Groundwater

Methods Brief/

An Agricultural Package for MODFLOW 6 Using the Application Programming Interface

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Abstract

An agricultural water use package has been developed for MODFLOW 6 using the MODFLOW Application Programming Interface (API). The MODFLOW API Agricultural Water Use Package (API-Ag) was based on the approach to simulate irrigation demand in the MODFLOW-NWT and GSFLOW Agricultural Water Use (AG) Package. The API-Ag Package differs from the previous approach by implementing new features and support for additional irrigation providers. New features include representation of deficit and over-irrigation, Multi-Aquifer Well and Lake Package irrigation providers, and support for structured, vertex, and unstructured grid models. Three example problems are presented that demonstrate how the API-Ag Package improves representation of highly managed systems and are further used to validate the irrigation demand and delivery formulations. Irrigation volumes simulated in the three example problems show excellent agreement with the MODFLOW-NWT AG Package.

Introduction

Surface-water and groundwater resources face increased pressures from population growth, economic development, climate change, and the expansion of irrigated agriculture (Liu et al. 2017; Tan et al. 2017). An estimated 4 billion people are affected by severe water scarcity, given the current demands on freshwater resources (Mekonnen and Hoekstra 2016). The increasing population will further exacerbate the growing divide between freshwater resources and demand (Fereres and Soriano 2006; Elliott et al. 2013; Mancosu et al. 2015; United Nations Department of Economic and Social Affairs 2022).

An estimated 70–75% of global water consumption is used to support agricultural production. (Wallace 2000; Rost et al. 2008). In the United States, combined surface-water and groundwater irrigation withdrawals accounted for 42% (about 450 million m^3/day) of total freshwater withdrawals in 2015 (Dieter et al. 2018). The large volume of agricultural freshwater consumption creates a disconnect where agricultural practices are necessary to support global food systems and growing populations; however, lack of sufficient water has already impaired sustainability in parts of the world (Forouzani and Karami 2011). As freshwater resources become more limited, it becomes more critical to evaluate water

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management strategies and scientific hypothesis using models (Fatichi et al. 2016).

Physics-based hydrologic modeling has long been used to simulate historical water use and availability, make relative predictions about future water resources, and test different water management strategies under historical and future conditions (Woolfenden and Nishikawa 2014; Faunt et al. 2015, 2016; Densmore et al. 2018; Kitlasten et al. 2021; Cromwell and Alzraiee 2022; Stamos-Pfeiffer et al. 2022; Morway et al. 2023). MODFLOW 6 is a physically based multi-model hydrologic simulator that is commonly used to assess hydrologic systems (Hughes et al. 2017). MODFLOW 6 is the current (2023) core release of MODFLOW. MODFLOW 6 consists of a Groundwater Flow (GWF) Model (Langevin et al. 2017) and a Groundwater Transport (GWT) Model (Langevin et al. 2022). The GWF and GWT models support regular and unstructured grids and have many new capabilities not available in previous versions of MODFLOW. The GWF Model in MODFLOW 6 currently supports simulation of groundwater and streamflow interactions; however, it does not yet employ a physically based method for simulating agricultural water use. The Water Mover (MVR) Package (Langevin et al. 2017) of the GWF Model can be used to simulate the hydrologic effects of agriculture through simplified assumptions and specified absolute rates of applied irrigation (Morway et al. 2021); however, the MVR Package is not capable of dynamically adjusting the amount of water transferred among its advanced flow packages based on the actual evapotranspiration deficit or soil water uptake from antecedent moisture conditions within the root zone.

An earlier version of MODFLOW, MODFLOW-NWT (Niswonger et al. 2011), and the integrated hydrologic model GSFLOW (Markstrom et al. 2008), each include packages that can represent irrigated agriculture using dynamic demands calculated from soil-water conditions. The Agricultural Water Use (AG) Package (Niswonger 2020) for MODFLOW-NWT and GSFLOW simulates surface-water and groundwater use on agricultural fields for a variety of common land-use scenarios and agricultural management regimes. MODFLOW-OWHM (Hanson et al. 2014; Boyce et al. 2020), which is another conceptualization of MODFLOW, includes the Farm Process (Schmid and Hanson 2009). The Farm Process represents many agricultural operations, such as irrigation return flows to surface-water diversions, anoxic soil conditions, and salinity management processes (Boyce et al. 2020). However, in the Farm Process irrigation demands are calculated based on the assumption that soil water content is well managed and under steady-state conditions (Hanson et al. 2014; Boyce et al. 2020). Although the AG Package and the Farm Process allow representation of agricultural water use, these packages are not compatible with MODFLOW 6. Other approaches to simulate agriculture in MODFLOW involve loosely coupling external models to MODFLOW by applying their output as boundary conditions. The Irrigation Demand Calculator (California Natural Resources Agency 2015) and the Soil-Water-Balance (Westenbroek et al. 2018) are two examples of code that have been used to loosely couple agricultural irrigation to MODFLOW (Stanton et al. 2013; Peterson et al. 2020; Fienen et al. 2022).

To extend the applicability of the core version of MODFLOW for irrigated areas, a new method for simulating agricultural water use was developed through the MODFLOW 6 Application Programming Interface (API; Hughes et al. 2022). The MODFLOW API can be used to tightly couple external processes and packages to MODFLOW 6 without the need to recompile the MODFLOW 6 source code. External processes (e.g., custom or existing software) can provide forcing data to MODFLOW and access internal variables, perform calculations, and update stresses within MODFLOW's outer iteration loop. The new MODFLOW 6 Agricultural Water Use Package (API-Ag; Larsen 2023) couples physically based agricultural water use processes to MODFLOW using the MODFLOW API. To test this coupling, a series of example problems have been developed and compared with solutions from the MODFLOW-NWT AG Package.

Methods

The API-Ag Package was developed as an installable Python package (software library) that leverages functionality from FloPy (Bakker et al. 2016, 2022; Hughes et al. 2023) and is a simulation driver for the MODFLOW API. Agricultural water-use processes are simulated by the API-Ag package, and the resulting water management decisions (MODFLOW "stresses") are applied to the simulation by overriding the behavior of the MVR Package, which distributes water from providers to receivers. That is, agricultural water use is simulated by transferring water from irrigation providers to irrigation receivers. Irrigation providers are model features that may include wells in the Well (WEL) Package, multi-aquifer wells from the Multi-Aquifer Well (MAW) Package, stream reaches from the Streamflow Routing (SFR) Package, and lakes defined using the Lake (LAK) Package. Irrigation receivers are unsaturated zone cells, defined by the user in the Unsaturated Zone Flow (UZF) Package, that are intended to represent agricultural fields.

The API-Ag Package calculates irrigation demand based on a modified version of the formulation presented by Niswonger (2020). The amount of available water that can be moved from a provider to a receiver is limited by the calculated amount of water available within the provider and the user-specified maximum irrigation rate. Irrigation demand for a receiver cell is calculated to minimize the difference between potential crop evapotranspiration ($ET_{\mathrm{o}}K_{\mathrm{c}}$) and actual evapotranspiration (ET_{a}), which is calculated by UZF (Niswonger et al. 2006; Langevin et al. 2017). The total volume of water consumed by a given crop (Q_{ET}) is calculated as follows:

$$Q_{\mathrm{ET}} = \sum_{n=1}^{n\mathrm{cell}} ET_{\mathrm{o}} K_{\mathrm{c}} A_{\mathrm{n}}, \tag{1}$$

where ET_o is the potential evapotranspiration flux, K_c is the crop coefficient (Allen et al. 1998), and A_n is the surface area of the model cell. The amount of water that must be supplied by agricultural providers is calculated by minimizing the evapotranspiration deficit (ET_d):

$$\min(ET_d) = ET_o K_c - ET_a. \tag{2}$$

A volumetric formulation for calculating the irrigation shortfall was presented by Niswonger (2020). This equation was adapted and modified to include an application factor (e_a) that enables the simulation of deficit and over-irrigation practices as follows:

$$Q_{c,i+1} = \left(Q_{c,i} + \frac{Q_{ET} - Q_{ET_{a,i}}}{\partial Q_{ET_{a,i}} / \partial Q_{c,i}} \right) * e_a, \tag{3}$$

where i is the outer iteration counter for a given MODFLOW timestep, Q_c is the calculated volumetric water demand, and Q_{ET_a} is the calculated volume of water available for evapotranspiration within the rooting zone. The volume of water available to be distributed from an agricultural provider $\left(Q_p\right)$ can be found with the relationship:

$$Q_p = \begin{cases} Q_p & Q_p \leq Q_{max} \\ Q_{max} & Q_p > Q_{max} \end{cases}, \tag{4}$$

where Q_{max} is the maximum user-supplied volumetric rate for an agricultural provider. Finally, the volume of water available to be moved from a provider to receivers (Q_A) is calculated as:

$$Q_A = \begin{cases} Q_{c,i+1} & Q_P > Q_{c,i+1} \\ Q_p & Q_P \leq Q_{c,i+1} \end{cases}. \tag{5}$$

Once Q_A is calculated, the irrigation flux that is applied to UZF receiver nodes (q_a) can be found from the relationship:

$$q_a = \frac{Q_A * e_i}{A_n}. \tag{6}$$

The irrigation efficiency factor (e_i) is used to account for losses due to inefficient transmission and irrigation methods (e.g., transmission losses due to evaporation, canopy interception, head losses, etc.). Irrigation losses (Q_L) simulated using e_i are calculated by

$$Q_L = (1 - e_i)\, Q_A, \tag{7}$$

and are removed from the model following Niswonger (2020).

In cases where q_a is greater than the vertical conductivity of the unsaturated zone, rejected infiltration calculated by the UZF Package can be routed to SFR reaches or LAK cells using the MVR Package (Langevin et al. 2017), which can be used to simulate irrigation return flows. In cases where a single provider supplies irrigation to multiple receiver nodes, q_a is split proportionally based on each receiver node's Q_{max} value.

Although the MODFLOW 6 API-Ag Package is based on the MODFLOW-NWT AG Package (Niswonger 2020), there are differences between the two approaches. The inclusion of the application factor (e_a) enables the simulation of both deficit and flush irrigation practices, which can be common in arid environments. The irrigation efficiency factor (e_i) in the API-Ag Package is inverse to the MODFLOW-NWT AG Package's definition of e_i. A value of 1 represents 100% irrigation efficiency in the API-Ag Package, whereas a value of 1 in the MODFLOW-NWT AG Package represents 0% irrigation efficiency. Surface-water providers represented with the SFR Package are represented as virtual diversions within API-Ag and transfer water from a given SFR reach without the need to alter or specify additional reaches within the SFR Package. This conceptualization can be used to represent a headgate that serves a specific field (or group of fields) and provides flexibility for specifying SFR Package agricultural providers, for example, a primary irrigation ditch with numerous headgates that divert from it. A user can also simulate surface-water transmission losses, such as evaporation from an irrigation canal or infiltration from an unlined canal, with the SFR Package by adding diversions to the existing stream network and specifying those reaches as agricultural providers.

Example Applications

Three example applications of the API-Ag Package are presented to illustrate the functionality of the package and validate results against the MODFLOW-NWT AG Package. The first example is a hypothetical basin with two small agricultural areas that are irrigated with a combination of surface water and groundwater. The second example is a modified version of the hypothetical Green Valley example problem, which has previously been presented in Prudic et al. (2004), Niswonger et al. (2006), and Niswonger (2020). The third example problem showcases the API-Ag Package with some of the advanced features in MODFLOW 6. The following sections describe the models and simulation results.

Agricultural Simulation Example 1

The first example application of the API-Ag Package is a simple 1 layer, 10 row, and 10 column model (Figure 1A). Four agricultural receiver cells (Figure 1A; green) are specified within the model and are grouped as two separate agricultural areas. These two groupings are referred to as irrigated area 1 (in model row 3) and irrigated area 2 (in model row 5). Each irrigated area is connected to two providers: an SFR reach (Figure 1; light blue) and a pumping well (represented by the WEL Package) that provides supplemental irrigation (Figure 1; red) when the SFR reach is unable to provide enough water to satisfy ET_d. Monthly average precipitation and potential evapotranspiration data from the California Irrigation Management Information System (CIMIS) station number 6 (California Department of Water Resources 2022) were

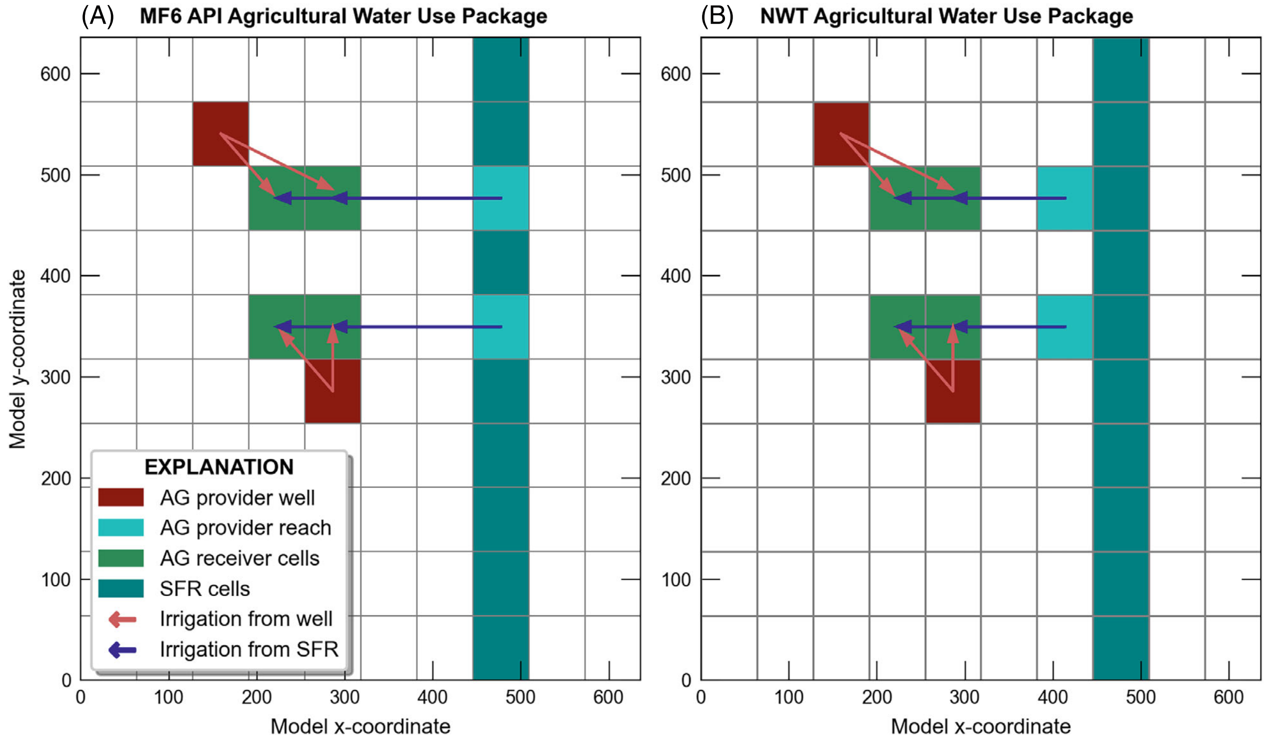

Figure 1. A conjunctive use example problem was developed for both the MODFLOW API Agricultural Water Use Package (API-Ag; A) and the MODFLOW-NWT Agricultural Water Use Package (AG; B). Differences in the Streamflow Routing (SFR) Package network are observed due to the simulation of diversions as "virtual links" in the API-Ag Package.

used to set evapotranspiration and precipitation parameters in the UZF Package. The model was run for 12 one-month stress periods, each of which has a daily time step. Starting head was set to 5 m below land surface elevation. A similar model was developed using the MODFLOW-NWT AG Package for comparison of the two simulation results (Figure 1B). Differences in stream network representations between MODFLOW 6 and MODFLOW-NWT are due to the API-Ag Package simulating diversions as virtual links, whereas diversions must be specified in the SFR Package for MODFLOW-NWT.

For the simulations, each agricultural area had different limitations set on maximum diversion rates ($Q_{\max}$) to test simulation of conjunctive use with surface-water diversions and groundwater pumpage. Irrigated area 1 had a maximum surface-water diversion rate of 20 m^3/day and irrigated area 2 had a maximum surface-water diversion rate of 10 m^3/day. The cumulative mass balance error in the simulation was 0.01%. Simulation results show excellent agreement between the API-Ag Package and the MODFLOW-NWT AG Package for each agricultural area. For each simulated agricultural area, correspondence with the MODFLOW-NWT irrigated volume has an r^2 value of 1.0 and a difference in irrigated water volume of 0.03 m^3 out of a total irrigated water volume of about 8996 m^3 ($\ll$0.01% difference) for the entire simulation period (Figure 2).

Agricultural Simulation Example 2

The hypothetical Green Valley example problem (Prudic et al. 2004; Niswonger et al. 2006; Niswonger 2020) was adapted as the second API-Ag Package example (Figure 3). The model represents a semi-arid alluvial basin where recharge is primarily driven by stream leakage. Water from Green Creek and Little Creek flows southward and flows into Blue River, which discharges near the southwestern corner of the model. The model has a rectilinear discretization and is composed of 1 layer, 15 rows, and 10 columns. As originally described in Niswonger (2020), six agricultural cells were specified adjacent to Green Creek (Figure 3). A single reach on Green Creek was specified as the surface-water provider for the agricultural receiver cells represented by the UZF Package. In addition, six wells provide supplemental irrigation when the SFR reach is unable to provide enough water to satisfy ET_{d}. The simulation was run three times, each with a separate application factor to evaluate the effects of deficit irrigation ($e_{\mathrm{a}} = 0.9$), optimal irrigation (base scenario; $e_{\mathrm{a}} = 1.0$), and over-irrigation ($e_{\mathrm{a}} = 1.1$).

Results from the base (optimal irrigation) scenario ($e_{\mathrm{a}} = 1.0$) were compared with the MODFLOW-NWT version of the model (Figure 4). The cumulative mass balance error for this model was 0.00%. Agricultural irrigation volumes from each simulation have an r^2 value of 1.0 with a difference in total volume of water used for irrigation of 0.7 m^3 out of about 525 m^3 for the entire simulation (0.1% difference). Total agricultural irrigation

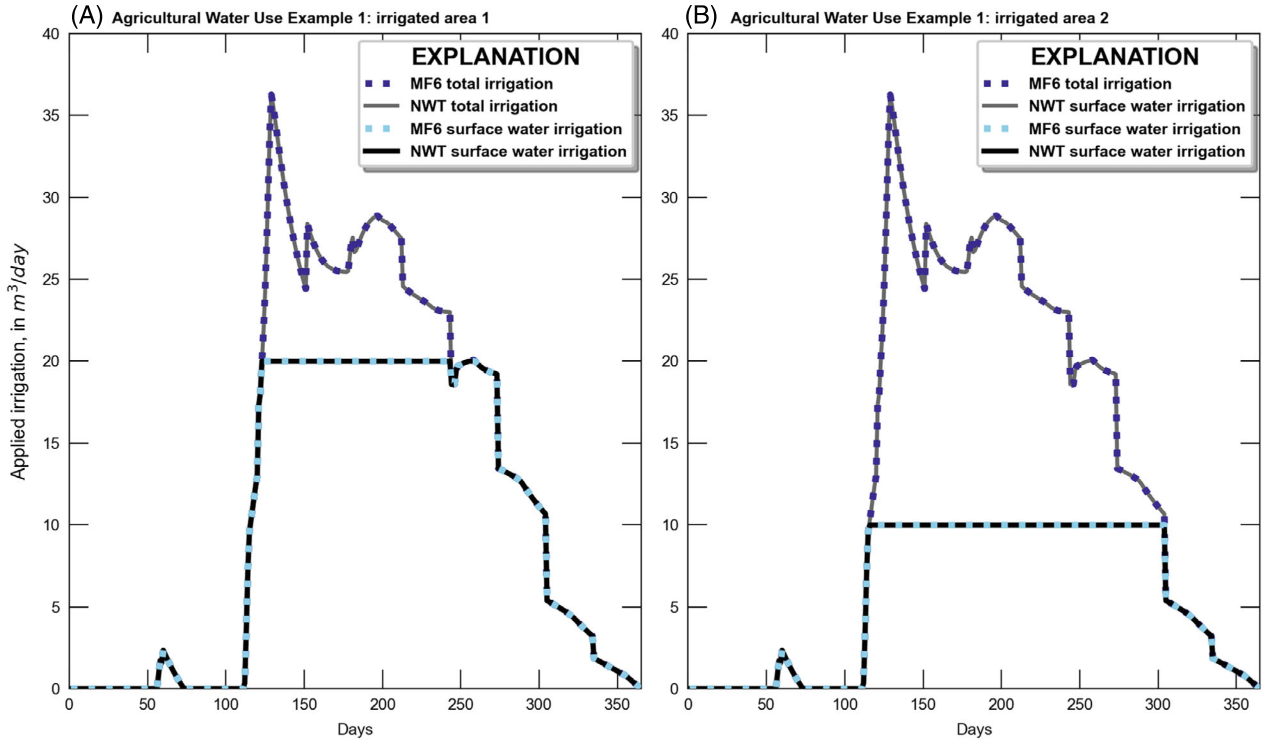

Figure 2. MODFLOW API Agricultural Water Use Package simulation results show excellent correspondence to simulation results from the MODFLOW-NWT Agricultural Water Use Package for both irrigated areas within the simulation (see Figure 1).

for the base scenario was about 526 m^3 (Figure 5). Total irrigation volumes for the deficit ($e_a = 0.9$) and over-irrigation ($e_a = 1.1$) scenarios were about 473 and 578 m^3, which is about a 10% change and was expected. Most of the additional water supplied to agricultural receiver cells in the over-irrigation scenario came from well providers, due to maximum diversion constraints imposed on the surface-water provider. Similarly, most of the reductions in irrigation demand that accompany the deficit irrigation scenario resulted in decreases in water provided to the well providers, and not the surface-water providers, due to ET_d being larger than the maximum surface-water diversion rate for ~100 days/year. The remainder of the year, ET_d was less than the maximum surface-water diversion rate and reductions in irrigation demand were realized by the surface-water providers.

Agricultural Simulation Example 3

The Green Valley example problem, shown in "Agricultural Simulation Example 2," was adapted into a 2-layer Voronoi grid discretization (Figure 6A). The model domain contains 470 cells per layer. In the northwest corner of the model, a lake was defined using the LAK Package and replaces a section of the SFR network. Agricultural receiver cells were defined by intersecting the Voronoi grid centroids with the previous example's agricultural receiver cells. Agricultural providers for this model include the lake and multi-aquifer wells (specified using the MAW Package). Other model inputs (e.g., horizontal hydraulic conductivity, model top) were resampled from the rectilinear discretization to the Voronoi grid using bilinear interpolation. The model was run for 13 stress periods, which corresponds to 1 cycle of updates to the UZF potential evapotranspiration and infiltration parameters.

Although the Voronoi grid representation of the Green Valley model is much different than the previous example, a comparison of irrigation volumes was made between the Voronoi grid representation of the API-Ag Package and the rectilinear MODFLOW-NWT version of the model shown in example 2 (Figure 6B). Before the comparison, the application factor was adjusted to 0.872 for the Voronoi grid model, because the number and total area of agricultural receiver cells in this example was larger than the previous example. The cumulative mass balance error reported by MODFLOW was 0%. The simulated total irrigation volume from the Voronoi Green Valley example problem was about 133 m^3 and the rectilinear MODFLOW-NWT model was about 131 m^3, which corresponds to a 1.3% difference in irrigated volume. Of note, surface-water irrigation provided from the LAK Package outlet was more than that provided by the SFR Package. The difference in irrigation volumes is due to irrigation diversion location. In example 2, irrigation was provided from Green Creek downstream of a diversion canal that routes available water to Little Creek and past the diversion location. Streamflow losses to the groundwater system before the diversion location in example 2 also contribute to the differences in surface-water irrigation volumes. Due to the

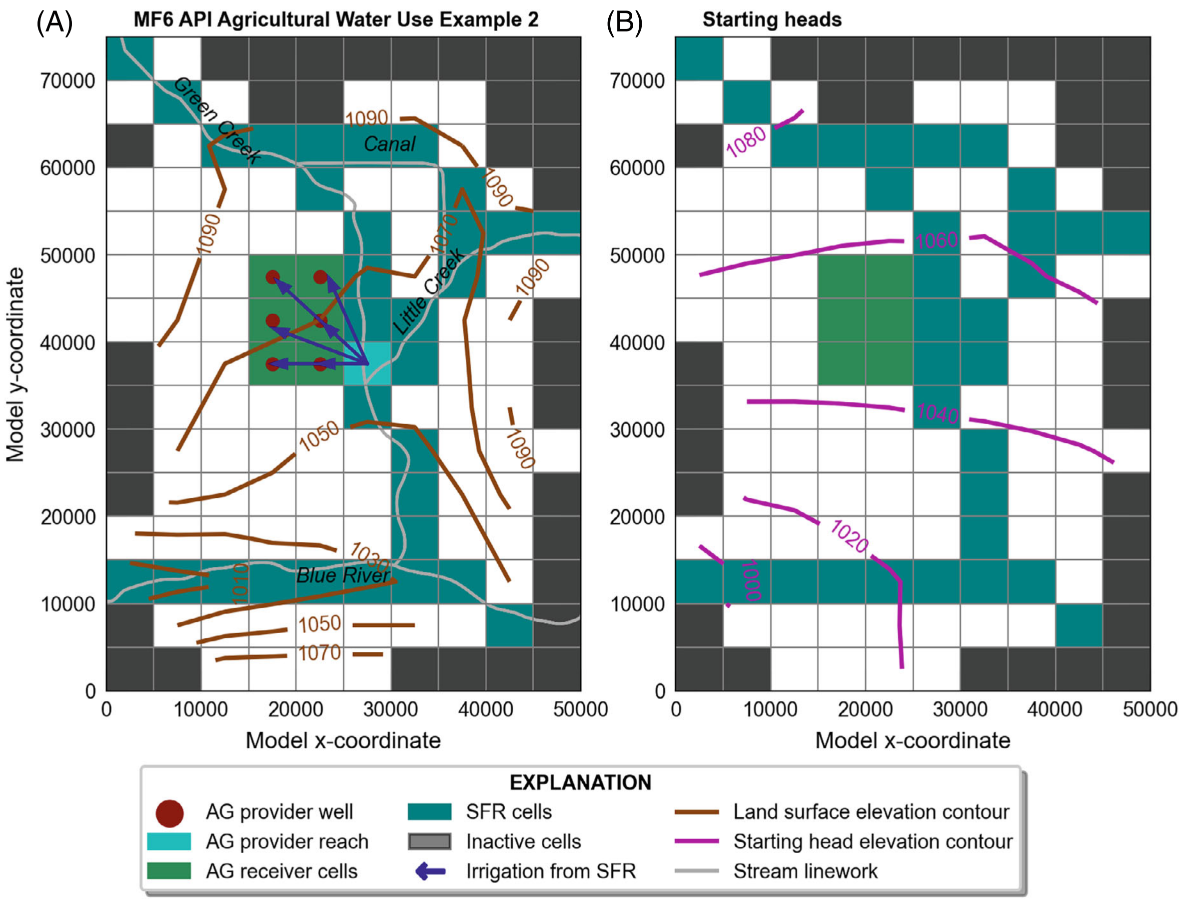

Figure 3. The Green Valley example problem (Prudic et al. 2004; Niswonger 2020) has been adapted for the MODFLOW API Agricultural Water Use Package (A). The adaptation presented here uses a virtual diversion link to supply surface-water irrigation to the agricultural cells. Starting head elevation contours are shown for the Green Valley example problem (B).

substantial differences in grid discretization and surface-water irrigation diversion location, no other comparisons were made.

Advantages and Limitations

The API-Ag Package was developed in Python and is coupled to MODFLOW 6 using the MODFLOW API. This coupling strategy allowed for rapid package development and testing because no changes to the MODFLOW 6 source code were needed. The API-Ag Package leverages the existing MVR Package behavior and replaces the MVR demand with the computed agricultural demand for each provider and receiver pair on each outer iteration. The design and structure of the Python package allows for iteration-level verification of equations. The approach also allows for future improvements or additional features to be easily integrated into API-Ag by future users without having to modify MODFLOW 6 source code. Moreover, the API-Ag Package is expected to be compatible with ongoing MODFLOW 6 development so that it can take advantage of new MODFLOW 6 features as they are released. The existing code improves upon an earlier approach by Niswonger (2020) by inverting the MODFLOW-NWT irrigation efficiency factor, incorporating an application factor, and by extending irrigation provider support to the MAW and LAK packages. The API-Ag Package also supports new features available in MODFLOW 6, such as the use of structured or unstructured grids, coupled flow and transport models, simulation of variable-density groundwater flow, and representation of full three-dimensional anisotropy (Provost et al. 2017).

The AG and the API-Ag Packages use a different scheme for representing evapotranspiration than the MODFLOW-OWHM Farm Process. In the Farm Process, the user can specify scale factors representing the split between crop covered area and bare soil that is used to partition evaporation from transpiration (Boyce et al. 2020). The API-Ag Package follows the approach presented by Niswonger (2020) and minimizes the difference between the user-supplied potential evapotranspiration and the actual evapotranspiration calculated by the UZF Package. The API-Ag package differs from the Farm Process in that it does not partition the actual evapotranspiration calculated by the UZF Package into evaporation and transpiration.

A limitation of the API-Ag Package is that conjunctive-use priority is fixed in the current version of the code. For example, when SFR and WEL both

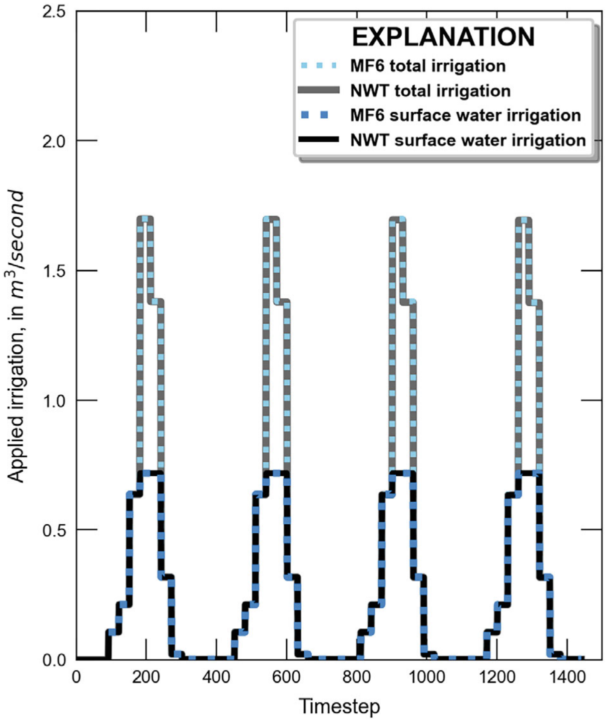

Figure 4. Simulated irrigation results from the MODFLOW API Agricultural Water Use Package Green Valley example problem show excellent correspondence ($r^2 = 1.0$) with the MODFLOW-NWT Agricultural Water Use Package.

provide water to the same irrigation receiver, SFR will provide water up to its maximum diversion rate before the WEL providing water. The irrigation priority for supported packages is LAK, SFR, MAW, and WEL. Future versions of the code could include methods for allowing the user to specify both irrigation provider priorities. Additionally, in complex agricultural systems (e.g., basins with water-rights allocation) irrigation priorities could be extended to agricultural receivers in future versions of the code.

Implementation of the API-Ag Package by leveraging the MVR Package and overriding its input through the MODFLOW API also has limitations. Q_P, Q_A, and Q_L must be calculated in Python and their values stored before adjusting the MVR Package's input values. The full output for these values is not easily accessible to the user in the MODFLOW list file or the binary cell budget file. The user could add observations using the MODFLOW OBS (Langevin et al. 2017) package to extract this information, but it would require additional user inputs to MODFLOW 6. Instead, this problem is solved by writing Q_P, Q_A, and Q_L directly to a separate ascii output file from the Python code. An additional limitation is that the irrigation demand is calculated in Python. While Python code can be written to be efficient, in certain cases it can be much slower than compiled code. However, given these limitations, the API-Ag Package provides a protype for future development and integration of agricultural processes into the MODFLOW source code.

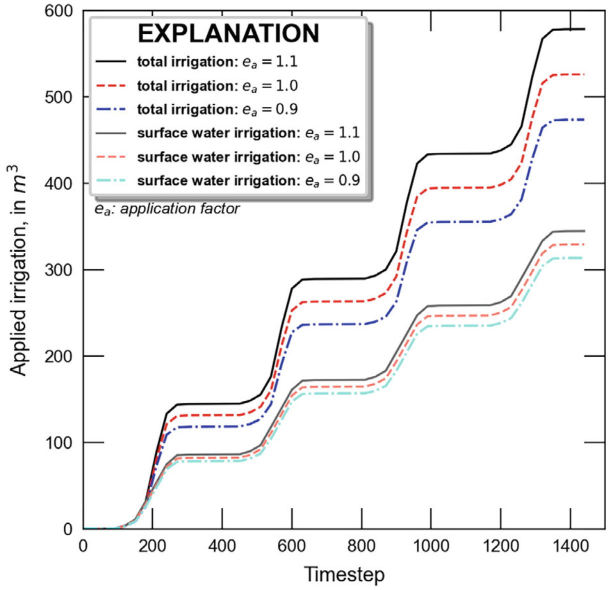

Figure 5. Cumulative infiltration profiles for three application factors (e_a) scenarios show that differences in total irrigation are primarily driven by supplementary groundwater pumping due to maximum irrigation constraints placed on the diversion.

Summary

A new approach for simulating irrigated agriculture was developed for MODFLOW 6 through the MODFLOW API. The MODFLOW API Agricultural Water Use Package is an installable Python package that leverages functionality from FloPy (Bakker et al. 2016, 2022) and the Water Mover Package (Langevin et al. 2017; Morway et al. 2021). Representation of agricultural processes within a MODFLOW 6 simulation is based on the MODFLOW-NWT AG Package (Niswonger 2020). The Agricultural Water Use Package improves on the MODFLOW-NWT AG approach by incorporating an application factor that allows simulation of deficit and over-irrigation. Additionally, the Agricultural Water Use Package extends irrigation provider support to the Multi-Aquifer Well and Lake Packages (Langevin et al. 2017).

Three example problems were presented that compared results from the MODFLOW API Agricultural Water Use Package to the previous approach. Example problems 1 and 2 were validated against the MODFLOW-NWT Agricultural Water Use Package and had excellent correspondence. In example problem 1, the measured difference between the two models total irrigated volumes was $0.03\,m^3$, and correspondence between applied irrigation had an r^2 value of 1.0. In example problem 2, the difference between total irrigated volumes was $0.7\,m^3$, and correspondence between applied irrigation values had an r^2 of 1.0. The third example problem adapted the Green Valley model as a Voronoi grid representation and showed irrigation from irrigation providers that were not available for use with the MODFLOW-NWT AG Package. Although there were substantial differences between the Voronoi grid representation and the MODFLOW-NWT

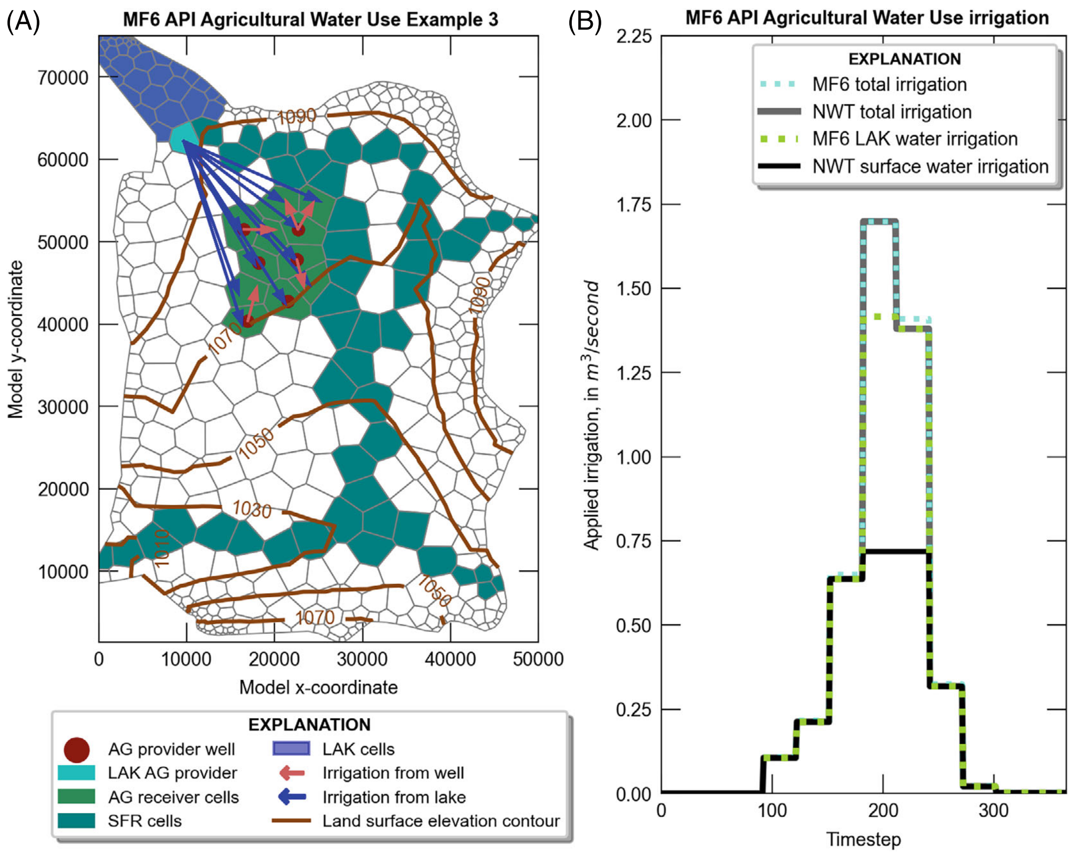

Figure 6. The Green Valley example problem (Prudic et al. 2004; Niswonger 2020) was adapted to a Voronoi grid discretization and modified to include lake (LAK) cells in the northwestern part of the model and to use multi-aquifer wells (MAW) as agricultural providers (A). Hand adjustments to the application factor allowed for a comparison between the MODFLOW-NWT irrigation volume and the modified example's irrigation volume (B).

version, with calibration of the application factor the difference between the total irrigation volumes of the two models was 2 m^3.

The MODFLOW API Agricultural Water Use Package is open source and can be downloaded from https://code.usgs.gov/cawsc/modflow-api-ag-package. This repository contains the source code, example problems, installation instructions, and documentation for the package.

DATA AVAILABILITY STATEMENT

The source code, examples, and data that support this study are openly available at https://doi.org/10.5066/P9K6UW9F

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