MODFLOW 6 GWE and API: New possibilities for modeling geothermal systems and heat pumps

Dávid Krčmář, Kamila Hodasová, Martin Zatlakovič, Natália Bahnová & Ivana Ondrejková

Comenius University Bratislava, Faculty of Natural Sciences, Department of Engineering Geology, Hydrogeology and Applied Geophysics, Ilkovičova 6, 842 15 Bratislava, Slovakia; david.krcmar@uniba.sk

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Abstract: Accurate numerical simulation of subsurface heat transport is fundamental for the design and management of shallow geothermal systems, such as Aquifer Thermal Energy Storage (ATES) and Borehole Heat Exchangers (BHEs). Historically, groundwater heat transport was modeled using solute-transport codes (e.g., MT3DMS) by applying mathematical analogies between mass and energy conservation equations. While functional, this proxy approach relied on calculating equivalent retardation factors to mimic thermal storage in the solid matrix and struggled to accurately represent heat conduction in unsaturated or hydraulically inactive zones. This paper reviews the transition to the newly released Groundwater Energy (GWE) code for MODFLOW 6, which provides a rigorous, physically based formulation for simulating heat transport through both fluid and solid phases. Furthermore, we demonstrate the transformative capabilities of the MODFLOW 6 Application Programming Interface (API) for overcoming the limitations of traditional file-based simulations. Through a case study of a geothermal well doublet, we show how the API's Extended Model Interface (XMI) enables dynamic feedback loops, allowing for the simulation of heat pumps operating with a constant temperature difference () rather than fixed injection temperatures. The results illustrate that coupling the explicit physics of the GWE code with the flexible control of the API significantly improves simulation accuracy and offers new possibilities for optimizing geothermal system operations under transient conditions.

Key words: subsurface heat transport, shallow geothermal energy, Aquifer Thermal Energy Storage (ATES), MODFLOW 6 GWE, Python API

1. INTRODUCTION

Subsurface heat transport has emerged as a critical frontier in hydrogeological research, driven by the accelerating global demand for renewable energy sources and the urgent need to understand the thermal dynamics of groundwater systems under changing climatic conditions. The subsurface is no longer viewed merely as a reservoir for drinking water; it is increasingly recognized as a thermal battery capable of decarbonizing heating and cooling sectors. Consequently, the ability to accurately model temperature variations within porous media is essential for designing efficient Aquifer Thermal Energy Storage (ATES) systems, managing shallow geothermal installations such as Borehole Heat Exchangers (BHEs), and assessing the ecological impacts of anthropogenic thermal anomalies on aquatic ecosystems (Morway et al., 2025). As the scale of geothermal utilization expands from single residential units to city-wide district heating networks, numerical modeling has become an indispensable tool for predicting system performance, optimizing well placement, and preventing thermal interference (Casasso, 2024).

Evolution of Modeling Capabilities

Historically, the hydrogeological community faced a scarcity of dedicated codes for simulating heat transport. To overcome this, researchers adapted well established solute-transport models, most notably MT3DMS and standard MODFLOW packages to solve the energy equation. This approach relies on the mathematical analogy between the advection-dispersion equation (ADE) for mass transport and the energy transport equation for heat (Langevin et al., 2010; Hecht-Méndez et al., 2010). In this "proxy" methodology, temperature is treated as a chemical species concentration, while the retardation factor is redefined to represent the ratio of the volumetric heat capacity of the solid matrix to that of the fluid. Specifically, the distribution coefficient () in the chemical reaction package is utilized to simulate the thermal inertia of the aquifer skeleton, effectively slowing the thermal front relative to the hydraulic velocity (Thorne et al., 2006).

While functional for basic scenarios, this proxy-based approach imposes significant limitations and requires extensive pre- and post-processing. Users must manually calculate "equivalent" parameters, converting thermal conductivity into diffusion coefficients and heat sources into mass fluxes. Furthermore, standard solute transport codes often struggle to account for complex, non-linear variations in thermal properties, particularly in the unsaturated zone (UZ) or under transient flow conditions where water content fluctuates (Morway et al., 2022). Despite these challenges, early integrated approaches, such as SEAWAT Version 4, marked a significant step forward by introducing capabilities to simulate simultaneous multispecies solute and heat transport, coupled with fluid density and viscosity variations (Langevin et al., 2008). These tools were validated against classic benchmarks, such as the Henry and Hilleke experiment, establishing a foundation for density-dependent thermal modeling (Langevin et al., 2010).

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Advances in Geothermal System Simulation

A major focus of recent literature has been the simulation of shallow geothermal systems, specifically the interaction between BHEs and the surrounding aquifer. Modeling these systems presents a unique computational challenge due to the huge scale disparity between the borehole diameter (centimeters) and the regional flow field (kilometers). To address this, researchers have moved beyond standard finite difference grids, adopting the Connected Linear Network (CLN) package within MODFLOW-USG. This methodology allows for the efficient simulation of vertical closed loop U pipes and multiple BHEs without the prohibitive computational cost of extremely fine discretization (Antelmi et al., 2021). Such approaches have been successfully applied to evaluate thermal perturbations in complex urban environments, for example in Milan, where the dense concentration of open loop and closed loop systems requires careful management to avoid thermal feedback and degradation of efficiency (Barbieri et al., 2022; Barbieri et al., 2025).

Furthermore, the integration of local heat transfer processes with field scale transport models has improved the prediction of dynamic heat pump efficiency. Coupling analytical borehole solutions with transport codes like MT3DMS has enabled the simulation of dynamic fluid temperatures (Zong et al., 2023). At the urban planning scale, agent-based modeling integrated with MODFLOW MT3DMS has been employed to investigate subsurface interactions between multiple ATES systems. These studies demonstrate that optimized well placement policies can maximize greenhouse gas emission reductions while maintaining individual system performance (Beernink et al., 2022). Additionally, innovative approaches now combine numerical modeling with machine learning algorithms to optimize ATES operations in depleted hydrocarbon reservoirs, significantly reducing computational time while maintaining high predictive accuracy (Abdulhaq et al., 2025).

Beyond energy extraction, heat acts as a robust natural tracer for characterizing hydrogeological parameters and surface water-groundwater interactions. Temperature profiles have been used to estimate vertical exchange fluxes in riverbeds, although studies suggest that 1D analytical solutions often underestimate total exchange fluxes compared to fully 3D numerical models when lateral flow is significant (Ghysels et al., 2021). In complex geological settings, such as karst aquifers, process based discrete continuum models (e.g., MODFLOW-CFPv2) have been used to jointly invert hydraulic, thermal, and chemical signals. These studies indicate that thermographs often contain more information about conduit geometry and transport properties than chemographs alone (Birk et al., 2006; Kavousi et al., 2020; Kavousi et al., 2023).

MODFLOW 6 GWE

Recognizing the limitations of proxy methods and the growing necessity for precise thermal modeling, the U.S. Geological Survey has recently introduced the Groundwater Energy (GWE) code for MODFLOW 6 (Morway et al., 2025). This represents a paradigm shift from ad-hoc adaptations to a rigorous, physically based formulation. The GWE code solves the energy transport equation directly, assuming Local Thermal Equilibrium (LTE) between the fluid and the porous matrix.

List of Symbols and Abbreviations

- c ($\mathrm{kg \cdot m^{-3}}$): Solute concentration
- C_m ($\mathrm{J \cdot m^{-3} \cdot K^{-1}}$): Volumetric heat capacity of the saturated porous medium (aquifer)
- c_s ($\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$): Specific heat capacity of the solid matrix
- C_w ($\mathrm{J \cdot m^{-3} \cdot K^{-1}}$): Volumetric heat capacity of water
- c_w ($\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$): Specific heat capacity of water
- D_h ($\mathrm{m^2 \cdot s^{-1}}$): Hydrodynamic dispersion tensor
- D_t ($\mathrm{m^2 \cdot s^{-1}}$): Thermal dispersion tensor
- $D_{t,diff}$ ($\mathrm{m^2 \cdot s^{-1}}$): Thermal diffusion coefficient
- ϵ (dimensionless): Porosity
- K_d ($\mathrm{m^3 \cdot kg^{-1}}$): Distribution coefficient
- λ_{bulk} ($\mathrm{W \cdot m^{-1} \cdot K^{-1}}$): Bulk thermal conductivity tensor
- λ_c ($\mathrm{s^{-1}}$): Decay coefficient (for solute)
- λ_s ($\mathrm{W \cdot m^{-1} \cdot K^{-1}}$): Thermal conductivity of the solid material
- λ_{vert} ($\mathrm{W \cdot m^{-1} \cdot K^{-1}}$): Effective vertical thermal conductivity of the overburden
- λ_w ($\mathrm{W \cdot m^{-1} \cdot K^{-1}}$): Thermal conductivity of water
- m (m): Aquifer thickness
- P_c ($\mathrm{kg \cdot m^{-3} \cdot s^{-1}}$): Source/sink term for the solute
- ϕ (dimensionless): Effective porosity
- ϕ_{cm} (dimensionless): Equivalent porosity
- P_t ($\mathrm{W \cdot m^{-3}}$): Heat source/sink term
- q ($\mathrm{m \cdot s^{-1}}$): Specific discharge or Darcy velocity vector
- q_E ($\mathrm{W \cdot m^{-3}}$): Energy source/sink term
- ρ_s ($\mathrm{kg \cdot m^{-3}}$): Density of the solid matrix
- ρ_w ($\mathrm{kg \cdot m^{-3}}$): Density of water
- T (K): Temperature
- ΔT (K): Temperature difference
- T_{rel} (K): Relative temperature ($T - T_{surface}$)
- v ($\mathrm{m \cdot s^{-1}}$): Fluid velocity vector

Unlike previous iterations, GWE is designed to run simultaneously with the Groundwater Flow (GWF) code on structured, vertex based, or unstructured grids (DIS, DISV, DISU), offering unprecedented flexibility for complex geometries (Langevin et al., 2022). It explicitly accounts for heat conduction, advection, and dispersion, treating thermal conductivity as a bulk parameter derived from volume weighted averages of the fluid and solid phases. This dedicated framework eliminates the need for parameter scaling and provides a standardized platform for simulating everything from deep geothermal doublets to the thermal buffering capacity of the unsaturated zone (Morway et al., 2023).

Static Models vs. Dynamic Systems

Despite these advancements in governing equations and grid flexibility, a fundamental gap remains in the operational simulation of geothermal systems. Traditional modeling workflows rely on static input files where boundary conditions such as injection temperatures or pumping rates are defined *a priori* for specific stress periods. However, real world geothermal systems, particularly heat pumps and ATES doublets, operate dynamically. The operation of a heat pump is governed by feedback loops: the injection temperature is rarely a fixed value; rather, it is a function of the extraction temperature and the instantaneous load of the building (e.g., a constant operation).

In a standard file based MODFLOW simulation, representing this feedback is problematic. If thermal breakthrough occurs and the extraction temperature rises, a standard model continues to inject water at the predefined temperature, failing to adjust the injection parameters in response to the changing system state. This limitation inhibits the accurate simulation of long-term system efficiency and thermal plume evolution, as it disconnects the subsurface model from the operational logic of the surface infrastructure.

Objectives and Scope

This paper explores the new possibilities offered by the MODFLOW 6 framework to bridge this gap. We aim to demonstrate the transition from traditional proxy-based modeling to the dedicated GWE code and to highlight the transformative potential of the MODFLOW 6 Application Programming Interface (API). By utilizing the Basic Model Interface (BMI, Hutton et al., 2020) and Extended Model Interface (XMI), we show how models can be coupled with external logic to simulate dynamic feedback loops that were previously impossible with static input files (Hughes et al., 2022).

To achieve these aims, the study first provides a synthesis of the transition from solute analogous heat transport modeling to the explicit GWE formulation. Furthermore, we demonstrate the implementation of the MODFLOW 6 API for controlling GWE simulations. Finally, we present a case study of a geothermal doublet where the API is used to enforce a dynamic temperature boundary condition (constant ΔT), illustrating the accuracy of this approach over traditional static modeling. By integrating the rigorous physics of the GWE code with the flexible control of the API, this work provides a roadmap for the next generation of hydrothermal simulations, capable of supporting the complex design requirements of modern geothermal energy systems.

2. THEORETICAL BACKGROUND: THE EVOLUTION OF HEAT TRANSPORT MODELING

The simulation of heat transport processes in subsurface environments has historically relied on numerical techniques primarily developed for solute transport, adapted for geothermal systems and aquifer heat storage. The numerical solution of the advective and conductive heat transport problem in porous media, encompassing both saturated and unsaturated zones, requires robust discretization strategies.

The foundational approach employed in early models was the Finite Difference Method (FDM). In this framework, the solution domain is discretized into prismatic cells linear for one dimensional problem and rectangular for two dimensional scenarios. The mean temperature, , assigned to the cell center, is calculated based on the physical heat balance expressed over all surfaces using linear approximations for advective, diffusive, and dispersive heat fluxes.

Time integration schemes in FDM have typically oscillated between explicit and implicit formulations. Explicit schemes, where fluxes are evaluated at the previous time level, must strictly satisfy stability criteria to prevent numerical oscillations. Specifically, the von Neumann criterion requires that diffusive and dispersive fluxes into any cell remain smaller than the rate of energy change within that cell. Furthermore, to mitigate numerical diffusion and oscillations, spatial and temporal discretization is constrained by the thermal grid Péclet number ( ) and the Courant number ( ). Alternatively, fully implicit or time centered Crank Nicolson schemes have been used, resulting in systems of linear equations typically solved using iterative techniques such as the biconjugate gradient solver.

For domains exhibiting irregular boundaries or requiring local refinement, the Finite Element Method (FEM) and Finite Volume Method (FVM) offered superior geometric flexibility. FEM discretizes the domain into elements (triangles, tetrahedra) using linear interpolation functions and applies the weighted residual method (Galerkin) to minimize errors (Mercer et al., 1975). Conversely, FVM divides the domain into small convex finite volumes, utilizing Gauss's divergence theorem to ensure that the sum of inflowing fluxes equals the rate of energy change within the volume (Russell et al., 2003; Rühaak et al., 2008).

To address advection dominated problems where standard methods suffer from numerical dispersion, operator splitting techniques such as the Method of Characteristics (MOC) and Random Walk were employed. MOC separates the transport step into a purely advective half step, solved via particle tracking, and a diffusive/dispersive half step. The Random Walk method simulates dispersion stochastically, displacing particles based on the velocity field and normally distributed random numbers (Kinzelbach & Uffink, 1991; Chevalier & Banton, 1999).

Prior to the release of dedicated heat transport codes within the MODFLOW suite, the utilization of existing numerical codes designed for solute transport (e.g., MT3DMS, FEFLOW in solute mode) was a common practice. This method exploits the mathematical isomorphism between the advection-dispersion equation for mass transport and the equation for energy transport in porous media.

To implement this analogy, a consistent mapping of physical parameters is required. The steady state solute transport equation with first order decay is defined as:

$$\nabla \cdot [D_h \nabla c] - \nabla \cdot [\mathbf{q}c] + P_c - \lambda_c c = 0 \quad (1)$$

This equation is compared to the steady state heat transport equation in a shallow regional aquifer for relative temperature $T_{rel} = T - T_{surface}$:

$$\nabla \cdot [D_t \nabla T_{rel}] - \nabla \cdot \left[\mathbf{q}\frac{C_w}{C_m}T_{rel}\right] + \frac{P_t}{C_m} - \frac{\lambda_{vert}}{C_m m}(T_{rel}) = 0 \quad (2)$$

By comparing the individual terms, specific equivalence relationships were established. The solute concentration corresponds to the relative temperature T_{rel}. Since concentration cannot be negative, T_{rel} represents the temperature increase relative to a reference value. In the solute equation, advection velocity is $\mathbf{q}/\phi$, whereas in the heat equation, the thermal front moves at a velocity determined by the ratio of heat capacities. To simulate thermal retardation without explicit retardation factors, an "equivalent porosity" ϕ_{cm} was defined as:

$$\phi_{cm} = \phi \frac{C_m}{C_w} \quad (3)$$

Additionally, the molecular diffusion coefficient is replaced by the thermal diffusion coefficient ($D_{t,diff} = \lambda_m / C_m$), and longitudinal/transverse dispersivities are mapped directly to thermal dispersivities. Vertical heat loss through the overburden is treated mathematically as first-order decay, with the equivalent decay coefficient calculated based on λ_{vert}, aquifer thickness, and depth to groundwater.

While the analogy described above allowed for heat transport simulation in codes like MT3DMS, it required the calculation of conforming coefficients. The retardation factor R in solute transport was used to mimic the thermal inertia of the solid matrix. In the Chemical Reaction Package of MT3DMS, this was implemented by defining a distribution coefficient K_d for a linear isotherm:

$$K_d = \frac{c_s}{\rho_w c_w} \quad (4)$$

Note that the produ $\rho_w c_w$ represents the volumetric heat capacity. Similarly, energy input/extraction rates had to be converted into equivalent mass-loading sources to maintain dimensional consistency, treating Temperature (K) as Concentration ($kg.m^{-3}$). While ingenious, this proxy approach was prone to errors during parameter conversion and lacked the rigorous physical representation of thermodynamic properties, particularly when dealing with transient density-dependent flows or unsaturated zones (Morway et al., 2022).

3. THE MODFLOW 6 GROUNDWATER ENERGY (GWE) MODEL

The Groundwater Energy (GWE) code represents a newly developed component of the MODFLOW 6 hydrologic simulator, explicitly designed to address the limitations of the proxy approach. Unlike previous methods that treated temperature as a chemical species, GWE introduces a dedicated "model type" that runs simultaneously with the Groundwater Flow (GWF) model. It accounts for heat conduction, advection, and dispersion, assuming Local Thermal Equilibrium (LTE) between the fluid and the solid matrix, meaning the temperature of the groundwater (T_w) and the porous matrix (T_s) are equal at any given point (Langevin et al., 2022; Morway et al., 2025).

The core of the GWE code is the energy transport equation derived from the principle of conservation of energy. According to Morway et al. (2025), the governing equation solved by GWE is:

$$\frac{\partial}{\partial t}\left[\epsilon\rho_w c_w + (1-\epsilon)\rho_s c_s\right]T + \nabla \cdot (\epsilon\rho_w c_w \mathbf{v}T) - \nabla \cdot (\lambda_{bulk}\nabla T) = q_E \quad (5)$$

Unlike the proxy methods, GWE explicitly handles the bulk properties of the aquifer. The term within the time derivative represents the bulk heat storage capacity. Similarly, thermal conductivity is treated as an effective bulk parameter, calculated as the volume-weighted average of the fluid and solid conductivities:

$$\lambda_{bulk} = \epsilon\lambda_w + (1-\epsilon)\lambda_s \quad (6)$$

This direct formulation ensures accurate mass and energy balance without the need for manual parameter scaling (Langevin et al., 2022).

Modules and Packages

Consistent with the modular architecture of MODFLOW 6, the GWE code utilizes specific packages to represent physical processes. These packages mirror the structure of the Groundwater Transport (GWT) code but are parameterized strictly for energy:

- **GWE-ADV (Advection Package):** Simulates the transport of heat via moving groundwater using flow fields calculated by the coupled GWF model.
- **GWE-CND (Conduction Package):** Represents thermal conduction through the aquifer (both water and solid matrix) driven by temperature gradients (Fourier's Law). This replaces the "Diffusion" package found in solute transport models.
- **GWE-EST (Energy Storage Package):** Defines the heat capacity and density of water and aquifer solids to calculate changes in stored energy over time.
- **GWE-SSM (Source Sink Mixing):** Handles energy inflow/outflow associated with standard flow boundary conditions, such as wells, drains, or rivers.

A significant advantage of the GWE code is its support for flexible geometry through the **GWE-DIS** packages. It supports structured (DIS), vertex-based (DISV), and unstructured

(DISU) grids. This capability is critical for geothermal applications, allowing for local mesh refinement around BHEs or complex geological features without the computational burden of globally fine grids (Morway et al., 2025). Furthermore, through coupling with advanced stress packages, GWE can simulate temperature regimes in lakes, streams, and the unsaturated zone, providing a holistic tool for thermal budget analysis.

4. THE MODFLOW 6 API

The MODFLOW 6 Application Programming Interface (API) marks a significant advancement in how groundwater models interact with external software. Unlike previous versions that relied heavily on file based coupling or monolithic code integration, MODFLOW 6 utilizes the Basic Model Interface (BMI) and the Extended Model Interface (XMI) to allow direct memory access and simulation control (Hughes et al., 2022). This architecture provides a robust framework for coupling heat transport simulations with external systems, such as geothermal plants or building energy models, and for performing advanced optimization tasks that require iterative feedback.

The core of the MODFLOW API is built upon standard BMI conventions, refactoring MODFLOW into a shared library (libmf6) that exposes standard functions for initialization, updating, and finalization. Crucially for heat transport applications, the API implements the Extended Model Interface (XMI). While standard BMI allows for time step coupling, XMI exposes the inner nonlinear convergence loop (Picard iterations). This capability allows external programs to modify model variables such as temperature boundary conditions or heat injection rates during the solution process of a single time step, ensuring numerical stability and rigorous coupling without the need for costly restarts (Hughes et al., 2022).

The integration of the Groundwater Energy (GWE) code into the MODFLOW 6 framework means it inherently supports all API functionalities available to the Flow (GWF) and Transport (GWT) models (Morway et al., 2025). To interact with the GWE code via the API, users address specific memory locations. For instance, the dependent variable, temperature ( ), can be accessed using the address GWE/X. Similarly, boundary condition parameters, such as the temperature of injected water in a well package, can be modified dynamically. This allows for the implementation of time varying heat injection controls that respond to the model's state, a feature critical for simulating systems with dynamic operational logic.

The API facilitates several advanced coupling capabilities:

• **Coupling with Surface Energy Systems:** Subsurface GWE models can be coupled with surface energy simulations (e.g., HVAC systems). An external script can calculate the building load and use *set_value* to update the injection temperature in the GWE code within the current time step.

• **Dynamic Feedback Loops:** Users can implement custom feedback loops that are not natively supported. For example, reading the simulated temperature field, applying a custom constitutive relationship to calculate temperature dependent properties, and updating matrix coefficients before the next iteration.

• **Optimization:** The API enables running the GWE code repeatedly without the necessity of reading and writing input files, making it ideal for optimization algorithms that iteratively adjust heat exchanger locations or pumping rates (Hughes et al., 2022).

5. DEMONSTRATION CASE STUDY: DYNAMIC FEEDBACK IN GEOTHERMAL SYSTEMS

To demonstrate the practical advantages of the API over traditional modeling workflows, we present a case study of a geothermal well doublet used for a heat pump system. This example highlights how dynamic feedback loops, enabled by the API, solve limitations inherent in static file-based simulations.

The system consists of an extraction (production) well and an injection (infiltration) well installed in a shallow aquifer. Groundwater is extracted, heated by a constant temperature difference (K) via a heat exchanger, and reinjected into the aquifer. This setup mimics a typical groundwater heat pump operating in heating mode, where the reinjected water is colder, or cooling mode, where it is warmer. For this demonstration, we simulate a heat injection scenario.

In standard "file-based" modeling workflows, boundary conditions must be defined *a priori*. For injection wells using the GWE-SSM package, the user must specify a concrete temperature value for every stress period. For example, the input file might define that from day 0 to day 365, the injection temperature is fixed at 15C.

This static definition creates a fundamental physical contradiction when thermal breakthrough occurs. If the thermal plume from the injection well migrates back to the extraction well, the extraction temperature ( ) rises (e.g., from 10C to 12C). A standard model, unaware of this change, continues to inject water at the predefined 15C. Consequently, the simulated temperature difference ( ) drops from 5 K to 3 K. This effectively simulates a heat pump with degrading performance, contradicting the operational reality where the system would maintain a constant by increasing the injection temperature to 17C. Standard MODFLOW execution lacks the internal mechanism to transfer data between boundary conditions (i.e., read and update) within a single time step.

Using the MODFLOW 6 API, we established a dynamic feedback loop to update boundary conditions at every time step during the simulation runtime. The logic proceeds as follows:

1. The current temperature at the extraction well ( ) is retrieved from the model memory using *get_value*.
2. The new injection temperature is calculated as (where K).
3. The source temperature for the injection well is updated using *set_value* before the solution advances to the next time step.

This approach was implemented using the xmipy Python wrapper, effectively bypassing the limitations of static input files.

A comparison of the thermal plumes reveals a significant difference in the extent and intensity of the thermal impact. In the

dynamic API-controlled simulation (Figure 1A), the thermal plume exhibits a larger spatial extent and higher temperatures compared to the traditional static approach (Figure 1B). This discrepancy is a direct physical consequence of the constant energy input maintained by the API. In the dynamic model, as the extraction temperature rises due to thermal breakthrough, the injection temperature is automatically increased to preserve the K condition. This results in a continuous and consistent injection of thermal energy into the aquifer.

Conversely, in the static model (Figure 1B), the injection temperature remains fixed despite the rising extraction temperature. As the temperature of the extracted water approaches the injection temperature, the effective of the system diminishes (K). This leads to a progressive reduction in the amount of thermal energy being injected into the aquifer over time.

Consequently, the traditional static approach underestimates the long-term thermal impact on the groundwater system, predicting a smaller and cooler plume than would occur in a real-world system operating under constant load conditions.

The quantitative advantage of the API approach is further demonstrated in Fig. 2, which compares the temperature evolution over time.

In the **traditional static model** (dashed lines in Figure 2), the fixed injection temperature causes the temperature difference to collapse as recirculation intensifies. In contrast, the **API-controlled simulation** (solid lines in Fig. 2) accurately maintains the operational parameters, predicting a higher total heat input and providing a more realistic basis for assessing environmental risks and system sustainability.

Explanations: The color gradient represents the temperature distribution, highlighting the migration of the heated front (thermal breakthrough) from the injection well toward the extraction well. A) This picture presents the new dynamic approach using MODFLOW 6 API, where a feedback loop adjusts injection temperature to maintain a constant ΔT. B) The traditional static approach (without API), where injection temperature is fixed regardless of extraction temperature changes.

Explanations: The dashed lines represent a standard

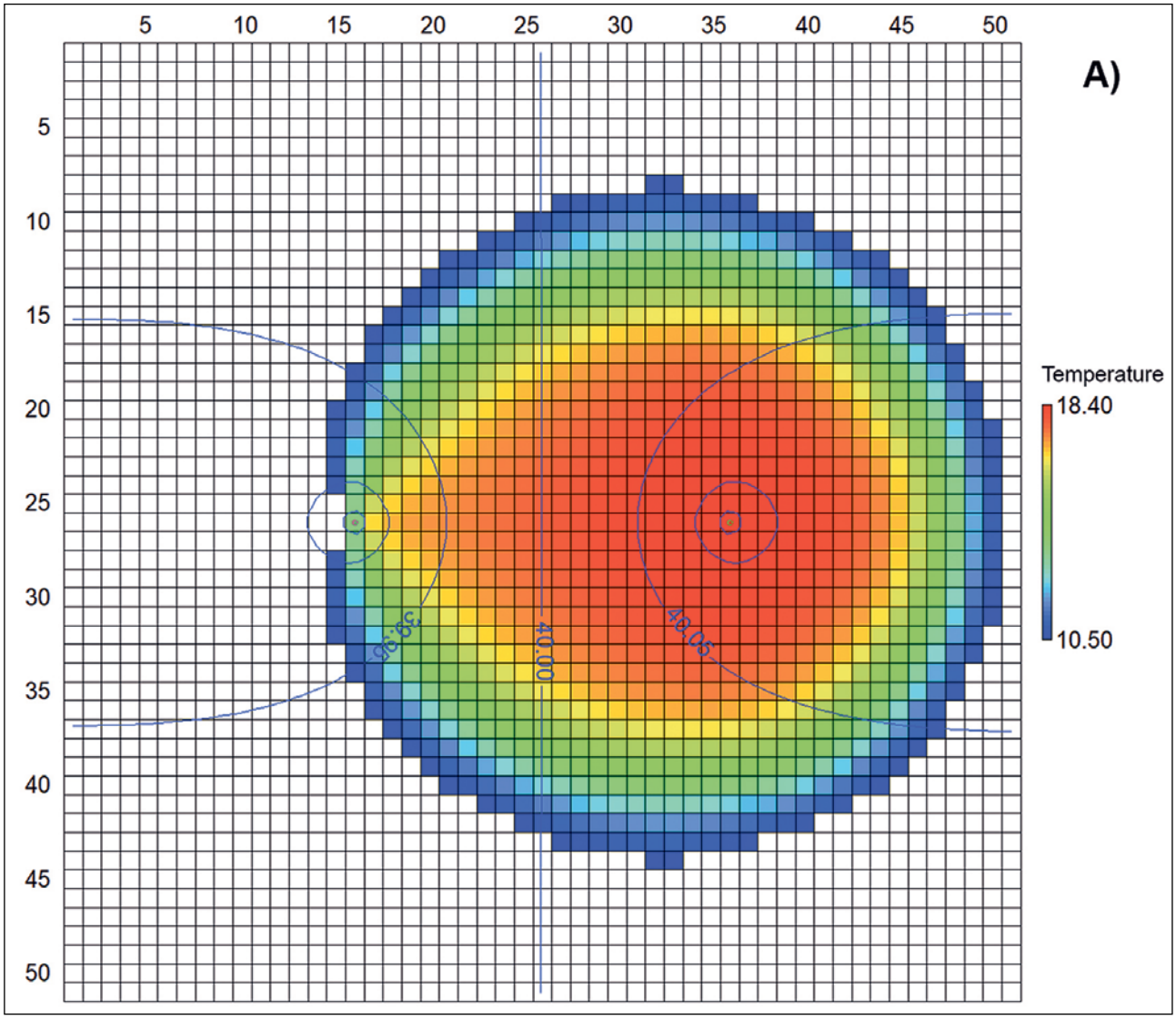

Fig. 1 illustrates the spatial distribution of the thermal plume for both simulation approaches. Over time, the heated water migrates from the injection well back toward the extraction well, leading to thermal interference (thermal breakthrough).

MODFLOW 6 simulation with fixed boundary conditions: as thermal breakthrough occurs and extraction temperature (blue dashed) rises, the static injection temperature (red dashed) remains constant at 15 °C, causing the system's thermal efficiency (ΔT) to degrade. In contrast, the solid lines show the API-controlled simulation where (red solid) is dynamically adjusted at each time step based on the simulated (blue solid) to maintain a constant temperature difference (ΔT = 5 K), accurately reflecting the operational logic of a heat pump.

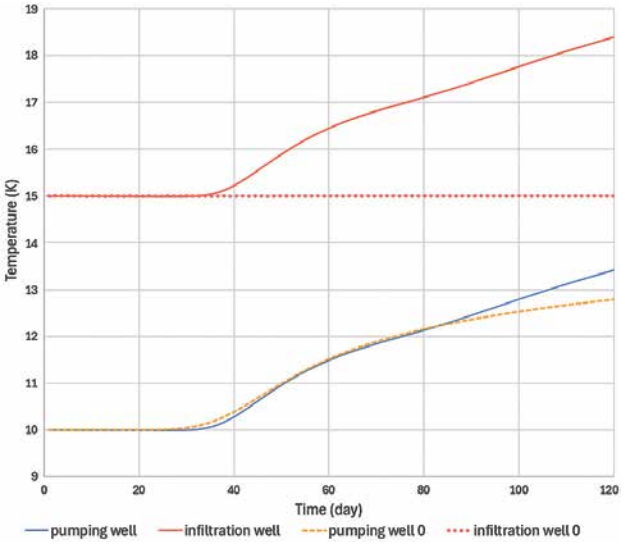

Fig. 2. Comparison of temperature evolution in a well doublet system using traditional static modeling versus dynamic API control.

6. DISCUSSION AND FUTURE OUTLOOK

The transition from proxy-based solute transport codes to the dedicated Groundwater Energy (GWE) code within MODFLOW 6 marks a pivotal advancement in hydrogeological modeling. While previous methods provided a functional workaround for basic geothermal problems, they often

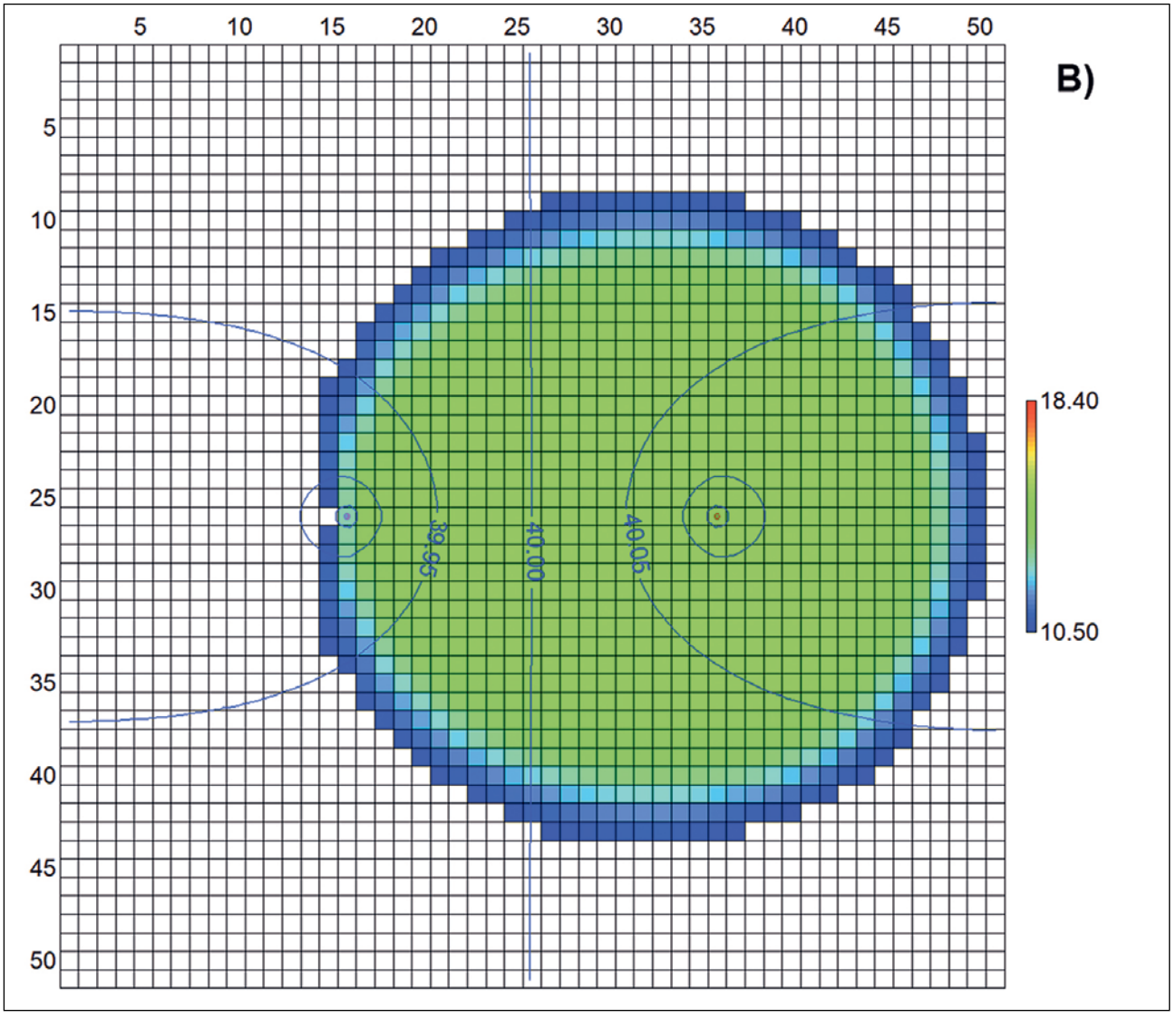

Fig. 1. Comparison of simulation approaches for a well doublet with spatial distribution of the thermal plume (based on modeled data).

struggled with physical consistency in complex environments. The introduction of GWE, coupled with the powerful MODFLOW 6 API, resolves several long-standing limitations and opens new avenues for research and engineering applications.

One of the most significant improvements offered by GWE is the rigorous treatment of heat transport through the rock matrix. In traditional solute transport proxies (e.g., MT3DMS), heat stored in the solid phase was simulated using a retardation factor. This approach inherently assumes that transport is dominated by advection within the pore space. A critical failure of this methodology occurs in "dry" or hydraulically inactive cells (NO-FLOW cells). In a solute model, if a cell becomes desaturated or dry, mass transport effectively ceases. However, in thermal physics, heat conduction continues through the solid rock matrix regardless of the water content.

The GWE code addresses this by decoupling the energy budget of the solid skeleton from the hydraulic saturation of the pore space. By solving the energy transport equation for the bulk porous medium, GWE allows for the simulation of conductive heat transfer even across zones with low or zero water saturation. This capability is particularly crucial for modeling the unsaturated zone (UZ), which acts as a thermal buffer between the atmosphere and the water table. As demonstrated by Morway et al. (2022), accurately capturing the thermal dampening effect of the UZ requires a model that can simulate conduction through the soil matrix when advective flux is minimal or absent.

Beyond governing equations, the integration with MODFLOW 6's Discretization via Vertices (DISV) and Unstructured Grid (DISU) packages offers a practical advantage for geothermal system design. Borehole Heat Exchangers (BHEs) create steep thermal gradients that require fine spatial resolution, while regional flow fields operate on kilometer scales. The ability to use unstructured grids allows for local mesh refinement around boreholes without the prohibitive computational cost of a globally fine finite difference grid. This flexibility, combined with the rigorous energy formulation, enables more accurate predictions of long-term system efficiency and thermal interference in dense urban settings (Barbieri et al., 2025).

The demonstration case study of the geothermal doublet highlights the transformative potential of the MODFLOW 6 API. Static simulations, while useful for initial sizing, fail to capture the dynamic operational logic of modern heating and cooling systems. Real world heat pumps operate based on feedback loops (e.g., maintaining a constant or meeting a varying building load). By utilizing the Extended Model Interface (XMI), researchers can now embed this control logic directly into the simulation loop. This capability transforms the groundwater model from a passive prediction tool into an active component of the HVAC design process, allowing for the optimization of pumping rates and injection temperatures in real-time response to aquifer conditions.

7. CONCLUSION

This article has synthesized the evolution of subsurface heat transport modeling, highlighting the shift from solute-analogous proxies to the physically rigorous Groundwater Energy (GWE) code. We have demonstrated that while historical methods served the community well, they lack the capability to address the complex, transient, and multi-phase thermal problems of the future. The GWE model provides a standardized platform that correctly solves the energy balance for both fluid and solid phases, resolving critical issues such as heat conduction in the unsaturated zone.

The primary scientific contribution of this work lies in establishing a methodological bridge between legacy solute-transport proxies and the physically rigorous Groundwater Energy (GWE) code. Unlike previous studies that primarily focused on governing equations, this paper provides a tangible demonstration of how to leverage the MODFLOW 6 API for practical engineering scenarios. By quantitatively defining the divergence between static and dynamic simulation approaches, we highlight the critical necessity of API-controlled feedback loops for accurate geothermal system design. Consequently, this work empowers the hydrogeological community to transition from simplified proxies to physically robust, operationally realistic thermal simulations.

Furthermore, the coupling of GWE with the MODFLOW 6 API represents a significant leap forward in simulation control. As shown in our case study, the API enables the simulation of dynamic feedback loops essential for modeling modern geothermal systems. These tools collectively empower hydrogeologists to design more efficient renewable energy systems and better understand the thermal dynamics of groundwater in a changing climate.

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