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Agent-based models of groundwater systems: A review of an emerging approach to simulate the interactions between groundwater and society

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ABSTRACT

Understanding how society can address and mitigate threats to groundwater sustainability remains a pressing challenge in the Anthropocene era. This article presents the first comprehensive and critical review of coupling Groundwater Models and Agent-Based Models (GW-ABMs) to address four key challenges: (1) adequately representing human behaviour, (2) capturing spatial and temporal variations, (3) integrating two-way feedback loops between social and physical systems, and (4) incorporating water governance structures. Our findings indicate a growing effort to model bounded rationality in human behaviour (Challenge 1 or C1) and a dominant focus on policy applications (C4). Future research should address data scarcity issues through Epstein's Backward approach (C2), capture feedbacks via tele-coupled GW-ABMs, and explore other modelling techniques like Analytic Elements Groundwater Models (C3). We conclude with recommendations to thrust future GW-ABMs to the highest standards, aiming to enhance their acceptance and impact in decision-making and policy formulation for sustainable groundwater management.

1. Introduction

Groundwater systems are essential for food and water security, ecosystem preservation, and human adaptation to climate change (Margat and Gun, 2013). They supply approximately 40% of the world's irrigation and serve as the primary drinking water source for over two billion people (Morris et al., 2003; Siebert et al., 2010). Current rates of groundwater use, however, are causing a rapid depletion of aquifers worldwide (Feng et al., 2013; McGuire, 2017; Rateb et al., 2020; Rodell et al., 2009; Scanlon et al., 2012, 2023; Voss et al., 2013), a situation that has attracted significant media attention, including a recent series in the New York Times highlighting the societal and policy implications of this global challenge (O'Neill et al., 2023; Rojanasakul et al., 2023; Searcey and Erdenesanaa, 2023). These impacts are predicted to intensify in the coming decades due to socio-economic development (Bierkens and Wada, 2019) and climate change-induced stress (Famiglietti, 2014; Ferroukhi et al., 2015; Wada et al., 2010). Concerningly, many of these endangered aquifers support vast agricultural regions

and major food production areas (Dalin et al., 2019), thereby posing a threat to global food security and 'virtual water' transfers embedded in international food trade (Dalin et al., 2017).

Sustainable groundwater management, which aims to ensure longterm, dynamic stability in the storage and flow of high-quality groundwater through fair, inclusive, and forward-thinking governance (Elshall et al., 2020; Gleeson et al., 2020), has emerged as a core challenge of the Anthropocene (Falkenmark et al., 2019; Lewis and Maslin, 2015; Rockström et al., 2014; Steffen et al., 2011). In this era, groundwater sustainability is impacted and determined not only by physical and environmental factors, but equally, and perhaps more importantly, by social and economic drivers. Many, if not all of these non-physical factors can be traced back to the decisions and behaviours of individuals and interest groups that depend on or have a stake in a given groundwater resource (An et al., 2021).

The study of groundwater sustainability has historically relied on groundwater modelling (Anderson et al., 2015a). Groundwater models

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(GWMs) provide information about the volume and the origin of water entering an aquifer, preferential flow paths, potential impacts due to groundwater extraction, and a full set of hydro-chemical features if solute transport is included as part of the modelling framework. As such, they can be used for water resource assessments, sustainable yield calculations, environmental impact assessments, and integrated water resource management. Among the various computer programs used to model groundwater systems, one of the most widely used and globally recognised tools is MODFLOW (Harbaugh, 2005), a numerical model which has been honed and vetted for almost 30 years (McDonald et al., 2003).

Numerical codeslike MODFLOW, while adept at simulating the physical aspects of groundwater systems, were not originally designed to simulate the non-physical drivers of groundwater sustainability, such as individuals' bounded rationality, cognitive biases, learning and memory, adaptability, social interactions, norms, and values. 'Integrated' modelling tools, including the Water Evaluation and Planning System (WEAP) (Yates et al., 2005), AQUATOOL (Andreu et al., 1996), Source IMS (Welsh et al., 2013), and MODSIM (Fredericks et al., 1998), while offering clear advantages in representing a range of physical processes within a unified framework, also do not inherently address these complex human and social drivers.

The MODFLOW One-Water Hydrologic Flow Model (MF-OWHM) (Boyce, 2020; Hanson et al., 2014) exemplifies an integrated hydrologic model that tightly couples groundwater flow, surface-water flow, landscape processes, aquifer compaction and subsidence, reservoir operations, and conduit (karst) flow. While this coupling results in a numerical modelling code capable of addressing fundamental, wateruse and sustainability issues, such as conjunctive-use and climatecrop-water linkages, it does not encompass the actions, learning, and adaptability of a heterogeneous population of water users in changing social and physical environments (Gilbert, 2020). Recognising this gap, the next section introduces coupled Groundwater Agent-Based Models (GW-ABMs), a promising methodological approach that complements traditional groundwater modelling by adding a layer of social and behavioural analysis through Agent-Based Modelling, thereby offering a more holistic view for groundwater management and sustainability.

2. Why ABMs? Overcoming challenges of traditional groundwater models

An Agent-Based Model is a computer simulation methodology in which individual elements of a social system are represented as distinct entities within the model (Edmonds and Meyer, 2017). This 'bottomup' modelling approach offers key advantages. Firstly, it enables the nuanced representation of individuals, and their dynamic cross-scale interactions within socially and spatially explicit environments (Furtado, 2022). Secondly, ABMs provide a platform for interdisciplinary communication and collaboration, facilitating the integration of data (empirical and tacit), theories, and methods from varied disciplines (Axelrod, 2006). By actively involving academics, public stakeholders, and policymakers in the model-building process, this collaborative platform can also enhance model credibility and legitimacy, allowing valuable knowledge, experiences, and perspectives to be incorporated (Baldwin et al., 2012; Basco-Carrera et al., 2017; Elshall et al., 2020). Thirdly, ABMs offer the ability to conduct experiments that would otherwise beinfeasible or impractical in real-world settings (due to fundamental limitations or challenges) (Gilbert, 2020; Kiel et al., 2021). By crafting fine-grained 'artificial societies' (Epstein and Axtell, 1996) within a controlled 'virtual laboratory', ABMs provide a safe environment to test policy interventions, evaluate potential outcomes, and delineate the space of what is possible (Edmonds and Ní Aodha, 2019). In the following, we discuss four major challenges (C1-C4) associated with traditional groundwater modelling approaches. For each challenge, we: (1) highlight the limitations it imposes on the analysis of real-world groundwater sustainability issues, (2) describe how ABMs

can help mitigate these constraints, and (3) explore the potential benefits and opportunities that arise from adopting a coupled GW-ABM modelling perspective (see Table 1). Following this, we turn our attention to the difficulties in developing and evaluating coupled GW-ABMs, which we frame under a fifth challenge (C5).

2.1. Representation of human behaviour (C1)

Traditional modelling frameworks often rely on simplifying assumptions that do not adequately capture the complex interplay of environmental, economic, social, and cultural factors influencing water users' decisions, and how these factors may interact and evolve over time. Such simplifications can lead to idealised conditions of "perfect rationality" assumed by *homo economicus* (economic man) models (Von Neumann and Morgenstern, 2004). In this idealised framework, agents are assumed to have complete information about the available options, perfect foresight, and the ability to solve a complex optimisation problem to identify the option that maximises their personal utility.

(1) Limitations. In real-world situations, however, humans exhibit bounded rationality (Simon, 1956, 1957, 1990): they can neither access nor fully process all the relevant information for making optimal decisions (Aumann, 1997). This limitation is particularly pronounced in the context of groundwater management, where water users face both cognitive and informational constraints when making decisions related to water use.

(2) Mitigation of constraints. Agent-Based Modelling allows for the explicit representation of bounded rationality, by providing a flexible framework to incorporate cognitive limitations, heuristics (Gigerenzer and Gaissmaier, 2011), rules of thumb, and biases into the decisionmaking processes of individual agents. When applied to groundwater management, an ABM can simulate how groundwater users make decisions based on their specific geographical, economic and social circumstances. This flexibilityallows for the accommodation of various influencing factors such as social norms and cultural values (e.g., Castilla-Rho et al., 2019; Rojas et al., 2022), economic incentives (e.g., Du et al., 2022), and peer pressure (e.g., Liu and Agusdinata, 2021).

(3) Potential benefits. By incorporating the bounded rationality of water users, an ABM enables a more nuanced and realistic representation of human behaviour. When coupled with GWMs, this combined approach can provide insights into how individual behaviour evolves in response to regulatory changes or environmental pressures, and its collective impact on the groundwater system.

2.2. Diversity of human behaviour and temporal aspects (C2)

Traditional modelling frameworks may not adequately represent the diversity (understood as spatial and temporal variation and/or heterogeneity) of human behaviour. This challenge mirrors what has been referred to as the "aggregation effect" in socio-hydrology (Baldassarre et al., 2019) — the process by which individual behaviours, actions, or characteristics are grouped together or "aggregated" to provide a simplified representation of the complex socio-hydrological system. Focusing on aggregated values, however, might overlook distributions across space (e.g., Du et al., 2022) and among distinct social groups (e.g., De Bruijn et al., 2023). This might result in models or assessments that are not fully representative of the nuanced dynamics of the socio-hydrological system.

(1) Limitations. In GWMs, this "aggregation" commonly occurs by clustering total water demands, evenly distributing pumping rates among users, or using pumping schedules that adhere to predetermined trends rather than responding to contextual variables. In contrast, in a real-world groundwater system we frequently find a wide array of actors that have a stake in a shared water resource (Kaiser et al., 2020), and who learn and adapt over time based on interactions with one another and their changing circumstances.

Description of the four major challenges (C1-C4) associated with traditional groundwater modelling methods and the benefits from adopting a coupled GW-ABM approach.

Challenge	Description	Benefits of a GW-ABM
C1. Representation of human behaviour	Traditional modelling frameworks often simplify human decision-making by assuming idealised incorrect conditions of perfectly rational behaviour.	ABMs offer the advantage of incorporating a more realistic representation of human behaviour by accounting for "bounded rationality" and various influencing factors (e.g., environmental, economic, social, and cultural).
C2. Diversity of human behaviour and temporal aspects	Traditional modelling frameworks often fall short in capturing human behaviour's heterogeneity and spatial-temporal variations.	ABMs offer the advantage of modelling the diverse actors that operate within groundwater systems, accounting for their location and dynamic adaptations.
C3. Two-way feedback loops	Traditional modelling frameworks often overlook the complex, time- and location-based interconnections between social and groundwater systems.	At each time-step, agents in an ABM can perceive and respond to hydrological and environmental changes, thereby enabling the coupled GW-ABM to capture two-way feedback loops between social and groundwater systems.
C4. Representation of groundwater governance and policy findings	Traditional modelling frameworks often lack the capability to adequately represent the structures and rules of water governance, as well as the institutions that enforce them.	ABMs can model the diverse governance structures that exist within groundwater systems, accounting for their spatial variations and temporal evolution.

(2) Mitigation of constraints. Agent-based modelling provides a flexible framework to explicitly represent this diversity, including the spatial and temporal variations. For example, ABMs can simulate a diverse set of groundwater users (e.g., agricultural, domestic, industrial and commercial) with unique characteristics (e.g., water demands, or financial resources), distinct preferences (e.g., crop types, water-saving technologies, or water sources), and varying perceptions (e.g., risk tolerance, environmental awareness, or trust in regulatory bodies). These agents can be programmed to learn from prior experiences or new information (e.g., García et al., 2019; Giordano et al., 2021; Nouri et al., 2022a), anticipate future trends (e.g., future crop prices and precipitation as in Hu et al., 2015a; Hu and Beattie, 2019), and modify their behaviours accordingly (e.g., switch to drought-resistant crops (Streefkerk et al., 2023), invest in water-efficient technologies (Mauser and Prasch, 2016), or switch between alternative water sources (Tamburino et al., 2020).

(3) Potential benefits. In practice, ABMs offer a flexible framework for simulating the diversity, temporal dynamics, and adaptive learning processes among different actors within a groundwater system. This, in turn, helps create a more nuanced understanding of these complex socio-hydrological systems.

2.3. Two-way feedback loops (C3)

Traditional modelling frameworks are not designed to capture the full gamut of interconnections — or co-evolutionary dynamics (Baldassarre et al., 2019; Sivapalan et al., 2012) — that exist between social and groundwater systems (Alam et al., 2022).

(1) Limitations. Groundwater codes such as MODFLOW are designed to represent one-way effects - the impact of water users' decisions on the water balance (e.g., draw-down of the water table, discharge to a wetland or river, land subsidence, etc.) - but not the other way around. Human stressors (such as pumping rates and landuse) are thus predetermined and provided as an input for a simulation scenario. This practice, however, assumes that hydrological state variables have no impact on human decisions (Srinivasan et al., 2016), which may omit critical feedbacks. For instance, substantial change in human behaviour follow from reduced groundwater availability due to excessive pumping, such as the adoption of water saving technologies (e.g., Streefkerk et al., 2023) or more cost-effective water supplies (e.g., Tamburino et al., 2020). Models that do not take this feedback into account would project the over-exploitation or even depletion of the aquifer due to the selfish behaviour of individuals, when this may not necessarily occur (Hardin, 1968; Ostrom, 1990).

(2) Mitigation of constraints. Coupled GW-ABMs can explicitly accommodate the two-way feedback loops between human behaviour and groundwater conditions. In practice, this means that agents can simultaneously perceive and react to changes in spatially-explicit hydrological and/or environmental conditions, at each time-step (Alam et al., 2022).

(3) Potential benefits. Having the ability to model these twoway feedback loops in a computationally tractable way is critical for developing recommendations and policies that are attuned to the interconnected and dynamic nature of coupled human-groundwater systems, and is probably one of the main strengths of coupling ABMs and groundwater models.

2.4. Representation of groundwater governance and policy findings (C4)

Traditional modelling frameworks focus on the physical dimensions of groundwater flow—they are not specifically designed to explicitly represent water governance arrangements, water regulations, and the hierarchy of institutions that support and/or enforce them.

(1) Limitations. In real-world contexts, water users dynamically interact with a nested hierarchy of institutions and governance structures (via policies and interventions) that affect their behaviour at multiple scales (Lippe et al., 2019). Although tools such as MF-OWHM and WEAP attempt to capture the role of certain regulations and governance instruments – such as water rights and the administrative controls that mediate the allocation of water resources in a catchment – the framework upon which these processes are represented is hardwired to the code. Thus, their ability to represent the relevant high-level social structures and institutions, along with the multiple stakeholders involved with a groundwater resource is not warranted (Castilla-Rho et al., 2019).

(2) Mitigation of constraints. ABMs have the flexibility to represent a range of operational governance structures. To illustrate, consider a hypothetical scenario featuring two countries (A and B), each with a unique approach to groundwater governance. Country A employs a centralised, top-down model, where the national government enforces stringent regulations and oversight. Conversely, Country B embraces a decentralised system, allowing local communities to exercise substantial control over groundwater resources, within the boundaries of state-level guidelines. An ABM can encode these governance structures through different rules and behaviours for regulatory agents. In Country A, for example, this agent could be programmed to enforce strict extraction quotas whenever groundwater levels fall below defined thresholds (e.g., Kuhn et al., 2016), whereas in Country B, multiple water resource management agents might implement distinct extraction limits within their own jurisdictions, leading to spatially-varying policies across the region (e.g., Du et al., 2022). Furthermore, the ABM can simulate changes in these governance structures over time. For instance, if over-extraction persists, the centralised agent in Country A may adapt existing quotas based on selected performance targets, aligning with the Adaptive Water Management framework (Pahl-Wostl et al., 2012; Varady et al., 2016). This adjustment could inform the integration of early-warning indicators in real-world planning scenarios (Edmonds and Ní Aodha, 2019). Conversely, agents in Country B could fine-tune quotas in response to perceived localised drought conditions (Du et al.,

2022). In both scenarios, the ABM would enable the evaluation of heterogeneous responses to policy interventions, while also considering the externalities affecting water users.

(3) Potential benefits. Overall, GW-ABMs provide a holistic framework to assess the interplay between human behaviour and groundwater systems, thereby facilitating the development of adaptive and geographically-attuned policies for sustainable groundwater management.

2.5. Methodological challenges in model development (C5)

The integration of GWMs and ABMs into a unified methodological tool offers a powerful approach. However, akin to other modelling and simulation endeavours, it also confronts various methodological challenges during model development, particularly in ensuring the model's quality and reliability (Manson et al., 2020). Given the distinct intellectual origins of GWMs and ABMs, there are contrasting differences in terminologies, standards, and practices. To harmonise these aspects, we adopt the 'Evaludation' framework as a unified methodology for evaluating the quality and reliability of coupled GW-ABMs (Augusiak et al., 2014). This framework serves as a *lingua franca* – a common language that bridges the methodological divides between GWMs and ABMs – while also facilitating interdisciplinary collaboration and dialogue among researchers, policy-makers, and stakeholders.

In C5, therefore, we place the spotlight on current practices over key aspects of the (coupled) model quality assurance process, throughout the iterative *modelling cycle* (see Section 3.3.6). This enables us to provide a comprehensive analysis of current practices in coupled GW-ABMs over these areas, emphasising contemporary challenges, innovative solutions, and actionable insights.

2.6. Objectives, contribution, and guiding review questions

Our aim is to present the first comprehensive and critical review on integrating traditional groundwater models with ABMs, to simulate, explore, and manage groundwater systems, including their social, economic, biophysical, and regulatory dimensions. The growing body of research in this area signals an expanding interest among researchers and policymakers in leveraging this combined modelling framework for sustainable groundwater management. This trend is further supported by the wider use of ABMs in interdisciplinary areas such as water resources (Kaiser et al., 2020), floods (Zhuo and Han, 2020), the food-energy-water nexus (Magliocca, 2020), agricultural policy (Kremmydas et al., 2018), fisheries governance (Lindkvist et al., 2020), socio-ecological systems (Lippe et al., 2019; Schulze et al., 2017), sustainability research (Aly et al., 2022; Shults and Wildman, 2020), and specially policy evaluation (e.g., Edmonds and Ní Aodha, 2019; Gilbert, 2008, 2020; Savin et al., 2023; Squazzoni et al., 2020). By synthesising and consolidating key insights from the literature on coupled GW-ABMs, our review serves as a seminal text for this methodology and a launchpad for practitioners. We identify current research gaps, outlining a focused research agenda including various promising avenues for future research together with actionable methodological recommendations. In doing so, we hope to contribute to the ongoing refinement of this emerging approach, and amplify its role in supporting sustainable groundwater management.

To achieve the above aims and contributions, our review will examine the literature using the following guiding review questions (RQs):

- RQ1 (Modelling purposes and typologies): What is the purpose and what are the issues or questions that have motivated the development of GW-ABMs?
- RQ2 (C1 Simplified Representation of human behaviour): What have been the subjects and objects of decision-making in coupled GW-ABMs? Which theories and levels of rationality have been used to simulate the behaviour and decisions of agents?

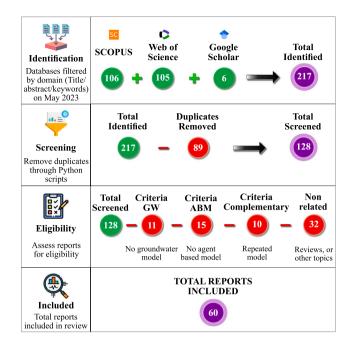


Fig. 1. The PRISMA protocol (PRISMA-P Group et al., 2015) as applied and adjusted for the current review.

- RQ3 (C2 Diversity of human behaviour and temporal aspects): Are various kinds of agents being simulated? Do agents stand for individual entities or are they grouped into clusters? Can agents actively learn and adapt during a simulation?
- RQ4 (C3 Two-way feedback loops): How is time and space represented in both GWMs and ABMs, and how is consistency in these scales maintained in the coupled model? What software is used to develop each model, and how are these coupled together?
- RQ5 (C4 Representation of groundwater governance and policy findings): How have water governance arrangements, water regulations, and the hierarchy of institutions been represented, if at all? What have been the main lessons, practical implications, or policy findings derived from GW-ABMs?
- RQ6 (C5 Methodological challenges in model development): Based on the critical assessment of GW-ABMs up-to-date – specifically in terms of best practices for model validation, calibration, sensitivity analysis, and documentation – what key lessons and opportunities emerge for implementing these coupled models in the future?

The paper is organised as follows. Section 3 outlines the methodology used for our systematic review of GW-ABMs. Section 4 presents the findings of this review. Section 5 builds on these results to re-examine and critically evaluate the progress that the coupled GW-ABM methodology has achieved in tackling each challenge, highlighting successful strategies, identifying gaps/unresolved issues, and suggesting directions for future research. Lastly, Section 6 offers concluding remarks.

3. Review methodology

Fig. 1 details the PRISMA protocol (PRISMA-P Group et al., 2015) employed for compiling a comprehensive database of scientific publications coupling groundwater and agent-based models. To guarantee thoroughness, comprehensibility, replicability, and systematic organisation of this review, we rely on the SALSA framework (Search, Appraisal, Synthesis, Analysis), which is commonly used for systematic literature reviews (Grant and Booth, 2009; Mengist et al., 2020).

3.1. Step 1 - Search

We designed a keyword search to capture all the different terminologies and spellings of our main concepts in the scientific literature. For the Agent-Based Modelling methodology, we included terms associated to both multi-agent systems (*multi-agent* or *multi agent*) and individual based systems (*individual-based* or *individual based*), since authors might use these terms indifferently. As our review focuses on groundwaterrelated issues, we narrowed results through the most commonly used terms in groundwater studies (i.e., groundwater or ground water or ground-water or hydrogeology or aquifer).

Taking into consideration that bibliographic databases do not cover journals in the same manner (Waltman, 2016), we performed our search using two major scientific databases: *Scopus* and *Clarivate Analytics Web of Science* (WOS). We then extended our search through Google Scholar to capture any other relevant study. We searched over articles' titles, abstracts and the authors' keywords, and then filtered these results by document type (articles, editorial materials and review documents), language (English), and source (Journals). We executed the search in September 2023, and obtained a total of 217 records which were retrieved and downloaded (106 from Scopus and 105 from WOS, and 6 from Google Scholar) (see Fig. 1). Next, we merged results using Python scripts, through which we detected and dropped about half of the documents as duplicates. The resulting 128 documents were collated into a single database and subjected to further inclusion criteria as detailed in the next step.

3.2. Step 2 - Appraisal

We examined the full-text articles from each record to determine their suitability for the literature review according to three criteria that together constrain our analysis to studies that have coupled ABMs with GWMs.

- Criteria GW Are groundwater processes explicitly modelled? We assessed how each study represented groundwater processes (e.g., using a physical or analytical GWM). If there was no representation of groundwater quantity and/or quality processes, we discarded the record from our review.
- Criteria ABM Is human behaviour explicitly modelled? We assessed whether the model developed in each article considered the explicit simulation of individuals (e.g., water users) and their behaviours. If there was no representation of the human agency, we discarded the record from our review.
- Criteria Complementary If an article presents a model previously covered without introducing new experiments, results, or parameterisations, it is placed in a separate database and used as a reference, but not included as part of the review.

By applying these inclusion and exclusion criteria, we identified and eliminated from the corpus those articles that were captured through our keyword search but did not align with our research focus. From the original 217 records, after the screening process, we were left with 60 documents for a comprehensive in-depth review in Section 4 (see Fig. 1).

3.3. Step 3 - Synthesis

We conducted a systematic analysis of the 60 studies based on sixreview topics: Modelling Purposes and Typologies (refer to Table A1) and the five listed challenges (see Table 2). In the following, we outline their significance and describe the methodology employed to assess them.

3.3.1. Modelling Purposes and Typologies

Our assessment started by identifying the purpose and objectives motivating the development of GW-ABMs (see RQ1). We adopted (Edmonds et al., 2019) classification system as a basis and expanded it to include studies introducing new modelling software (refer to Table A1 for detailed definitions of each category). Then, we sorted the articles into two general categories of application: Agriculture or Water Supply. Studies focusing on different topics were grouped under the Other label (e.g., Aquifer Thermal Energy Storage systems). Lastly, since the modelling purpose informs the choice of a suitable GWM, we classified each GWM using two taxonomies (see Table 2): (1) Type --- physically-driven (relies on processes and principles of physics to represent groundwater flows), data-driven (relies on relations derived from empirical data to predict physical variables), hybrid (combines both previous approaches, such as a physically-based model used to train a data-driven model), or Other (any other modelling approach) — and (2) Sub-type — numerical (solves the groundwater governing equations through numerical methods), analytical (uses simpler forms of the groundwater governing equations to compute physical variables), Other (any other modelling approach).

3.3.2. (C1) Representation of human behaviour

Our second analytical lens sought to determine what have been the subjects and objects of decision-making in coupled GW-ABMs, and what has been the behavioural underpinning (theoretical basis) and rationality level of the simulated artificial agents (see RQ2). For the former, we documented the agent types reported in each article and grouped them by the functional categories proposed by Kaiser et al. (2020) for ABMs in water resource management. This classification included three types of water users (namely, urban/domestic, industrial, and agricultural), three types of water providers (namely, regulator, water utility, and reservoir manager), any interest group, economic institution, and a category titled other to capture any agents not included by the previous classifications. Lastly, to assess rationality, we classified each article based on whether the simulated individuals make decisions following a fully-rational (i.e., using optimisation-only procedures), boundedly rational (i.e., using heuristics under limited knowledge and cognitive capacity), or a mixed behaviour (i.e., agents might rely on optimisation, but have limited knowledge and cognitive capacities).

3.3.3. (C2) diversity of human behaviour and temporal aspects

In complex systems, diversity is typically defined in three ways. Firstly, as the *differences within* a specific type or category (e.g., the distribution of groundwater entitlements and allocations assigned to a population of water users). Secondly, as the *differences across types* (e.g., the different individuals, groups, institutions, and stakeholders involved in water resources management). Thirdly, as the *differences in composition*, referring to how these types are arranged or assembled (Page, 2011).

To capture these multiple dimensions of diversity and gain insights into how it has been represented in coupled GW-ABMs (see RQ3), we defined and used several measures. For *diversity within an agent type*, we investigated whether the primary agent-type simulated in each article (i.e., farmers or domestic urban water users for agricultural and water supply applications respectively) was aggregated into clusters, groups, or super-agents. For *diversity across agent types*, we used Kaiser et al. (2020) classification system. Finally, we did not quantify the *diversity of composition* in our review, since computational experimentation with GW-ABMs always resulted in variations of agents and their state variables through defined scenarios.

To capture the temporal aspect of decision-making, we examined each article to extract whether *learning* or *adaptation* mechanisms were explicitly simulated and how. Given there is no universal agreement in the relevant literature on how to distinguish between these two processes (Müller et al., 2013), we assessed both indistinctly.

Classification system and categories used	d in this review for each of the challenges. Note the first row sets the context by outlining modelling purposes and typologies.
Challenge	Classification and actooption

Challenge	Classification and categories	
Modelling purposes and typologies	 * General application: (i) Agriculture, (ii) Water Supply, (iii) Other. * Modelling purposes: (i) Prediction, (ii) Explanation, (iii) Description, (iv) Theoretical Exploration, (v) Illustration, (vi) Analogy, (vii) Social Learning, (viii) New Modelling Software (refer to Table A1). * GWM types: (i) Process or Physically-based, (ii) Data-driven or Black-box, (iii) Hybrid, (iv) Other. * GWM sub-types: (i) Numerical, (ii) Analytical, (iii) Other. 	
(C1) Representation of human behaviour	 * Subjects of decisions: (i) Agricultural water user, (ii) Urban/Domestic water user, (iii) Industrial water user, (iv) Regulator, (v) Water Utility, (vi) Reservoir Manager, (vii) Interest Group, (viii) Economic Institution, (ix) Other. * Rationality level: (i) Fully-rational, (ii) Boundedly Rational, (iii) Mixed. 	
(C2) Diversity of human behaviour and temporal aspects	 * Diversity across (see "Subjects of Decisions" in C1). * Temporal aspects (Learning/Adaptation): (i) Included, (ii) Not included. 	
(C3) Two-way feedback loops	 * GWM - Treatment of space: (i) Distributed, (ii) Semi-distributed, (iii) Lumped/Aggregated, (iv) Other. * GWM - Treatment of time: (i) Transient, (ii) Steady-state, (iii) Not Applicable. * ABM - Treatment of space: (i) Spatially-Explicit, (ii) Spatially-Implicit. * ABM - Treatment of space - Type: (i) Continuously, (ii) Grid-based, (iii) Network-Based, (iv) Geographical Information System. * GWM/ABM - Software: (i) Proprietary, (ii) Open-source, (iii) Not Clear. * Model coupling: (i) Loosely coupled, (ii) Tightly/Closely coupled, (iii) Integrated. 	
(C4) Representation of groundwater governance and policy findings	★ Groundwater policies (refer to Table 4).	
(C5) Methodological challenges in model development	 * GWM - Model output verification: (i) Performed, (ii) Not Performed, (iii) Not clear, (iv) Not mentioned. * GWM - Model output verification - Type: (i) Automated, (ii) Manual, (iii) Not clear, (iv) Not applicable. * ABM - Model output verification: (i) Performed, (ii) Not Performed, (iii) Not clear, (iv) Not mentioned. * GWM - Model output corroboration: (i) Performed, (ii) Not Performed, (iii) Not clear, (iv) Not mentioned. * GWM - Model output corroboration: (i) Performed, (ii) Not Performed, (iii) Not clear. * ABM - Model output corroboration: (i) Performed, (ii) Not Performed, (iii) Not clear, (iv) Not mentioned. * ABM - Model output corroboration: - Technique: (i) Structural Validation, (ii) Extreme and Sensitivity Tests, (iii) Participatory Modelling, (iv) Pattern-Oriented Modelling, and/or (v) Empirical Output Validation. * Model analysis (Refer to Table 3). * Model documentation (ODD): (i) Fully Used, (ii) Partially Used, (iii) Not Used. 	

3.3.4. (C3) two-way feedback loops

To enable a richer discussion on two-way feedback loops (see RO4), we first assessed the spatial and temporal scales, and the software used in both GWMs and ABMs. We first classified GWMs based on how they treated time (i.e., transient or steady-state approach) and included details on the temporal resolution (time-step). Then, we analysed how they treated space, classifying them as either Distributed (i.e., the model considers spatial variations in the aquifer's properties), Semidistributed (i.e., the model divides the spatial domain into units that are assumed to be internally homogeneous, but can vary from one another), Lumped/Aggregated (i.e., space is treated in an aggregated or averaged manner), or Other (any other representation of space), and further documented the number of spatial dimensions (namely, 3D, 2D, 1D, or N.A.), the size of the cell (if applies), and the total extent. Analogously, for ABMs, we categorised them based on whether they included space (spatially-explicit) or not (spatially-implicit), and how it was represented (continuously, grid-based, network-based, or through a Geographical Information System). In terms of time, however, given agents make decisions at varying time scales, we chose not to classify ABMs by a single time scale as this could lead to misunderstandings in cross-article comparisons. Lastly, we separately recorded the software used to develop the GWM and the ABM in each study, and then further classified each article as either proprietary or open-source (free) based on the licenses that govern the software used. With all this information, we then proceeded to examine the coupling (at the software level) between each GWM and ABM as explained below.

Coupling standards, frameworks, and initiatives aimed at promoting interoperability of developed models in various fields exist and are well developed (e.g., The Open Modeling Interface (OpenMI) used in hydrology (Harpham et al., 2019) or the Bespoke Framework Generator (BFG) for Climate Models (Armstrong et al., 2009)), yet we did not find any records that utilised them. During our review, we did notice the use of terms such as *loosely, tightly/closely*, and *integrated*, to describe the different types of connections between GWMs and ABMs. Although this terminology neatly synthesises the coupling level to a single category, as highlighted by Bithell and Brasington (2009), it can be ambiguous

when multiple and simultaneous feedback loops exist. For instance, a GWM might be integrated spatially to an ABM (i.e. agents and the simulated physical system share the same coordinate system and spatial resolution), whilst simultaneously be loosely coupled temporally (i.e., the GWM operates at a different time scale than the ABM) to fit a restricted computational budget or to reach numerical stability. Resolving this ambiguity would require complete access to the source code of each model (which is often lacking), and sufficient disciplinary expertise on each type of programming language and software package. Given the effort and nuance that would be needed to accomplish this task, we opted for a qualitative assessment using Antle et al. (2001) terminology of loosely coupled (i.e., the GWM and ABM are executed sequentially, passing information between each other as data files), tightly/closely coupled (i.e., relevant processes of the GWM and the ABM are coded and linked together on the same programming system), and Integrated (i.e., the GWM and the ABM share the same set of drivers and scales, making processes endogenous) and informed by our previous evaluation of spatio-temporal scales and software used (see Table 2).

3.3.5. (C4) representation of groundwater governance and policy findings

Groundwater governance can be understood as the framework encompassing the processes, interactions, and institutions, in which actors (i.e. government, private sector, civil society, academia, etc.) participate and decide on the management of groundwater within and across multiple geographic (i.e. sub-national, national, transboundary, and global) and institutional/sectoral levels (Villholth and Conti, 2018). Despite the numerous legal frameworks and policies in place for the regulation of groundwater, these often assume that perfect compliance from individuals can be achieved at no cost, while compliance and enforcement still remains a major global issue (see Holley et al., 2020, and references therein). We began by examining the role of actors simulated in coupled GW-ABMs. In this review topic, however, we took a closer look at how the compliance behaviours of individuals has been represented so far, if at all, and the role of enforcement (from official or unofficial parties and institutions). Concurrently, to understand the role of coupled GW-ABMs in policy assessment (see RQ5), we categorised

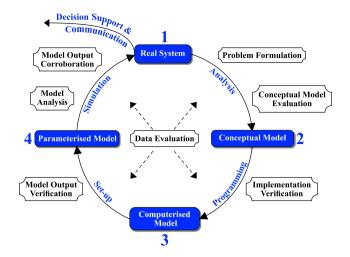


Fig. 2. The six elements of the 'Evaludation' framework (see black italics titles) mapped to a simplified representation of the modelling cycle (see blue boxes) as presented in the original figure (Augusiak et al., 2014), plus the elements analysed during this review (see purple titles).

which groundwater policies have been simulated and assessed to date (refer to Table 4 for a description of each), documenting the key findings that emerged from studies and their implications for the design and improvement of these policies.

3.3.6. (C5) methodological challenges in model development

The 'Evaludation' framework (Fig. 2) integrates the different elements that need to be addressed during model development to establish quality and credibility. Among its six elements, we centred our review on four backbone components: Model Output Verification (calibration), Model Output Corroboration (validation), Model Analysis (through sensitivity analysis), and Model Documentation (part of Data Evaluation). This focused approach aimed for an insightful and actionable assessment, to highlight best practices, common difficulties, and innovative solutions (see RO6). While both the Conceptual Model Evaluation and Implementation Verification elements are also essential for quality assurance, both are particularly difficult to assess. The former, with a plethora of methods, is also inherently subjective, while the latter requires an understanding and access to the source code and software used to develop the coupled model. In the following, we first briefly define each element reviewed and contextualise it from the context of groundwater modelling and Agent-Based Modelling. Grounded on this comparative explanation, we then present our review approach which synthesises our understanding of each element for coupled GW-ABMs.

During the Model Output Verification stage, a critical assessment is performed on how well model outputs (predictions) match (system) observations and the role of calibration in obtaining adequate fits (Augusiak et al., 2014). In groundwater modelling, this procedure is termedsolving the "inverse problem", as parameter values are estimated and assigned based on measurements of what is being modelled (Carrera et al., 2005; Zhou et al., 2014). While it has been extensively investigated since the early 1970s, this process continues to present significant challenges including computational burden due to the requirement of multiple model realisations, scale inconsistencies between field measurements and the model's discretisation, and the problems of non-uniqueness, non-existence and non-steadiness of solutions (Anderson et al., 2015b; Doherty, 2015). For ABMs, however, the considerable amount of individual-level behavioural information that is needed for fine-tuning parameters, makes this "calibration" process a major challenge (An et al., 2021). Furthermore, given observations of relevant outputs are usually not available, parameter values are commonly fit to reproduce instead patterns observed in reality, as

described in "pattern-oriented parameterisation" (Grimm et al., 2005; Grimm and Railsback, 2012; Jakoby et al., 2014).

Based on these definitions, we first examined whether *history matching* was performed on each GWM and whether this was performed *manually* or through *automated* algorithms. Then we recorded any efforts to perform parameter fitting to match existing data sets or patterns on each ABM. In both cases, to gain further insights into current trends, pitfalls, and opportunities, we also examined which parameters were fine-tuned, how well model output matched the observations, and how the results were presented. With this information, we then classified the ABM and GWM of each record into the categories presented on Table 2.

Model Output Corroboration refers to the comparison of model predictions with independent data and patterns that were not used while the model was developed, parameterised, and verified (Augusiak et al., 2014). In groundwater modelling this comparison is common practice, despite debates suggesting a GWM cannot be completely validated (see Anderson et al., 2015a; Konikow and Bredehoeft, 1992, and references therein). For ABMs, however, there is a lack of official common standard protocols, resulting in a multitude of available methodologies and frameworks (Kang, 2018; Rand and Rust, 2011; Troost et al., 2023). Hence, with the aim to understand current practices for coupled GW-ABMs, we examined whether any comparison to independent data or patterns was performed and whether scholars mentioned any validation attempt in their studies. Based on the techniques used for the ABMs in particular, we classified them into (see Table 2): (1) Structural Validation - the process of ensuring realism in the conceptual model by analysing assumptions and simplifications (Manson, 2002)- (2) Extreme and Sensitivity Tests, (3) Participatory Modelling (i.e., relying on workshops, surveys, or other participatory techniques (Voinov et al., 2018)), (4) Pattern-Oriented Modelling (Grimm et al., 2005), and (5) Empirical Output Validation (North and Macal, 2007; Rand and Rust, 2011).

Model Analysis includes the assessment of how sensitive model outputs are to parameter variations, a process known as Sensitivity Analysis (SA) (Saltelli, 2004). While Uncertainty Analysis (UA) often complements SA for exploring, managing, and evaluating uncertainty during Model Analysis (Saltelli et al., 2019; Saltelli, 2008), we do not cover it in this review. We chose to concentrate solely on SA because assessing the diverse uncertainties in data input, model structure, and parameter estimation methods is a substantial endeavour which would significantly extend the scope and length of this review. Future work should take a specific focus on this aspect, and provide the necessary platform to dissect and explore it in detail.

In terms of *Model Analysis*, then, we first classified articles based on whether they *performed* or not a SA. We recorded the SA methods used, and categorised each article following the classification system shown in Table 3. Firstly, to uncover the *purpose* of each SA (the *why*), we used the 'settings' proposed by Saltelli (2004) and Saltelli (2008). Similar to Borgonovo and Plischke (2016), we included a *Model Building* setting to capture those studies aimed to assist in any of the various phases of the modelling cycle. Secondly, to understand the implementation of each SA (the *how*), we followed Pianosi et al. (2016), Saltelli et al. (2019) and Song et al. (2015) to distinguish between *quantitative* or *qualitative* techniques, and the *sampling strategies* as either *Local* or *Global*. Lastly, we recorded whether the *input factors* and the *outcomes measured* during the SA, targeted either the *social system*, the *physical system*, or a combination of both.

In terms of *Model Documentation*, transparent description of a model's structure not only enables accurate replication but also fosters seamless communication within and across disciplines (Grimm et al., 2020). Given its interdisciplinary nature, a primary challenge for GW-ABMs is the establishment of a unified and standard protocol that covers every facet of the coupled model development (e.g., conceptualisation, parameterisation, analysis, and evaluation). The ODD (Overview, Design concepts, Detail) protocol (Grimm et al., 2010) and its successive extensions (Grimm et al., 2020; Laatabi et al., 2018; Müller et al., 2013) have become the accepted standard for describing

Classification system and categories used for classifying articles on the Model Analysis element of the 'Evaludation' framework.

Classification	Sub-categories and descriptions		
Purpose	 * Factor prioritisation and screening: Aimed to either obtain insights about the most important input factors (i.e., the <i>factor prioritisation/ranking setting</i>), or find those least influential ones (i.e., the <i>factor fixing/screening</i> setting). * Model building: Aimed to guide model development in any of the various phases of the modelling cycle (e.g., model output corroboration, model output verification, etc.), thereby improving the model's credibility and reliability. * Model exploration: Aimed to identify critical or interesting regions in the space of the input factors, or trace how an output of interest is generated, or study which values of the input factors lead to model realisations in a given range of the output space (i.e., the <i>factor mapping setting</i>). * Other: This category captures any other purpose not included in the previous ones. 		
Sampling strategy	 * Local sensitivity analysis (LSA): The SA explored how deviations in a single input affect the variability of the results while holding all other inputs constant. This includes the traditional One-At-A-Time (OAT) design. * Global sensitivity analysis (GSA): Explores the whole input space, analysing outcome variability both due to single input and interactions (Ligmann-Zielinska et al., 2020; Saltelli, 2004). * Hybrid: This category captures those Sensitivity Analysis that do not fit on the previous ones. 		
Method type	 ★ Quantitative: Each input factor is associated with a quantitative and reproducible evaluation of its relative influence, normally through a set of sensitivity indices. ★ Qualitative: The sensitivity was assessed qualitatively by visual inspection of model predictions or by specific graphs (e.g., tornado plots, scatter visualisations, etc.). 		
Input(s)/Output(s) targeted ^a	 * Physical system: The input factors varied during the SA (or in turn, the selected outcomes), were associated with the hydrology or the groundwater system (or target outcome measures associated to it). * Social system: The input factors varied during the SA (or in turn, the selected outcomes), were associated with the social system (or target outcome measures associated to it). * Both: The input factors varied during the SA (or in turn, the selected outcomes), were associated with the groundwater system and the social system (or target outcome measures associated to it). 		

^a Note we assessed separately the input factors and the output measures in terms of which system they target.

ABMs, and now are included within the TRACE protocol (Grimm et al., 2014), which documents the different elements defined in the 'Evaludation' framework. Therefore, we first examined the methods that modellers have employed to document their coupled GW-ABMs. Then, we specifically extracted information as to whether the ODD protocol was used and how extensively, classifying each article into one of the following categories: (1) *Fully-used* (i.e., the entire ODD protocol is given), (2) *Partially-used* (i.e., the protocol is used only for guiding the model's description in the article, but it is not fully covered, neither delivered), or (3) *Not used* (see Table 2).

3.4. Step 4 - Analysis

We conducted a thorough review of each article in the corpus, guided by the review topics and methodology outlined in Section 3.3. This review resulted in the creation of a databasecontaining categorical and multi-nominal variables. To address our research questions, we carried out quantitative analyses of these variables, and presented the findings through visualisations tailored for multi-dimensional data.

4. Results

The earliest instance of a coupled GW-ABM dates back to 2003 with the SINUSE model (Feuillette et al., 2003). As shown in Fig. 3, GW-ABM applications garnered limited attention during the first decade (2003– 2013). However, this trend shifted dramatically in the subsequent decade (2014–2023), with notable bursts in research activity occurring in 2015 and 2019. This upward trajectory indicates a growing scholarly interest in this interdisciplinary topic, aligning with prior observations that groundwater systems are under-researched and highlighting the potential of ABMs to address this gap (see Gorelick and Zheng, 2015). Regarding geographical focus, the majority of case studies were situated in catchments in Iran (17), the USA (14), China (4), and the Republic of Kiribati (3). Notably, most of these countries are grappling with similar threats to groundwater sustainability stemming from the combined effect of over-pumping and climate change (see Rodell et al., 2018; Wu et al., 2020).

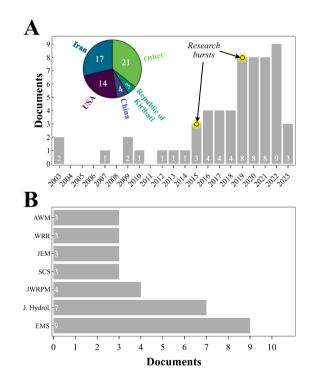


Fig. 3. A. Bar chart displaying the annual scientific production of the reviewed corpus. Highlighted are two periods in time in which a significant increase in the number of articles published takes place (called research bursts). The pie chart highlights the number or articles per country, based on the location of the case studies. B. Bar chart displaying the most frequent journals (note we intentionally leave out of this chart those journals with less than three articles).

4.1. Modelling purposes and typologies

The majority of the reviewed studies focused on simulating the behaviours and interactions of either farmers (32 articles, 53%) or urban water users (10 papers, 17%), with some addressing both (14 papers, 23%) —refer to the "Agriculture", "Water Supply", and "Both" categories depicted in Fig. 4-A. As to agriculturally-focused GW-ABMs,

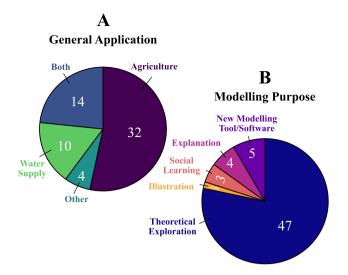


Fig. 4. GW-ABM studies were classified based on: A. the general application (i.e., Agriculture, Water Supply, Both, or Other), and B. the modelling purpose using the criteria put forward by Edmonds et al. (2019).

we detected several methodological innovations and *hybrid* modelling approaches, aimed to enhance the representation of human decisionmaking such as Bayesian Cognitive Maps (Pope and Gimblett, 2015), Fuzzy Cognitive Maps (Mehryar et al., 2019), Fuzzy Inference Systems (Nouri et al., 2019), Social Network Analysis (Giordano et al., 2021), and data-driven Directed Information Graphs combined with Boosted Regression Trees (Hu et al., 2017).

As tourban Water Supply, studies have targeted a wide range of issues in managing urban groundwater systems, such as the effects of different degrees of urban clustering on groundwater levels (Zellner and Reeves, 2012), the relationship between urbanisation and water vulnerability to water shortages (Srinivasan et al., 2013), the interactions between water supply and water consumer networks and their structural heterogeneities (Zhang et al., 2023), and decentralised systems for micro-trading harvested rainwater (Bolton and Berglund, 2023). Overall, these studies have deepened our understanding of groundwater in urban settings, thereby improving our ability to manage them effectively.

The remaining 4 articles (7%), classified as "Other", have investigated a range of topics, such as system-level emergent outcomes and feedback between groundwater and urban Aquifer Thermal Energy Storage systems (Beernink et al., 2022; Jaxa-Rozen et al., 2019), the social impacts of mining (Liu and Agusdinata, 2021), and the role that changes in natural spring flows may have played on hominin movement (Cuthbert et al., 2017). This diversity of applications highlights the potential of ABMs in addressing pressing issues that require an acknowledgement of the complexities of human behaviour and regulatory institutions.

Finally, we observed the development of large modelling frameworks designed to integrate the multiple aspects of water resources and their multi-scale linkages to other sectors into a single computational decision-support tool (García et al., 2019; Martin et al., 2016; Mauser and Prasch, 2016; Phetheet et al., 2021; Yoon et al., 2021). While these integrated models represent ambitious and long-term endeavours, they possess the capabilities to unravel the trade-offs and synergies inherent in groundwater management interventions. Consequently, they can facilitate more informed decision-making processes that can lead to sustainable pathways.

In 47 studies (78% of the corpus), GW-ABMs were developed to explore how different modelling assumptions produce different outcomes (see *Theoretical Exploration* on Fig. 4-B and Table A1). Interestingly, most of these studies took a policy focus, as 42 of these 47 articles

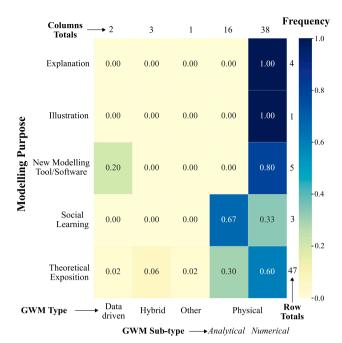


Fig. 5. Heatmap representations of the distribution of groundwater model types and sub-types combinations (columns, see also Table 2), as they pertain to distinct modelling purposes (rows). Darker cell colours illuminate higher frequencies after normalisation of values based on each modelling purpose (rows).

explicitly simulated, experimented, and assessed the effects of potential management or policy interventions at the group and/or individuallevel (see Table 4). Remarkably, we identified a total of 16 studies (27%) using a participatory/collaborative modelling approach (Voinov et al., 2018) during model development, and a total of 3 studies (5%) aimed to build a model that encapsulates a shared understanding of a group of people to promote *social learning* (Reed et al., 2010). This latter category has included the development of a novel digital platform that enables on-the-fly execution of a coupled GW-ABM (Rojas et al., 2022), and a computer-assisted role-playing game aimed to facilitate dialogue (Dray et al., 2007; Perez et al., 2003).

We identified 5 articles that introduced new modelling tools and software for developing coupled GW-ABMs. Castilla-Rho et al. (2015) unveiled FlowLogo, an interactive NetLogo-based modelling environment that deploys the 2D finite-difference solution of the governing equations for groundwater flow. Bakarji et al. (2017) offered an extendable and modular computational package that combines social, economic, and physical components (using the Finite Element Heat and Mass Transfer code). Jaxa-Rozen et al. (2019) presented a Python-based architecture coupling NetLogo with MODFLOW/SEAWAT, thereby facilitating the exploration of socio-hydrological dynamics involving complex subsurface processes. Phetheet et al. (2021) provided the Food-Energy-Water Calculator (FEWCalc), an ABM designed to project farm incomes based on crop selection, irrigation practices, groundwater availability, renewable energy investment, and historical and projected environmental conditions. More recently, De Bruijn et al. (2023) introduced the Geographical, Environmental and Behavioural model (GEB), capable of simulating millions of individual household agents within independent hydrological environments and dynamically linked to the spatially-distributed CWatM hydrological model. Although a comprehensive comparison of these tools falls beyond the scope of this review, it is important to underscore their pivotal role in expanding what is methodologically feasible, and in facilitating and broadening the applicability of coupled GW-ABMs to other research and policy-making contexts.

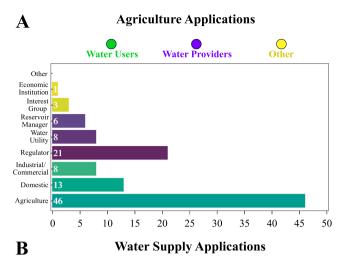
In terms of groundwater modelling, overall we observed a prevalence of *physically-based* GWMs (54 studies), from which most are numerical in nature (38 articles). These models dominate across various modelling purposes. They are, in fact, the exclusive choice for Explanation, Illustration, and Social Learning purposes (see Fig. 5). A subset of studies also explored hybrid or data-driven approaches, which typically integrate an Artificial Neural Network (ANN), trained on a physicallybased numerical GWM, to estimate groundwater levels (Anbari et al., 2021; Bakhtiari et al., 2020; Elhamian et al., 2022; Farhadi et al., 2016). All these approaches, however, have less frequently been used, as seen by the sparse entries in Fig. 5, suggesting their potential might still be largely unexplored. Finally, while prediction of future impacts has been a traditional objective of groundwater models, our review revealed no GW-ABMs specifically aimed at this modelling purpose. This absence, however, aligns well with acknowledged difficulties of making predictions in complex and wicked systems, given the lack of data, the ontological diversity, and the variety of algorithmic approaches to simulating human behaviour (Edmonds et al., 2019; Squazzoni et al., 2020). Similarly, we detected very limited attention to Groundwater Quality issues (5 studies), and no study representing complex coupled processes of flow in porous media, chemical reactions, transport and/or heat transfer (e.g., coastal saltwater intrusion or energy storage), which concurs with prior findings (see Jaxa-Rozen et al., 2019).

4.2. (C1) representation of human behaviour

For agricultural GW-ABM applications (see Fig. 6-A), although the subjects of decisions are mostly individual farmer agents (e.g., Du et al., 2022; Mehryar et al., 2019; Pope and Gimblett, 2015; Tamburino et al., 2020), studies have also *aggregated* these up to groups or clusters of farmers (e.g., Giordano et al., 2021; Khan and Brown, 2019; Mulligan et al., 2014), counties (e.g., Hu et al., 2015b, 2017; Hu and Beattie, 2019), and even extensive management regions (e.g., Farhadi et al., 2016). We also evidenced an extensive range of simulated objects of decisions, both direct and indirect, including which crops to plant and grow, how much land to irrigate, water use levels and sources (groundwater, surface water and tanker water), irrigation scheduling, water trading, and other investment decisions (e.g., adopting renewable energy or new irrigation technologies).

Urban Water Supply GW-ABMs (see Fig. 6-B) have simulated different entities at multiple hierarchical levels, from individual consumers, residents, and households (e.g., Bolton and Berglund, 2023; Zhang et al., 2023), up to groups of water consumers (e.g., Bakhtiari et al., 2020) and entire cities (e.g., Al-Amin et al., 2018). The key simulated decisions regarding all these agent types is how to supply water for respective water uses (e.g., piped water, domestic groundwater well, water bought from water tank trucks, domestic rainwater tanks, or water trade), and whether to engage in water-related investments such as innovation technologies (Mauser and Prasch, 2016) or long-term water infrastructure (Srinivasan et al., 2013). As expected from the classical urban water supply problem, public management agencies (e.g., municipalities, state services, provincial governments, water utilities, water agencies, etc.), and the role of water utility managers is also simulated in almost all these GW-ABMs. Their main role is to distribute water for the agents throughout the simulation (e.g., Bakhtiari et al., 2020; Lachaut et al., 2022; Yoon et al., 2021), and enact and enforce water restrictions (e.g., Al-Amin et al., 2018; Allain et al., 2018; Martin et al., 2016).

Most GW-ABM studies have aimed to test the effects of potential policy interventions. Consequently, a regulatory agency is usually included as an agent, with oversight on water rights, water caps, and water allocations (e.g., Anbari et al., 2021; Farhadi et al., 2016; Giordano et al., 2021; Nouri et al., 2019), monitoring and controlling illegal water withdrawal (e.g., Aghaie et al., 2020a,b; Castilla-Rho et al., 2019; Rojas et al., 2022), implementing local water taxes (e.g., Du et al., 2022), and enacting laws related to the formation and operation of water markets (e.g., Nouri et al., 2022a). In Agricultural applications, studies have also introduced *Interest group* agents. These agents have



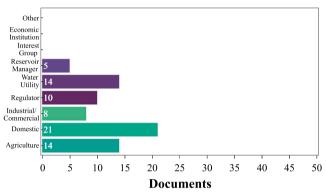


Fig. 6. Number of agent types simulated in A. Agriculture, and B. Water Supply GW-ABMs using the classification system put forward by Kaiser et al. (2020).

represented agricultural institutions that aim to improve irrigation efficiency either by disseminating knowledge (De Bruijn et al., 2023) or by offering economic incentives (Anbari et al., 2021). They have also represented environmental institutions that focus on raising awareness about aquifer over-exploitation (Nouri et al., 2022b) or aim to minimise groundwater drawdown (Farhadi et al., 2016).

As to the simulated agents' level of rationality in coupled GW-ABMs (Fig. 7), we found a tendency towards a boundedly rational behaviour (48% of the corpus), through the inclusion of cognitive limitations (e.g., constrained knowledge of the groundwater system, limited foresight of environmental conditions or the consequences of their actions, finite memory, and different learning/adaptation processes), various biases (e.g., risk aversion, loss aversion, and susceptibility to social influences), and the use of heuristics (e.g., imitation and social norms, rules of thumb, and satisficing behaviours). Furthermore, when examining the research timeline, we found that the first decade (2003-2013) showed an equal preference for both boundedly rational and fully-rational agents, each making up 38% of the corpus. However, in the subsequent decade (2014-2023), the proportion of studies featuring boundedly rational agents (50%) more than doubled those with fullyrational agents (21%). This shift suggests a growing effort to more accurately represent human decision-making in coupled GW-ABMs.

Despite the numerous behavioural theories developed in Social Sciences, Behavioural Economics, and other scientific fields, we only detected a few studies making explicit use of them to model human decision-making. For instance, the Theory of Planned Behaviour (Giordano et al., 2021; Mauser and Prasch, 2016; Zhang et al., 2023; Zolfagharipoor and Ahmadi, 2021), Protection Motivation Theory (Streefkerk et al., 2023), Dempster–Shafer Belief Theory (Allain et al., 2018; Martin et al., 2016), Cultural Theory (Castilla-Rho et al., 2019;

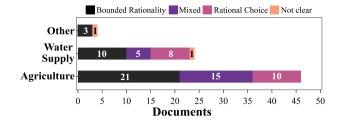


Fig. 7. Bar chart displaying the number of publications with a model of human behaviour classified as either *fully-rational, boundedly rational, mixed,* or *not clear*. We present the results for each specific application separately (namely, *Agriculture, Water Supply,* or *Other*). Note 14 publications are classified as *both* Agriculture and Water Supply. Since these are presented in both columns separately in the chart, then the total number of studies presented reaches to 74.

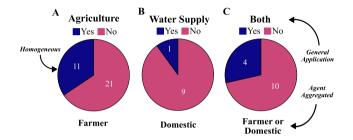


Fig. 8. Number of GW-ABM studies in which the main agent type is represented as an individual (i.e., "No") or aggregated (i.e., "Yes"). Results are presented for A. Agriculture-only applications (i.e., farmers), B. Water Supply-only applications (i.e., domestic water users), and C. Both (i.e., either farmers or domestic water users are aggregated or not).

Rojas et al., 2022) and Hofstede's Cultural Dimensions Theory (Tamburino et al., 2020). The rest of the studies have relied instead on social or behavioural constraints that complement the traditional profitoptimisation approach, by using IF-THEN rules (e.g., Mehryar et al., 2019; Noël and Cai, 2017; Ohab-Yazdi and Ahmadi, 2018) or Fuzzy rules (e.g., Nouri et al., 2019, 2022b). Other studies have ventured into the application and use of Machine Learning techniques (e.g., Bayesian cognitive mapping and boosted regression trees) to adequately capture behavioural stochasticity (Hu et al., 2017; Pope and Gimblett, 2015).

4.3. (C2) diversity of human behaviour and temporal aspects

With our first diversity lens – termed *diversity within* – we aimed to uncover the level of aggregation at which the primary agent-type has been simulated. Overall, we evidenced substantially more disaggregation (44 studies or 73% of the corpus). However, agriculture applications tend to rely more on aggregated agents (see Fig. 8-A) than *Water Supply* studies (see Fig. 8-B). Quoting the terms employed by the scholars, this aggregation is made to fit available data (Hu et al., 2015b, 2017; Hu and Beattie, 2019), to reflect independent management areas (Nouri et al., 2019, 2022b,a) or actual partitions in the landscape (Giordano et al., 2021), or to reduce computational time (Elhamian et al., 2022; Farhadi et al., 2016).

Our analysis under the second lens – termed *diversity across* – uncovered that multiple agent types are commonly simulated in the literature. This is evident from the densely interconnected co-occurrence network shown in Fig. 9-A, which has a density of 0.81 (note also 65% of the articles included more than one agent type). The most frequently represented agent types are "Agriculture" under the Water Users class and "Regulator" under the Water Providers class (see Fig. 9-B). Notably, the linkages between Agriculture-Regulator and Domestic-Water Utility are among the three most frequent, suggesting a thematic focus on groundwater regulation in non-urban areas and urban water supply respectively. Interestingly, Regulator agents were

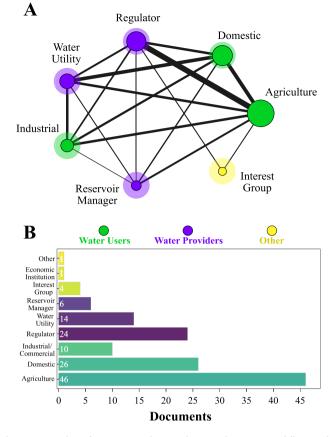


Fig. 9. A. Number of GW-ABM studies simulating each agent type following the classification of Kaiser et al. (2020). Note under the label *other* we capture a single study that simulates individuals that do not consume water, but only seek for it (Cuthbert et al., 2017). B. Co-occurrence network of agent types. Nodes (agent types) are scaled to the number of occurrences as per A, while edges' thickness indicate more frequent co-occurrence between agent types. In both cases, we apply a power function to adjust the data distribution.

only introduced in 2015, while Water Utilities have been consistently represented since 2003. We hypothesise that the increased focus on regulatory agents may stem from growing societal concerns about groundwater depletion in the agricultural sector, and related shifts in groundwater policy.

As to learning and adaptation, we found 30 studies (50% of the corpus) explicitly simulating these behavioural processes. These have been captured through a "best-mean imitation" heuristic - imitate the strategy of whichever neighbour is doing best, exploit the current strategy if better, and explore a new strategy occasionally (Castilla-Rho et al., 2019; Rojas et al., 2022) ----, reinforcement learning --- implement the same strategy of the previous year, until this strategy proofs to be not satisfactory (Giordano et al., 2021)-, bayesian learning (e.g., Hu and Beattie, 2019), and mostly through the agents' memories of previous experiences such as attained crop profits (Aghaie et al., 2020a; Nouri et al., 2019), crop yields (Tamburino et al., 2020), crop productions (Allain et al., 2018), and aquifer conditions (Jaxa-Rozen et al., 2019). The explicit inclusion of these mechanisms has allowed agents' decisions to evolve in response to changing circumstances, knowledge, and experiences, which overall provides a richer representation of human heterogeneity.

4.4. (C3) two-way feedback loops

The multiple intricate bidirectional feedback loops that exist between social and groundwater systems can be conceptualised, simulated, and explored through the coupled GW-ABM methodological

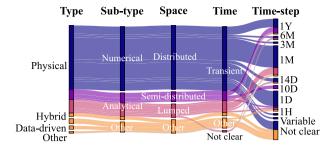


Fig. 10. Parallel categories diagram displaying the type (namely, *Physical, Hybrid, Data-driven,* or *Other*) and sub-type (namely, *Numerical, Analytical, Other*) of each groundwater model reviewed, and how they treat space (namely, *Distributed, Semi-distributed, Lumped, Other*) and time (*transient* or *other,* and time-step used). Note ribbons are coloured based on the treatment of space (third column).

approach. However, linking separate models to enable close interconnections and synchronous exchanges of data requires reaching a consistent spatial and temporal scale between the models. The representation of space in groundwater models has been prominently distributed (38 studies, see blue ribbon in Fig. 10), as scholars have mostly relied on physically-based numerical GWMs. In contrast, 8 studies Aggregated the aquifer to a single unit (see red ribbon in Fig. 10), by using Analytical methods (mostly mass balances). Although these analytical models are computationally less demanding compared to physically-based models, they assume that an aquifer responds uniformly and instantly to groundwater pumping (Brozović et al., 2010) and thus are not able to capture the aquifer's heterogeneity and the spatially-varying responses to human action. In between these two extremes, we detected 6 articles using Semi-Distributed GWMs (see purple ribbon in Fig. 10), which divide the aquifer into different regions with distinct physical properties (e.g., Darbandsari et al., 2020; Moradikian et al., 2022). Remarkably, with the goal of striking a balance between efficiency and accuracy, researchers have ventured into the use of Hybrid approaches by developing a physically-based distributed model that then trains an ANN (e.g., Farhadi et al., 2016) to predict groundwater flows while acknowledging space variability. Likewise, other scholars have ventured into the design of Data-Driven approaches that either train an ANN from available data (e.g., Anbari et al., 2021) or rely on simpler linear regressions (e.g., Phetheet et al., 2021). Since in these cases groundwater properties are obtained only at specific locations in space (usually around features of interest), the aquifer's spatial heterogeneity is simplified (see yellow ribbon in Fig. 10).

Although most studies have considered spatial variability in the aquifer system (see Fig. 10), this has been done at vastly different levels. For instance, most of the spatially-explicit models (i.e., *Distributed* or *Semi-Distributed*) have opted for a 3D model with a *cell size* in the range of 0 km² to 0,5 km², and covering a total geographical area between 100 km² and 10.000 km² (see larger bars on each axis or column in Fig. 11). These results suggest case studies have mostly taken a catchment-level focus instead of a regional, national, or even global scale, which are also common in the broader groundwater modelling literature (e.g., Gleeson et al., 2012; Scanlon et al., 2023; Wada and Bierkens, 2014). We believe this might be partially due to computational limitations of the coupled architectures, and the complexities associated with accessing, designing, and further calibrating and validating larger GWMs.

In terms of the temporal dimension, the reviewed corpus reveals a clear tendency towards the development and use of *transient* GWMs (53 articles or 88% of the corpus, see Fig. 10). Among the *Other* category, the dynamic response of the aquifer has been captured in several ways. For instance, *Hybrid* GWMs have deployed *transient* physical GWMs to train an ANN (e.g., Elhamian et al., 2022), while *Data-driven* GWMs have relied either on time-series data of piezometers (Anbari

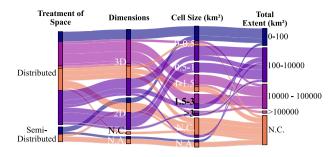


Fig. 11. Parallel categories diagram displaying, for the spatially explicit groundwater models in the corpus reviewed (i.e., those *Distributed* or *Semi-Distributed*, as highlighted on the first column), the number of dimensions (namely, *3D*, *2D*, *Not* Applicable or N.A., and *Not Clear* or N.C.), the size of the cell (in km^2), and the total geographical area or extent covered by the model (in km^2). Note ribbons are coloured based on this last column (total geographical extent) to display the spatial scale of the study.

et al., 2021) or reported groundwater use in time (Phetheet et al., 2021). In terms of temporal resolution, we evidenced a considerable variability, with 11, 17, and 9 studies relying on daily, monthly, or yearly time-steps respectively, while the rest of transient models (16 articles) relying on temporal resolutions in between these values (see right column on Fig. 10). We believe this variability might respond to the variety of modelling purposes and research questions being addressed by scholars, the specific characteristics of the systems, computational efficiency, and data availability.

In terms of spatial considerations in ABMs, the majority of the corpus reviewed (78%) defined an *explicit spatial environment* to simulate the positions and movements of agents. The spatial dimension thus takes a prominent role in the dynamics of these coupled GW-ABM, as the spatial relationships of agents determine their interactions and decision-making processes. This feature, however, has been represented in various ways. Overall, most of the studies (53%) used *grids*, which divide the spatial environment into cells. We believe this choice is partially influenced by the ease of integrating real-world GIS data – as demonstrated by 27% articles that integrated geographical maps or satellite imagery – and the consistency this design offers with distributed GWMs as a direct linkage can take place between the cells of the ABM and the GWM (and vice-versa). However, the choice of grid size can significantly affect both computational run-time and simulation outcomes (e.g., Jaxa-Rozen et al., 2019).

In the corpus we only detected 2 studies (3%) that have allowed agents to move freely within a continuous space, by locating their agents through a coordinate system (x, y) (Bithell and Brasington, 2009; Noël and Cai, 2017). Remarkably, 20 studies used a network-based representation, although mostly in conjunction with other representation of space (14 articles). These networks were used to represent the social relationships between agents (e.g., Castilla-Rho et al., 2019; Darbandsari et al., 2020; De Bruijn et al., 2023; García et al., 2019; Mauser and Prasch, 2016; Nouri et al., 2022a), or the buyer-seller connections in a formal or informal water market (e.g., Aghaie et al., 2021; Bolton and Berglund, 2023). Those studies that relied exclusively on a network to represent space (6 studies), deployed either a spatiallyexplicit node-link distribution system (see Avisse et al., 2020; Kuhn et al., 2016; Lachaut et al., 2022; Yoon et al., 2021), or a spatiallyimplicit social network approach (see Moradikian et al., 2022; Zhang et al., 2023).

From the toolkits available for the development of ABMs (Abar et al., 2017), scholars have mostly relied on NetLogo, followed by Python – through packages such as Mesa (Kazil et al., 2020), Honeybees (De Bruijn et al., 2023), and Pynsim (Knox et al., 2018) – and Java (see Fig. 12-A). We found similar results over groundwater modelling software (see Fig. 12-B), with the physically-based MODFLOW model being the most commonly employed (34% of the corpus), followed by NetLogo (mostly through the FlowLogo environment developed

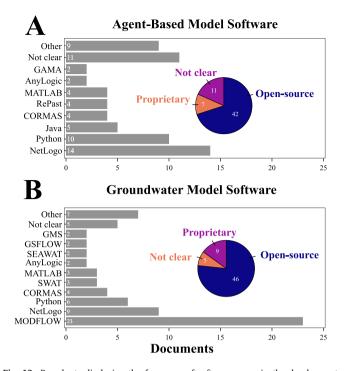


Fig. 12. Bar charts displaying the frequency of software usage in the development of A. ABMs and B. GWMs. Accompanying pie charts in each sub-figure illustrate the proportion of studies that employ either *open-source or proprietary* software for the A. ABMs or B. GWMs. Note that if a study relies on multiple software platforms, each instance is counted separately in the bar charts, but the study is classified only once in pie charts. The label '*Not Clear*' includes all studies that do not specify the software used, while the '*Other*' category aggregates software that is used in one study or less.

by Castilla-Rho et al., 2015), and Python (mostly through the FloPy package developed by Bakker et al., 2016). These results also highlight a prevalent use of *open-source* over *proprietary* software in the development of both GWMs and ABMs, accounting for 77% and 70% of the corpus respectively (see pie charts in Fig. 12). This trend towards *open-source* is substantiated by various software linkages, such as between NetLogo and MODFLOW (Jaxa-Rozen et al., 2019), NetLogo and Python (Jaxa-Rozen and Kwakkel, 2018), and Python and MODFLOW (Bakker et al., 2016). This preference for *open-source* platforms may likely stem from their inherent flexibility (allowing to tailor software to specific research needs), cost-effectiveness, and transparency (critical for verification and replicability). However, this trend may also signal that the field is still in a maturing phase.

In regard to the connection between GWMs and ABMs, our review found that only two articles allowed a high degree of interaction and feedback between the models. These *integrated* architectures achieved consistent spatial and temporal alignments, and shared a unique set of drivers and internal variables and highlight the technical complexity required to align spatio-temporal scales and integrate them cohesively (Allain et al., 2018; Martin et al., 2016; Mauser and Prasch, 2016).

Not all modelling purposes, however, require a completely integrated and holistic modelling framework. During our review, GWMs and ABMs were instead predominantly *closely/tightly* coupled (48% of the corpus). In these studies, the spatial consistency was achieved by either defining a single grid to simulate both physical and social processes, as seen in applications using NetLogo (Aghaie et al., 2020a,b, 2021; Castilla-Rho et al., 2015; Liu and Agusdinata, 2021; Zolfagharipoor and Ahmadi, 2021) and CORMAS (Dray et al., 2006, 2007; Moglia et al., 2010), or by linking the grid of the GWM to ABM grid in a direct one-to-one relationship (e.g., see Du et al., 2020, 2022; Streefkerk et al., 2023). We also observed a clear trend over the last decade (2013–2023) towards *loosely* coupled GW-ABMs (14 articles out of the total 15 in the corpus). Although this type of connection can be

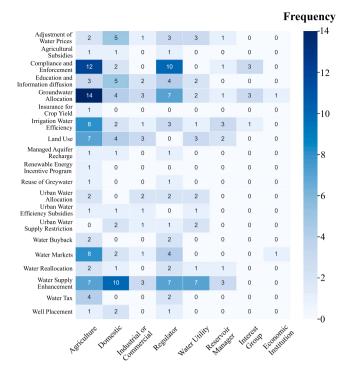


Fig. 13. Heatmap representation displaying the distribution of analysed policies in coupled GW-ABMs (rows), with different agent types (columns). Darker cell colours indicate higher number of co-occurrences between each policy-agent combination. The label *Other* includes all policies with under 5 appearances.

computationally expensive (see Castilla-Rho et al., 2015, and references therein), its flexible modular design can harness powerful specialised models like MODFLOW.

4.5. (C4) representation of groundwater governance and policy findings

Overall, most of the studies took a policy-oriented focus (83% of the corpus), in which the effectiveness, efficiency, and the various strengths, weaknesses, and limitations of policies were assessed through carefully designed simulations (e.g., Du et al., 2020, 2022; Mulligan et al., 2014). By acknowledging the diversity of the human response (e.g., groundwater use) and the multiple interconnections to the groundwater system (e.g., changes on the groundwater table), these studies illustrate the potential of coupled GW-ABM in informing policy design and implementation (see Table 4 for details of each groundwater policy assessed, and Fig. 13 for the distribution of policies studied in function of different agent types). For instance, in the design of a groundwater tax, Mulligan et al. (2014) showcased how an uniformly applied tax tends to yield sub-optimal outcomes both economically and environmentally when tested against a more realistic population that includes heterogeneous, short-term-focused, and self-interested individuals. Similarly, Du et al. (2020) demonstrated that local hydrological conditions (closeness to a stream and depth to groundwater table) can significantly affect the performance of a groundwater tax, generating non-linear relationships that highlight the need for spatially varied and temporally dynamic policies. In a subsequent study, they showed it is feasible to adjust a groundwater tax over time (i.e., changing from wet to dry years) and across space (i.e., set differently between irrigation districts) to improve hydrological outcomes without adversely reducing the total water supply (Du et al., 2022)

The simulation of the enforcement of water rules by official or unofficial parties, and the resulting compliance response of individual water users, has also been explicitly simulated in various studies (22% of the corpus). This regulatory issue has been mostly examined in

P

Policies analysed in coup	led GW-ABMs to date	. Note that individual	studies often assess	multiple policies,	resulting in a cum	ulative total of 95.

Policy name	Description	Total
Adjustment of Water Prices	Modification of pricing schemes or rates for using surface or groundwater.	5
Agricultural Subsidies	Financial measures designed to support farmers economically.	1
Compliance and Enforcement	Simulation of the enforcement of water rules by various parties and the resulting compliance behaviour of individuals.	13
Education and Information Diffusion	Policies aimed at educating and informing key groups about the status, significance, or management of water resources across various contexts.	6
Groundwater Allocation	Methods for adjusting water user permits to regulate groundwater extraction and prevent overuse.	15
Insurance for Crop Yield	Financial risk-management programs that provide farmers with compensation for crop losses due to unforeseen events (e.g., droughts).	1
Irrigation Water Efficiency	Measures and practices aimed to optimise water use in agricultural irrigation.	8
Land Use	Regulations directing land development, allocation, and management in areas such as agriculture, urban planning, and environmental conservation.	7
Managed Aquifer Recharge	Methods aimed to maintain, enhance, and secure groundwater systems by intentionally replenishing groundwater into aquifers.	2
Renewable Energy Incentive Program	Financial and regulatory measures designed to promote the adoption and production of renewable energy sources.	1
Reuse of Greywater	Policies focused on the systematic collection, treatment, and repurposing of wastewater generated from non-sanitary sources.	1
Urban Water Allocation	Mechanism design for the distribution and allocation of water resources among water users in urban areas.	2
Urban Water Efficiency Subsidies	Financial incentives to promote water-saving behaviours and technologies in urban settings.	1
Urban Water Supply Restriction	Regulations to limit specific water uses in urban areas, particularly during droughts, affecting sectors such as residential, commercial, and industrial.	2
Water Buyback	Initiatives where water rights are acquired from users and then reallocated for other purposes (e.g., environmental conservation).	2
Water Market	Simulation of the trading of water-related rights, licenses, allocations, or any other similar water product (e.g., tanker groundwater, recharged rainwater, etc.).	9
Water Reallocation	Transfer of water allocations between different users, often requiring adjustments to legal rights or permits.	2
Water Supply Enhancement	Measures aimed to increase the available water supply for diverse uses (e.g., construction of wastewater treatment facilities, or desalination plants).	11
Water Tax	Simulation of a groundwater tax (i.e., resource fee) that individuals need to pay for each unit of groundwater.	4
Well Placement	Interventions that change the location and spacing of wells for groundwater extraction.	2

relation to the over-extraction of groundwater with respect to defined extraction limits (e.g., water rights, water permits, or water allocations). For instance, in Kuhn et al. (2016), agricultural agents' water use was regulated through non-tradable water permits that defined the individual allowed abstractions and a Water Allocation Plan (WAP) that limited these based on lake water levels. In Castilla-Rho et al. (2017, 2019), a groundwater constrained system (i.e., allocations set as 20% of farmers' needs) was explored across four levels of regulatory enforcement that varied the proportion of monitored farmer agents (10% or 50%) and fine magnitudes (10% or 90% of farmers' profits), over three case studies. Interestingly, in their model both a random monitoring style and a risk-based audit system were assessed, showing that an increase in the proportion of farmers inspected did not lead to substantial increases in compliance. Further, random monitoring proved to be more effective at dissuading illegal behaviour than targeted monitoring in all the case studies assessed. In a follow-up study Rojas et al. (2022) parameterised the same behavioural model (Castilla-Rho et al., 2019) to the Copiapó River Basin in Chile, and coupled it to a hydrological model to explore farmers' compliance response against imposed caps on groundwater allocations. In this case study, simulation results showed that at least 20% of the groundwater users have to be monitored if a cap on groundwater extraction was imposed by the regulator. Aghaie et al. (2020b) further expanded the original farmers' behavioural model by Castilla-Rho et al. (2017) (Groundwater Commons Game) to include and simulate a market institution that, beyond monitoring, enforcement, and defining the yearly caps over water permits, also operated a double-auction groundwater market by pairing buyers-sellers, and a water buyback program from the government. By analysing different scenarios of monitoring level, they found that

the appropriate monitoring and enforcement settings can lead to the emergence of a social norm that is enough to discourage violation and can bring about a functioning market. Similarly, Nouri et al. (2022b) developed a coupled GW-ABM in which agricultural agents were able to over-extract groundwater based on their knowledge of the aquifer level and the behaviour of their peers. Various regulator agents, on the other end, were simulated to determine water rights, and penalise farmers in proportion to the magnitude of their over-exploitation. In a follow-up study, Nouri et al. (2022a) showed that when a groundwater cap or water trade is included along with a penalty policy, total overextraction increases, as farmer agents tend to take more profit by behaving selfishly and trading the over-extracted groundwater volume.

Lastly, in Du et al. (2020, 2022), the cost of groundwater use is based on a groundwater tax (price for each unit of groundwater), pumping costs (a function of pumping lift), and a penalty fee whenever the aquifer is under over-exploitation conditions (that is, the water table decline exceeds an imposed limit). Farmer agents rely exclusively on an economic optimisation approach to select the most economic water source to irrigate their crops. Their model assumes the monitoring of every pumping well in the basin, and the enforcement of policies by each regional manager, has no cost.

4.6. (C5) methodological challenges in model development

In this section, we present findings related to different aspects of the 'Evaludation' framework as described on Section 3.3.6.

i. Model Output Verification: Overall, the majority of GWMs reviewed have undergone calibration (33 studies or 55% of the corpus), and mostly through *automated* methodologies (23 studies or 70% of the

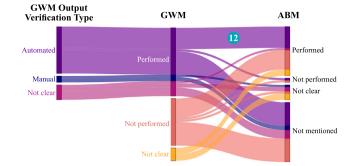


Fig. 14. Parallel categories diagram displaying the relative frequency of co-occurrence of model output verification efforts over the GWM (see middle categories), and ABM (see right side categories) of each study. The left side axis presents the type of methodology used, that is, either *manual* regularisation, or *automated* (i.e., mathematically performed through algorithms). The label '*Not Clear*' includes all models (GWMs or ABMs) where it is not possible to identify how this process takes place nor its results, while the category '*Not mentioned*' groups all models were the term 'calibration' is not mentioned. In a teal-coloured circle we highlight the number of articles that performed model output verification on both the ABM and the GWM.

calibrated GWMs) like PEST (Doherty, 2018a,b), rather than iterative manual trial-and-error procedures (3 studies or 9% of the calibrated GWMs, see Fig. 14). In contrast, most ABMs in the corpus lacked a documented 'calibration' step (28 studies or 47% of the corpus). Among the 23 studies that described a 'calibration' process, we found 10 applications of the inverse modelling approach (Allain et al., 2018; Darbandsari et al., 2020: Kuhn et al., 2016: Lachaut et al., 2022: Martin et al., 2016: Nouri et al., 2019, 2022b,a: Yoon et al., 2021: Zhang et al., 2023). Interestingly, 4 studies adopted a Pattern-Oriented approach (García et al., 2019; Liu and Agusdinata, 2021; Noël and Cai, 2017; Topping et al., 2012), while 2 made use of Participatory workshops for calibration purposes, including developing and populating Bayesian cognitive maps for agents (Pope and Gimblett, 2015) and calibrating the bidding behaviour of farmer agents in a water market (Straton et al., 2009). It is worth noting that surveys (e.g., Al-Amin et al., 2018; Srinivasan et al., 2013) and semi-structured questionnaires (e.g., Castilla-Rho et al., 2019; Rojas et al., 2022; Streefkerk et al., 2023) have also been used to parameterise the initial populations of artificial agents.

ii. Model Output Corroboration: A total of 27 GWMs (45% of the corpus, see Fig. 15-A) compared simulated with observed empirical data (e.g., heads or flows), synthesising results mostly through statistical metrics (e.g., RMAE, MAE, Nash-Sutclife coefficient, etc.). Interestingly, while the vast majority of these GWMs were grounded in physical processes (23 studies), 30 physical GWMs did not perform any model output corroboration, which suggests there still remains a gap in practice.

In terms of ABMs, we found 20 studies (33% of the corpus) explicitly addressing and explaining a validation process. Scholars have used a variety of different and complementary methods, which included (see Fig. 15-B): (1) Structural Validation (Manson, 2002), (2) Extreme and Sensitivity Tests, (3) Participatory Modelling, (4) Pattern-Oriented Modelling (Grimm et al., 2005), and (5) Empirical Output Validation (North and Macal, 2007; Rand and Rust, 2011). Structural validation, i.e., the process of ensuring realism in the conceptual model by analysing assumptions and simplifications, was explicitly mentioned in 3 articles. However, this process reflects a conceptual evaluation (Bert et al., 2014) rather than the Model Output Corroboration targeted in this section. Similarly, extreme and sensitivity tests give insights into model behaviour through designed scenarios, thus aligning better to Model Analysis (see Fig. 2). For participatory modelling methods, the studies relied on interviews (Giordano et al., 2021; Hu et al., 2017), workshops (Allain et al., 2018; García et al., 2019; Martin et al., 2016; Moglia et al., 2010), or computer-assisted role-playing games to facilitate

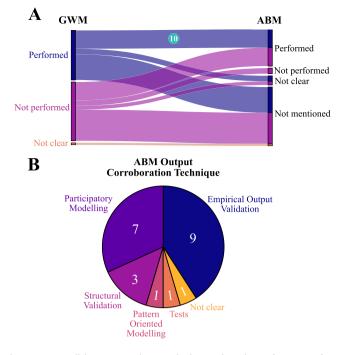


Fig. 15. A. Parallel categories diagram displaying the relative frequency of cooccurrence of model output corroboration of GWMs (see left-side categories) and ABMs (see right-side categories), coloured by the former. In a teal-coloured circle we highlight the number of articles that performed model output corroboration on both the ABM and the GWM. B. Pie chart presenting the distribution of methodologies used for model output corroboration of ABMs.

dialogue (Dray et al., 2007) with diverse experts, stakeholders, and technical advisors. Overall, all these studies reported satisfactory results from these interactions, which helped build confidence in the model and its results.

The comparison of ABMs outputs to real-world empirical data formodel output corroboration purposes was performed on a total of 8 studies, and encompassed arange of methods to compare predicted versus observed values. For example: García et al. (2019) assessed the decrease in the number of active farmers, increase in average area operated by active farmers, and rise in the number of farms and total area operated by tenants through qualitative comparisons; Castilla-Rho et al. (2017, 2019) used statistical measures (mean, interquartile ranges) to compare simulated compliance on water restrictions against observed statistics from survey data; Liu and Agusdinata (2021) used qualitative methods to compare trends and patterns in simulated social stress against the actual timeline of mobilisation events documented in ethnographic studies; Avisse et al. (2020) employed correlation coefficients to compare predicted storage levels against remote sensing observations over the 1998-2015 period; Noël and Cai (2017) used Root Mean Square Error (RMSE) and Coefficient of Variation (CV) to compare predicted long-term average corn yields against countylevel historical corn yields; Yoon et al. (2021) fitted an ordinary least squares regression to match water consumption outputs for urban and agricultural water users with observed data; Zhang et al. (2023) applied the RMSE and Nash-Sutcliffe Efficiency (NSE) coefficients to compare simulated against historical annual water demand data between 2010 and 2018; Beernink et al. (2022) benchmarked model outputs against energy demand monitoring data of two buildings. These results attest to a clear commitment to model output corroboration, albeit to varying degrees and with different methods, both qualitative and quantitative. However, nearly half of the studies did not document any validation efforts, highlighting a critical need for enhancement in this area.

iii. Model Analysis: Overall, 47% of the reviewed studies performed a Sensitivity Analysis (see Fig. 16-A), suggesting it is a common practice by modellers of coupled GW-ABMs. This prevalence however has only appeared recently, as 71% of these studies were published in the last 5 years. A total of 13 studies relied on *local* sampling methods (see the LSA tag on the second column of Fig. 16-B) despite its documented limitations (see Ligmann-Zielinska et al., 2020; Saltelli et al., 2019). Surprisingly, from the 14 studies that deployed a *global* sampling, 8 preferred a *qualitative* rather than a *quantitative* analysis, through a *graphical* examination of the response surface. The 6 studies that relied on *global quantitative* indices, used the Sobol (Streefkerk et al., 2023), Morris (Allain et al., 2018; Jaxa-Rozen et al., 2019; Martin et al., 2016), Latin-Hypercube One-At-a-Time (LH-OAT) (Giri et al., 2018), and Polynomial Chaos Expansion variance-based decomposition (Hu et al., 2015b) methods.

The most commonly examined parameters through SA have been related to the Social System under study (see third column on Fig. 16-B) (Bolton and Berglund, 2023; Liu and Agusdinata, 2021; Streefkerk et al., 2023; Tamburino et al., 2020). Interestingly, in terms of outcomes assessed during the SA, scholars have mostly considered both the physical and the social systems during their assessments. For instance, Castilla-Rho et al. (2019) quantified the effects of increasing monitoring and enforcement powers in a catchment by measuring the evolution of mean groundwater depletion, cumulative illegal extractions, the average social properties of the population (social norms), and overall compliance. Hu et al. (2015b) measured both crop profits and total groundwater depletion. Allain et al. (2018) and Martin et al. (2016) measured various performance metrics of the physical system (e.g., percolation and shallow aquifers content) and of the social system (e.g., daily farmers work and crop yields). Khan and Brown (2019) measured farmers' gains from trading, their pumping costs, and the proportion of streamflow violations (i.e., when modelled flow falls below target levels in specific cells). These examples demonstrate that the coupled GW-ABM methodology can facilitate the identification of critical factors that can determine the behaviour and sustainability of a groundwater system, and which may exist in the physical system, the social system, or in the dynamic interconnections between the two.

From the three defined purposes of SA (Factor Prioritisation and Screening, Model Building, and Model Exploration, see Fig. 16-A), most of the studies aimed to *explore* the dynamic model responses to specified variations in a group of input parameters (e.g., Bolton and Berglund, 2023; Feuillette et al., 2003; Khan and Brown, 2019). Remarkably, in a total of 7 studies the SA was used to guide model development (see *Model Building* category on Fig. 16-A), whereas in 6 studies the SA was used to determine the most or least significant input(s) (see *Factor Prioritisation and Screening* label on Fig. 16-A). These results highlight the positive impact of performing SA to increase a GW-ABM model's credibility and reliability.

iv. Model Documentation: From the 58 studies reviewed after the creation of the ODD in 2006, only 10 fully-used any version of the protocol, while 6 used the ODD+D extension recommended for effectively describing human decision-making (Müller et al., 2013). Reviewing these articles' structures, underlying assumptions, theoretical foundations, and the robustness and scopes of their results, was a vastly easier task compared to the rest of the corpus, and as such we emphasise the critical importance of adopting a common language during model documentation efforts. On the other hand, 7 studies used the ODD for guiding the model description in the article, but did not deliver the complete protocol (namely, partially-used category), while the majority (41 articles) did not use nor mention the protocol at all (namely, not-used category). Interestingly, to share their model documentations and software, scholars have relied on various platforms such as the COMSES OpenABM community-of-practice repository (see Castilla-Rho et al., 2015, 2019; Mehryar et al., 2019), the HydroShare platform (Khan and Brown, 2019), the GitHub distribution software (Bakarji et al., 2017; Castilla-Rho et al., 2015; De Bruijn et al., 2023; Jaxa-Rozen et al., 2019; Phetheet et al., 2021), and other external digital repositories (Avisse et al., 2020; Yoon et al., 2021). As with the ODD, however, none of these have received substantial adoption.

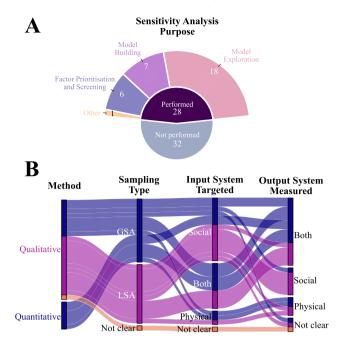


Fig. 16. A. Sunburst graph displaying the number of articles where a Sensitivity Analysis was *performed* (internal circle), and their distribution across various *purposes* (outer circle). Note some Sensitivity Analyses served multiple purposes, causing the total count in the outer circle to exceed that of the '*Performed*' category in the inner circle. B. Parallel categories diagram displaying from left to right, the type of SA method used (namely, *Quantitative* or *Qualitative*), the type of sampling performed (namely, *Social, Physical,* or *Both*) for each study reviewed.

5. Discussion

In this section we re-examine and critically evaluate the progress that the coupled GW-ABM methodology has achieved in tackling each of the challenges discussed in Section 2. We highlight current successful strategies, identify gaps or unresolved issues, suggest promising directions for future research, and discuss the broader implications for policy. Table 5 synthesises this discussion through a set of key messages for scholars, practitioners, decision-makers, and stakeholders interested in developing and applying coupled GW-ABMs for studying and managing groundwater systems.

5.1. (C1) representation of human behaviour

Our review reveals a growing trend towards the simulation of 'bounded rational' agents, which more faithfully replicate the complexities of human reasoning compared to the purely rational behaviour that is typical of most traditional frameworks. However, we found only a few studies that utilise established behavioural theories, or that explicitly compare different human decision models (Hu et al., 2015b, 2017; Hu and Beattie, 2019). This absence of theoretical grounding has also been recognised in other reviews of Agent-Based Modelling applications (Alam et al., 2022; Groeneveld et al., 2017; Rounsevell et al., 2012; Zhuo and Han, 2020). Given that a key advantage of the Agent-Based Modelling approach is its capacity to capture and model human behaviour with the necessary level of detail (An et al., 2021), the limited use and evaluation of various behavioural theories can potentially undermine the ability of ABMs to uncover emergent patterns, feedback loops, and cross-scale interactions. These elements may be crucial for the development of robust policies and interventions that can effectively manage the complexities and uncertainties inherent in human behaviour.

Summary of gaps (G), recommendations (further classified as methodological \mathbb{R}^M or implementation-focused \mathbb{R}^I), and future research areas (F) for advancing coupled GW-ABMs across challenges. Recommendations and future research directions are indented to indicate their association with specific gaps.

Challenges	Gaps (G), Recommendations (R), and Future Research Directions $\left(F\right)$
C1 Representation of human behaviour	G: Lack of guidance on the rationale for behavioural theory selection (<i>why</i>), identification of appropriate contexts (<i>when</i>), and determination of suitable application methods (<i>how</i>). \mathbf{R}^{M} : Adopt the "Human Behaviour - Cognition in Context" (HuB-CC) framework (Constantino et al., 2021) for the design, testing, and implementation of theoretically robust virtual agents within groundwater systems.
C2 Diversity of human behaviour and temporal aspects	 G^a: Lack of detailed behavioural data to represent social heterogeneity. R^M: Employ the inverse approach (Epstein, 2023) to find agents' specifications and behaviours that can generate specific macro-level targets (e.g., patterns, trends, or desirable future outcomes). G: Incorporating adaptive and learning mechanisms into individual agents remains a challenge, especially at the institutional or management level, where applications are notably limited. F: Explore the use of artificial intelligence and data science techniques to enable agents to learn and adapt. R^M: Integrate the Institutional Grammar approach to GW-ABMs to capture the emergence and dynamics of institutions (e.g., through the MAIA framework (Ghorbani et al., 2013)).
C3 Two-way feedback loops	 G: Lack of coupled GW-ABMs operating at large spatial scales (e.g., multiple catchments or countries, up to continents or global-scale). F: Use the Telecoupling framework to develop Tele-coupled GW-ABMs. F: Develop and couple a mesh-free Analytic Element Groundwater Model to an ABM. R^M: Generate a tightly coupled GW-ABM using the MODFLOW API.
C4 Representation of groundwater governance and policy findings	 G: While the wider regulatory scholarship has developed multiple theories and approaches, a unified strategy for ensuring compliance and enforcement is still lacking (Black and Baldwin, 2010; Gunningham, 2011). The absence of consensus becomes even more problematic in the realm of groundwater regulation, where these theories remain also largely unexplored and untested (Holley et al., 2020). F: Harness interdisciplinary insights from the broader regulatory scholarship to develop a comprehensive framework that models the compliance behaviour of water users, and facilitates the simulation and evaluation of alternative enforcement strategies employed by regulatory agencies. R': Adequately plan and document <i>who</i> (which groups of stakeholders) needs to be involved in which steps of the model development and use process, to <i>what extent</i> (level of involvement) and <i>how</i> (see useful guidelines on Voinov et al., 2016, 2018).
C5 Methodological challenges in model development	 R^M: In case of re-using an existing GWM, critically assess and document the rationale for its validity in the context of the new GW-ABM study, specifying any recalibration efforts undertaken to ensure the model is fit-for-purpose. R^{M.a}: In situations of data scarcity, make use of the Pattern Oriented Modelling framework for inverse <i>calibration</i> over known patterns. R^M: Develop guidelines or adopt existing ones for <i>Model Output Corroboration</i> (e.g., Troost et al., 2023). R^M: Use global instead of local sampling techniques for SA. Document key design decisions, including the rationale behind the selection of minimum sampling size and methods for ensuring variance stability. Critically assess the adoption of existing systematic frameworks for SA (e.g., Borgonovo et al., 2022; Ligmann-Zielinska et al., 2020). R^M: Adopt a combined TRACE-ODD+D approach for <i>Model Documentation</i>, and make the source code of the model available.

^a The lack of empirical data is transversal to all challenges, and as such we highlight it with this symbol.

Designing and executing an ABM rooted in a behavioural theory is a challenging and resource-intensive endeavour that demands numerous considerations, especially when faced with the limited time and resources common to real-world management scenarios. Schlüter et al. (2017) outlines three key issues to consider. Firstly, accurately mirroring behavioural processes requires extensive empirical data. Depending on the selected theory, this might encompass spatially-distributed demographic information such as socio-economic status, dynamic environmental data such as land and water use, and attitudinal metrics capturing preferences, attitudes, and beliefs. Secondly, it calls for a multidisciplinary approach, given theories about human behaviour are scattered across various specialised domains (e.g., psychology, anthropology, political sciences, economics, etc.). Thirdly, theories are often not complete, requiring tailored conceptualisations and modelling assumptions when translated into computer code for specific problems and applications. This process might also entail making explicit assumptions about processes and mechanisms to establish clear causal relationships driving human decision-making.

Drawing from our own experience in developing GW-ABMs, we have pinpointed a crucial impediment in achieving a theoretically robust representation of human behaviour within these models. Despite various scholars conducting reviews of modelling approaches and techniques for simulating human behaviour at diverse decision-making scales (e.g., Kwon and Silva, 2020; Müller-Hansen et al., 2017), guidance remains scarce on the rationale for theory selection (*why*), identification of appropriate contexts (*when*), and determination of suitable application methods (*how*). The Modelling Human Behavior (MoHuB) framework (Schlüter et al., 2017) was conceived to address these issues, but falls short in capturing dynamic processes and the broader social and biophysical context that may sway agents' decision-making within groundwater systems. To fill this gap, a refined version — the Human Behaviour - Cognition in Context framework (HuB-CC)

— was developed. Grounded in cognitive psychology, HuB-CC aims to encapsulate essential features and processes that underlie perception, judgement, and decision-making (Constantino et al., 2021).

Within the realm of GW-ABMs, the HuB-CC framework offers a promising structured approach to ground agents' decisions on the substantial body of theoretical knowledge on human behaviour, thereby addressing critical gaps in theory selection and contextual application. By mapping 31 theories from behavioural and social sciences to decision-making elements, the framework serves as a gateway for more nuanced, theoretically-grounded models in resource management. As an illustration, consider a modelling scenario that aims to simulate farmers' decisions about groundwater extraction within the confines of regulated quotas and a shared resource. Using the mapping proposed by HuB-CC, we can identify a suite of theories that encapsulate critical and relevant aspects to this modelling scenario, such as Habitual Behaviour (Graybiel, 2008), Embodied Cognition (Wilson, 2002), Choice Architecture (Johnson et al., 2012), Trust and Reciprocity (Berg et al., 1995), Reinforcement Learning (Sutton and Barto, 1998), Social Norms (Bicchieri, 2005), Attention Restoration Theory (Kaplan and Kaplan, 1989), Affordance Theory (Gibson, 1979), Selective Attention (Posner and Petersen, 1990), Psychological Risk Dimensions (Fischhoff et al., 1978), and Prospect Theory (Kahneman and Tversky, 1979). To facilitate the framework's practical application, we have linked the database by Constantino et al. (2021) with current applications in GW-ABMs (see Table 6). By doing so, we hope to set the stage for the design, testing, and implementation of theoretically robust virtual agents within Agent-Based Models.

5.2. (C2) diversity of human behaviour and temporal aspects

Results from this review revealed significant advancements in incorporating and simulating social heterogeneity in coupled GW-ABMs, as

Mapping of theories to reviewed GW-ABMs. The first column sorts theories into four classes based on how they deviate from traditional rational choice theory: acknowl-edging cognitive constraints, recognising multiple goals, accounting for learning, or factoring in the broader contexts.

Conceptual origin	Theory name	GW-ABMs
Constraints	Bounded Rationality	Castilla-Rho et al. (2019) and Giordano et al. (2021)
Context (social)	Social Norms	Giordano et al. (2021)
Dynamics	Reinforcement Learning	Giordano et al. (2021)
Multiplicity	Theory of Planned Behaviour	Giordano et al. (2021), Mauser and Prasch (2016), Zhang et al. (2023) and Zolfagharipoor and Ahmadi (2021)
Constraints	Protection Motivation Theory ^a	Streefkerk et al. (2023)
Constraints	Dempster-Shafer Belief Theory ^a	Allain et al. (2018)
Context	Cultural Theory ^a	Castilla-Rho et al. (2019) and Rojas et al. (2022)
Context	Hofstede's Cultural Dimensions Theory ^a	Tamburino et al. (2020)

^a Theories used within GW-ABMs that were not found in the original table by Constantino et al. (2021). These have been included following the structural and conceptual guidelines of the initial framework.

studies predominantly opted to simulate each single individual instead of relying on spatial aggregations (see Fig. 8), and also multiple agent types rather than a single uniform type (see Fig. 9). These studies, however, also showed that collecting the detailed behavioural data required to populate ABMs is still a significant challenge.

All ABMs examined in this review have followed what is referred to as the forward approach (Epstein and Axtell, 1996), where carefully handcrafted agents (the micro) are created to represent real-world entities (such as farmers or households) and their behaviours (such as water use decisions). These agents are then placed within an environment (the groundwater system/aquifer) where they interact and make decisions based on specified rules. Researchers then study how these agents affect the coupled system (the macro) by exploring its dynamic response through relevant performance metrics (e.g., groundwater drawdowns). While insightful, this approach poses a significant challenge when data about individual behaviours are scarce or incomplete. To address this limitation, the inverse or backward problem emerges as a promising approach (Epstein, 2023). Here, the macro-level targets are first defined - including patterns, trends, and desirable future outcomes, informed or not by empirical data. Then the agents' behaviours, often guided by theory, are allowed to evolve within an evolutionary framework such as genetic programming (Gunaratne et al., 2023; Vu et al., 2023). This model discovery process results in a rich landscape of possible agents' behaviours that can generate the selected macro-level targets.

During our examination of the human diversity challenge, we emphasised the essential role that learning and adaptation play in evolving individuals' decisions in response to changing circumstances (e.g., weather, policies, social interactions, etc.), and thus steering the dynamics of a groundwater system. Accordingly, we analysed whether these dynamic processes have been explicitly simulated in coupled GW-ABMs to date, and documented the techniques used by scholars. Results indicated a tendency towards the explicit inclusion of learning and adaptation mechanisms within GW-ABMs. However, the multitude of methods used to program these mechanisms highlights the continuing challenge of including these aspects (Kiel et al., 2021; Filatova et al., 2013). To bridge this gap, promising avenues for future research are coming from artificial intelligence and data science, such as the use of reinforcement learning and convolutional neural networks to equip agents with the intelligence of self-learning their behaviour rules directly from data (An et al., 2023).

We also uncovered that only a few studies have introduced management-level agents capable of adapting their policies during a simulation, particularly in response to droughts and local hydraulic properties (Du et al., 2020, 2022). This focus on institutional adaptation is noteworthy because Agent-Based Modelling scholarship has often overlooked the role of regulators and management institutions (Lippe et al., 2019). Adaptation at this level, however, has been advocated for more than a decade, and is at the forefront of modern water resources management approaches such as Adaptive Water Management (Pahl-Wostl, 2006; Pahl-Wostl et al., 2012; Schoeman et al., 2014; Varady et al., 2016) and Dynamic Adaptive Policy Pathways (DAPP) (Haasnoot et al., 2013).

To facilitate the adoption of management-level adaptation, we propose leveraging the well-established Institutional Grammar approach (Crawford and Ostrom, 1995), which decomposes institutions into five key elements: Attributes, Deontic, aIm, Conditions, and Or else (ADICO). This approach has been refined over the last four decades (Dunlop et al., 2019), and has gained significant traction in the Agent-Based Modelling community (Ebenhöh and Pahl-Wostl, 2008; Frantz et al., 2016: Ghorbani and Bravo, 2016: Ghorbani et al., 2017: Powers et al., 2018; Smajgl et al., 2008), especially for formalising institutions related to Common Pool Resource problems (Pitt et al., 2012; Lewis and Ekart, 2017; Kurka and Pitt, 2017). The MAIA meta-model framework (Ghorbani et al., 2013) builds upon this approach to systematically incorporate institutions into ABMs, as demonstrated in recent flood risk management models (Abebe et al., 2019). These developments underscore the untapped potential of integrating Institutional Grammar into GW-ABMs, a sentiment echoed in recent literature reviews for ABMs (Siddiki et al., 2022). By doing so, we can develop more comprehensive policy scenarios and explore how institutions evolve within the systems they influence (Ghorbani, 2022).

Lastly, given the differences between learning and adaptation are not universally agreed upon in the literature, future research could expand the scope and depth of this review by reviewing each concept separately

5.3. (C3) two-way feedback loops

Our results showcased a prevalent use of 3D physically-based distributed and transient GWMs, along with a grid-based and GIS-backed social space in the ABMs. In other words, to date, coupled GW-ABMs have relied on an accurately simulated aquifer which dynamically and spatially heterogeneously responds to the action of geographicallyplaced agents, steering their decisions and interactions. Although these findings reveal technical and capable models, there are in our view exciting future research directions that can bring novel insights into the interconnections between groundwater and social systems.

Firstly, critical policy issues such as climate change, water and food security, operate at spatial scales larger than catchments, spanning multiple distant regions in an increasingly interconnected world. While there has been a proliferation of continental to global scale studies of groundwater systems during the last decade (Gleeson et al., 2020), these studies often incorporate human impacts into global hydrological models using a water balance approach rather than directly simulating groundwater fluxes and heads (Condon et al., 2021). A coupled GW-ABM offers several advantages over this traditional approach given its flexible design (Heppenstall et al., 2021), that cater to a holistic understanding of the interplay between social and groundwater systems, and thus have been proposed in the field of global hydrology (Bierkens, 2015). GW-ABMs operating on a large spatial scale (defined for simplicity as above 100.000 km²), however, are exceptionally rare. We believe the absence of coupled GW-ABMs operating at large scales can be partially explained by current methodological challenges, including model parameterisation demands, uncertainty quantification, and the taxing computational costs of such endeavours (Heppenstall et al., 2021; Manson et al., 2020).

A promising way forward to overcome these challenges has emerged in the broader Sustainability Sciences under the tele-coupling framework (Kapsar et al., 2019; Liu et al., 2013). This framework provides a hierarchical model and a common terminology to identify and understand distant (i.e., "tele") interactions in and among systems. The framework has been used and advocated for both water resources (Yang et al., 2016) and groundwater management (Luetkemeier et al., 2021), and has been adapted for an Agent-Based Modelling architecture (Dou et al., 2020), followed by calls for a new generation of Telecoupled ABMs in a recent article (An et al., 2021). By connecting multiple GW-ABMs, it becomes possible to simulate, for instance, how water extraction decisions by farmers (agents) in one region (sending system) impact the groundwater levels and agricultural practices in another region (receiving system), mediated by trade, policies, technology transfer, and climatic influences (flows). This telecoupled model would directly capture the underlying motivations and interactions of agents (causes) and the broader socio-economic and hydrological impacts (effects) within and beyond the two main systems (i.e., spillover systems). By gradually expanding the spatial scale under a coherent conceptual framework, tele-coupled GW-ABMs can enable an integrated analysis of how human decisions, grounded in localised contexts, can reverberate through the intricate web of interconnections that link distant groundwater systems.

Secondly, GWMs are complex tools that demand high levels of data for proper characterisation and obtaining reliable predictions for scenario analysis. Alternatives to these complex and data-demanding physically-based groundwater models are possible by using Analytic Element Groundwater Models (AEGWMs) (Strack and Haitjema, 1981a,b). In our review, we did not detect any use of the AEGWMs, despite current advancements in open-source libraries that would facilitate the coupling with ABMs (see Bakker and Kelson, 2009). AEGWMs come with advantages and disadvantages (Bakker and Strack, 2003; Bakker, 2006, 2013a,b; Fitts et al., 2015; McLane, 2012). For example, AEGWMs are known for their computational efficiency and flexibility, precise representation of complex hydrogeological features without the need for a computational grid, and can handle problems with an infinite or semi-infinite domain. On the downside, AEGWMs struggle with non-linear problems (e.g., unsaturated and density-dependent flow) and may not be suitable for problems where aquifer heterogeneity is relevant. Considering these disadvantages, coupling an ABM with an AEGWM can therefore offer several opportunities including: a less computationally demanding coupled model, making it more feasible for large-scale or long-term simulations; the absence of a restrictive mesh or grid, which can be advantageous when working with ABMs that often require to represent complex spatial interactions between agents. However, it is important to note that the coupling of ABMs and AEGWMs can also present challenges, such as the need for extensive data, the complexity of model integration, and potential issues with model output corroboration and uncertainty.

Thirdly, the rapidly evolving landscape of groundwater modelling opens multiple avenues for the future development of coupled GW-ABMs. From the untapped potential of versatile software, such as COMSOL Multiphysics (Li et al., 2009), to novel machine learning techniques and methods applied to simulate groundwater dynamics (Hussein et al., 2020; Tao et al., 2022). Notably, an Application Programming Interface (API) has been recently introduced for MODFLOW (Hughes et al., 2022), the prevalent software used by developers of GW-ABMs, which allows for direct interaction with this program without the need to alter its source code. For many existing MODFLOW coupling applications, the data provided to MODFLOW needs to be updated multiple times within a single time step which in our experience severely impacts memory usage and model run times. This makes the MODFLOW API a powerful tool for socio-hydrologists and other professionals who need to model groundwater flow and integrate these models with ABMs. Interfacing an ABM with a GWM using the MODFLOW API presents both advantages and challenges. On the advantage side, the API allows for a seamless integration of the two models, enabling the ABM to interact with the GWM in real-time and adjust variables without modifying the source code. This can lead to more accurate and dynamic simulations of complex systems, where human actions and groundwater responses interact. However, there are also challenges associated with this approach. The integration of two complex models can be computationally intensive and may require significant technical skill and computational resources. Furthermore, the process of interfacing the models can be complex, requiring a deep understanding of both the ABM and GWM, as well as the MODFLOW API itself. Additionally, the need to update information multiple times within a single time step, as required by many MODFLOW coupling applications, can add another layer of complexity and computational overhead to the modelling process. Despite these challenges, the potential benefits of a tightly coupled ABM and GWM, facilitated by the MODFLOW API, can offer significant research opportunities.

5.4. (C4) representation of groundwater governance and policy findings

Groundwater sustainability challenges can be traced back to the decisions and behaviours of autonomous agents (An et al., 2021). Through computational experimentation of possible alternative futures, simulation models provide a pathway to explore the outcomes of different policies and thus inform resource management efforts (Gilbert et al., 2018; Squazzoni et al., 2020). However, traditional simulation tools are often not prepared to represent the diverse set of groundwater regulations and the hierarchy of groups and institutions that support and/or enforce them. To understand the progress of coupled GW-ABMs towards facing this challenge, we concurrently reviewed and documented which policies have been evaluated to date, and whether the compliance behaviour of individuals and the role of enforcement have been represented. Remarkably, our review revealed a prevalent policy-oriented focus of coupled GW-ABMs (83% of the corpus), and a landscape filled with examples of policy evaluations (see Fig. 13), which show what happens when we move outside the realm of simplistic models and assumptions to capture complex phenomena. Inspired by these efforts, we identify various gaps and areas for future research.

Managed aquifer recharge (MAR) comprise a wide and growing range of methods aimed to support active management of groundwater resources at the local and basin level (Bouwer, 2002). MAR systems have had a remarkable growth in applications in the past 60 years given its potential to replenish over-allocated and restore brackish aquifers, and even enable energy recovery (Dillon et al., 2019). As a demand-side management strategy, MAR systems rely on the actions of individuals for their success. With legislation now allowing individuals to bank treated storm-water or wastewater, and to also market the resulting credits (Lall et al., 2020), it becomes an interesting area of future research to critically assess the circumstances which favour the adoption of these practices, and the overall effect of the human component on their success in restoring or maintaining groundwater sustainability and quality (e.g., see the study of Bolton and Berglund (2023) assessed in this review).

The pressing issue of anthropogenic groundwater contamination demands an understanding of both the intricate physical processes involved (flow and transport of contaminants), and the social drivers that underpin this degradation, including the values, norms, and decisions of water users. In this context, we anticipate a growing trend in the application of coupled GW-ABMs to simulate the role of farmers (e.g., decisions about the application of fertilisers, pesticides, hormones, antibiotics, and steroids consumed by livestock), households (e.g., usage of treated and untreated wastewater, septic systems, and other land treatment of solid and liquid wastes), and commercial/industrial (e.g., discharge or injection of a wide range of chemicals into groundwater) water users (Lall et al., 2020). These applications also hold promise for coastal aquifers, where the intricate saltwater intrusion processes add another layer of complexity to the transport of contaminants from land-based sources, placing them at more risk (Elshall et al., 2022).

The enforcement of groundwater rules and regulations is seen as a cornerstone component of effective groundwater governance systems (Closas and Villholth, 2020; Rodella et al., 2023), with compliance serving as an essential pillar in sustaining any policy effort (Felbab-Brown, 2017; Rouillard et al., 2022). While our review revealed the explicit simulation of water users compliance behaviours and dynamic responses to enforcement (e.g., see Castilla-Rho et al., 2017), there remains a noticeable gap in understanding the role and the effects of the hierarchy of institutions and enforcement strategies in achieving compliance, which resonates with findings of previous research (e.g., see Kaiser et al., 2020; Lippe et al., 2019) and emphasises the need for focused exploration in this area. Notably, this gap is also reflected in the wider regulatory scholarship on compliance and enforcement, where numerous proposals have been put forth to address a key challenge faced by regulatory agencies: how to intervene in the affairs of regulated enterprises to foster compliance, such as graduated, responsive, smart, meta, and risk-based regulation (Black, 2010a,b; Coglianese, 2017; Gunningham, 2010). Furthermore, there has also been a significant progress in understanding the motivations of regulated entities to comply (Parker and Nielsen, 2011, 2017; Parker, 2021), and in particular with groundwater allocations (Holley et al., 2020).

This situation presents a timely opportunity for coupled GW-ABMs to synthesise interdisciplinary knowledge, establish a robust behavioural framework for simulating water users, and computationally experiment and test the efficacy of competing regulatory strategies. Indeed, the widespread failure to comply with enacted groundwater legislation in many countries, along with inadequate enforcement power (Food and Agriculture Organization of the United Nations, 2016), makes the insights from these analyses particularly valuable. A GW-ABM, for example, can help elucidate who (water user type), where (geographical location), when (such as during dry or wet periods), and why (motives) complies or not with a given groundwater policy, and reveal the aggregated effect on the sustainability of the underlying groundwater system. The complexity of grounding the behaviours and attributes of virtual agents in conceptual theories, however, underscores the need for active collaboration with stakeholders throughout the modelling process.

Building on this, our review revealed that many studies have actively involved stakeholders during model development (16 studies), aligning with the growing momentum and agreement on stakeholder integration in managing challenges related to surface water (Carr et al., 2012), groundwater (Elshall et al., 2022; Hynds et al., 2018; Simpson and De Loë, 2020), and natural resources (see Perrone et al., 2023, and references therein). Certainly, appropriate stakeholder participation has been recognised as the most critical piece (Elshall et al., 2020) and essential prerequisite (Barthel et al., 2017) for successful groundwater management. A view that is endorsed by numerous global organisations (e.g., Food and Agriculture Organization of the United Nations, 2016; UNESCO and Sánchez, 2022; UNESCO World Water Assessment Programme, 2023; Rodella et al., 2023; Wijnen et al., 2012), and reflected in modern groundwater regulations (e.g., the California Sustainable Groundwater Management Act, the EU Water Framework Directive, among many others).

The benefits of including stakeholders broadly include saliency, credibility, and legitimacy (see Elshall et al., 2020, and references therein), a shared understanding among diverse participants (social learning and co-learning), and a greater adoption in practice (see Baldwin et al., 2012; Basco-Carrera et al., 2017, and references therein). These benefits extend also to integrated modelling efforts (Voinov et al., 2020), and resonate with calls within the Agent-Based Modelling community for extensive collaboration between public stakeholders and academic scholars to *co-design* models (Squazzoni et al., 2020). Thus, we urge practitioners to adequately plan and document *who*

(which groups of stakeholders) needs to be involved in which steps of the model development and use process, to *what extent* (level of involvement) and *how* (see useful guidelines on Voinov et al., 2016, 2018). Lastly, since our review did not evaluated the quality of the participatory processes or their outcomes, future research could explore these areas. For instance, by using the framework developed by Basco-Carrera et al. (2017), which provides a systematic way to choose a participatory approach based on a ladder of *participation* levels, different types of *cooperation*, and other relevant factors.

5.5. (C5) methodological challenges in model development

In the Introduction section we highlighted several methodological issues that coupled GW-ABMs face, which determine their quality and credibility. Then, in the Methods section we proposed and adopted the 'Evaludation' framework as an integrative approach under which to group and consider these issues, and subsequently defined and reviewed four of its six elements. Now, we weave key results from this assessment to highlight gaps and present future research directions under each of these elements.

i. Model Output Verification: Calibrating the GWMs is a necessary step (Poeter and Hill, 1997), especially in the face of limited data, which can amplify the uncertainty in model predictions (Zhou et al., 2014). Our review revealed that while distributed numerical GWMs are widely used, only 54% of them have undergone calibration. Furthermore, in many coupled GW-ABMs, the employed GWM originated from prior research. If the original GWM was designed for a different objective, however, a re-calibration could be essential before integrating it with an ABM. Yet, our review found only one study acknowledging this limitation (see García et al., 2019). This gap may be attributed to the substantial resources required for a re-calibration exercise. Thus, it is paramount that modellers critically assess and document the reasons why the re-use of an existing GWM is valid for coupling it with an ABM.

The lack of individual-level behavioural data, compounded by the taxing and complex resulting GW-ABM coupled architectures, creates substantial difficulties for performing rigorous parameterisation (An et al., 2021), especially if both systems (physical and social) are targeted jointly (note only 12 studies performed these on both, as highlighted on Fig. 14). In line with previous reviews of ABMs (Thiele et al., 2014), we also found an overall low adoption of model output verification efforts. However, given coupled GW-ABMs are gaining traction in regulatory and legal contexts, the importance of these efforts cannot be overstated (Bair and Metheny, 2011). To address these challenges, we recommend that future modellers explore and harness the established Pattern Oriented Modelling framework. When used for model output verification, each pattern can act as a selective filter for parameter values, discarding those that do not generate the observed phenomena according to selected criteria (Grimm and Railsback, 2012). In the context of a GW-ABM, these patterns may relate to physical or social aspects. By focusing on and accurately reproducing multiple tangible and recognisable patterns, this approach can enhance the robustness and reliability of GW-ABMs, thereby facilitating their acceptance and adoption by decision-makers (Topping et al., 2012).

ii. Model Output Corroboration: ABMs attempt to model complex social systems for which there is usually no independent data against which to compare selected model outputs to assert validation (Kiel et al., 2021). This difficulty has led to a heated debate and multiple re-definitions of *what* is required from a model to be deemed credible and fit-for-purpose, and *how* to achieve this milestone for different modelling purposes (e.g., see An et al., 2021; Heppenstall et al., 2021; Sargent, 2013; Troost et al., 2023). To provide relevant insights while navigating this complex and contentious issue (Heckbert et al., 2010), we focused our review towards (1) understanding what ABM 'validation' means to modellers, and (2) capturing the current techniques used, including the matching of simulation to empirical data (included in the model output corroboration element of

the 'Evaludation' framework). Interestingly, our results showed that various interdependent approaches are being used altogether, targeting both conceptual and empirical aspects, which aligns with previous recommendations (e.g., see Bert et al., 2014; Daly et al., 2022).

The methodological diversity uncovered by our review, featuring different approaches applied in various combinations and to varying degrees, suggests an absence of standard guidelines for selecting suitable methods pertinent to a specific context or modelling purpose. Hence, an encouraging research direction to help progress the validity, credibility, and uptake of GW-ABMs could lie in the development of such standards for model output corroboration. In this vein, a promising framework was recently introduced by Troost et al. (2023), aimed to assist modellers in making appropriate choices during simulation analysis and to substantiate them with sound reasoning. Their "Keep It Adequate" (KIA) framework consists of 12 questions that (i) define the modelling context, (ii) argue the adequate selection of models and methods for model inference and uncertainty documentation, and (iii) properly derive and interpret simulation results and their uncertainty. Policyoriented coupled GW-ABMs, in particular, might derive significant benefits from adopting frameworks like KIA, as it offers a structured approach that promotes transparency, fosters trust, and ensures models are tailored to the policy context. Careful evaluation and discretion should be exercised however when implementing this framework, particularly in budget-constrained scenarios, as its detailed structure might result in a time-consuming and resource-intensive modelling process. A critical issue that has been highlighted, for instance, in the traditional ODD protocol (Grimm et al., 2020).

iii. Model Analysis: Most of the GW-ABMs assessed in this review aimed to simulate and assess the performance of a policy using SA results as a key input to aid in decision-making. However, we detected a lack of methodological transparency with respect to the SA. For instance, critical design decisions, such as the selection of the minimum sampling size and variance stability (Lee et al., 2015), that are known to determine the resulting sensitivity assessment (Haghnegahdar et al., 2017; Razavi et al., 2021), were not clearly explained. Furthermore, our review revealed widespread use of Local sampling methods.While these might provide a fast initial exploration, they are less effective in systems exhibiting non-linear behaviour and interactions, characteristics typical in ABMs. Such techniques generally underestimate uncertainty and incorrectly estimate sensitivities, issues that are compounded by the lack of robust numerical methods and unrealistic model formulations (Kavetski and Clark, 2011), ultimately compromising the reliability, robustness, and credibility of the model results (Saltelli et al., 2019).

Given the crucial role SA plays in supporting policy and decisionmaking processes (Razavi et al., 2021), we recommend modellers to use the vast range of existing global SA techniques, such as variance-based (e.g., Sobol, 2001, Fourier Amplitude Sensitivity Test (FAST) Cukier et al., 1973, Random Balance Designs Fourier Amplitude Sensitivity Test Tarantola et al., 2006, etc.), derivative-based (e.g., Morris Morris, 1991, Distributed Evaluation of Local Sensitivity Analysis (DELSA) Rakovec et al., 2014, Derivative-based Global Sensitivity Measures Sobol' and Kucherenko, 2009, etc.), density-based (e.g., Delta Plischke et al., 2013, PAWN Pianosi and Wagener, 2015, etc.), variogrambased (Razavi and Gupta, 2016a,b; Razavi et al., 2019), among others. As to the lack of common methodological practices for conducting sensitivity analyses over coupled GW-ABMs, rather than pushing for a standardisation that might overshadow the need for flexibility of each modelling effort, we instead refer interested readers to some of the systematic frameworks that have been recently developed for ABMs, such as the six-step methodology proposed by Borgonovo et al. (2022) and the mixed-method approach proposed by Ligmann-Zielinska et al. (2020).

In our review, we consciously chose not to engage in a detailed exploration of how uncertainty permeates the modelling process of a GW-ABM, and its influence on the process of communicating the model and its results to the broader community. This decision stemmed from the expansive and complex nature of such an analysis, which would extend beyond the intended scope of our current work. However, we recognise that addressing uncertainty is crucial in the development and application of GW-ABMs. Thus, future research should focus on a systematic exploration of these uncertainties, the challenges they present, and their implications. Notably, while groundwater modelling has a rich tradition of uncertainty analysis with tools like PEST (Doherty, 2018a,b) and DAKOTA (Dalbey et al., 2020), such practices are less common in ABMs, possibly due to limited empirical data on individual level human behaviours (Heppenstall et al., 2021), as indicated by our findings (see the transversal gap in Table 5). This gap underscores the potential for significant advancements in integrating uncertainty quantification and analysis into GW-ABMs, paving the way for more robust and reliable models.

iv. Model Documentation: The absence of universally accepted standards for model documentation can make coupled GW-ABMs difficult to maintain, improve, and reuse (Daly et al., 2022; Voinov et al., 2020). Adequate documentation of the model's structure and analysis plays a pivotal role in promoting transparency, facilitating communication, and enabling proper evaluation and reuse, all recognised bottleneck problems within the Agent-Based Modelling community (An et al., 2020, 2021). In our review, we examined the methods that modellers have employed to document their models across the different stages of the modelling cycle, and focused on the current uptake of the ODD protocol. Our findings revealed a lack of common documentation standards, with researchers employing various tools (e.g., HydroShare and OpenABM) to different extents. Interestingly, the adoption of the ODD protocol among GW-ABM practitioners was strikingly higher than in the broader Agent-Based Modelling field - 29% over the 9.9% reported by Daly et al. (2022) - which suggests a growing acceptance of this documentation approach.

Building on the insights of this review and our own hands-on experience developing coupled GW-ABMs, we have identified various promising methodological directions that can instil a consistent and effective documentation culture that spans all the stages of the iterative modelling cycle. Firstly, we urge practitioners to produce a TRACE document (Daly et al., 2022; Schulze et al., 2017), which provides a comprehensive and standard format for documenting all the major elements of model development, testing, and use (Augusiak et al., 2014; Grimm et al., 2014; Schmolke et al., 2010). To communicate the Model description element of TRACE, we advise modellers to adopt the refined ODD+D protocol, which includes a rigorous basis (theoretical and empirical) for the selection of the human decision-making model (Müller et al., 2013). The adoption of this unified approach would not only promote transparency but also streamline good modelling practices within the field. Given the complexity and the resource-intensive nature of the implementation of these protocols, we anticipate this might result in substantial barriers to newcomers. Considering however its benefits we go as far as to suggest that publishers establish this combined TRACE-ODD+D as a prerequisite for publication of future coupled GW-ABMs.

Secondly, in line with the FAIR Principles for Research Software initiative (Chue Hong et al., 2022; Janssen, 2017; Janssen et al., 2020; Wilkinson et al., 2016), we recommend to make the source code of the model available. This can be published in community-of-practice repositories (e.g., CoMSES OpenABM, HydroShare, etc.) or through free-distribution platforms (e.g., GitHub or BitBucket).

6. Conclusions

Groundwater sustainability hinges on the decisions and behaviours of autonomous agents (An et al., 2021; Vörösmarty et al., 2013). The complexity in groundwater management arises from several factors: the uncertainty of human behaviour (C1); a heterogeneous social system comprising various water users and stakeholders (C2); intricate bidirectional feedback loops connecting social systems to groundwater dynamics (C3); and the multifaceted nature of groundwater regulations and the hierarchy of groups and institutions that enforces them (C4). Historically, computational and simulation models have aimed to guide policy development to steer groundwater systems towards sustainable trajectories. These methods, however, often fall short in addressing these challenges, leading to 'unintended consequences' (Merton, 1936), interventions that 'backfire' (Hammond, 2015), and the subsequent impacts on the social, economic, and environmental systems that critically depend on groundwater resources.

In this research, we present the first comprehensive and critical review of the state of knowledge of coupling Agent-Based Groundwater Models to study and manage linked human-groundwater systems. Our review unearthed key findings across the aforementioned challenges. We identified a crucial obstacle to achieving a theoretically robust depiction of human behaviour (C1), and suggested adopting the "Human Behaviour - Cognition in Context" (HuB-CC) framework (Constantino et al., 2021) for the design, testing, and implementation of virtual agents within groundwater systems. To address data scarcity issues for populating social system heterogeneity (C2), we proposed using Epstein (2023) backward method. This approach aims to find families of agents that are able to grow specified macro-level targets. We also highlighted promising avenues to capture critical feedback loops between groundwater and social systems (C3), such as the development of tele-coupled GW-ABMs, and GW-ABMs using Analytic Elements GWMs as well as the MODFLOW API. Our review also exposed a prevalent policy-oriented focus of GW-ABMs (C4), and a landscape filled with policy evaluations that illustrate the effects of stepping beyond the realm of simplistic models and frameworks.

In order to thrust future GW-ABMs to the highest standards of model development, transparency, and rigour for replicability and reusability, we offer a set of methodological recommendations favouring the use of global sensitivity analysis and model documentation following a combination of the TRACE and ODD+D protocols. We further provide promising avenues for future research for model output verification based on the established Pattern Oriented Modelling framework, and for GW-ABMs corroboration using the KIA framework for coupled model validation.

In a world where groundwater resources are increasingly strained by competing demands, climate change, and human interventions, the development of coupled GW-ABMs emerge as a critical tool for unravelling the drivers of groundwater sustainability and crafting more effective responses to this urgent issue. By integrating human behaviour with hydrological dynamics, GW-ABMs offer a comprehensive framework for modelling complex socio-hydrological systems. Through our review, we identify challenges, gaps and delineate a compelling agenda for future research, in the hope of inspiring readers to explore and harness this methodology and contribute to the sustainable management of our groundwater resources.

CRediT authorship contribution statement

Marcos Canales: Conceptualization, Data curation, Formal analysis, Methodology, Visualization, Writing – original draft. Juan Castilla-Rho: Conceptualization, Formal analysis, Writing – original draft. Rodrigo Rojas: Writing – review & editing. Sebastian Vicuña: Supervision, Writing – review & editing. James Ball: Supervision, Writing – review & editing.

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

I have shared the link to my data in the Attach file section

Agent-Based Models of groundwater systems - Database (HydroShare) https://doi.org/10.4211/hs.5e6cc59ec95b4aa2bcc8f0be8f8832fb

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT from OpenAI in order to assist in the writing and editing process. After using this service, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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Appendix A. Supplementary data

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