intrusion problems but also to examine, for example, the effects of climate changes on the management of coastal aquifers.

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