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Towards Best Practices in Isotope-Enabled Hydrological Modelling Applications

Final Report of a Coordinated Research Project

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TOWARDS BEST PRACTICES IN ISOTOPE-ENABLED HYDROLOGICAL MODELLING APPLICATIONS

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FINAL REPORT OF A COORDINATED RESEARCH PROJECT

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FOREWORD

The increase in frequency and intensity of extreme climatic events around the world since the early 2000s — such as droughts in California, United States of America (2011), Melbourne, Australia (2015), and Cape Town, South Africa (2017), and floods in Haiti (2004), Patna, India (2016), Cologne, Germany (2021), and Durban, South Africa (2022) — has highlighted the importance of hydrological forecasting under increasing climate variability. Recognizing the need for adaptive strategies used to ameliorate the effects of climate change on water resources, the IAEA has developed guidelines on the use and application of isotope-enabled hydrological models, which can enhance the predictive power of modelling catchment systems for hydrological forecasting and support more realistic water flux and storage simulations of the natural environment.

In recent years the advancement in hydrological modelling has allowed models to explore and develop complex environmental linkages, driving the predictive capacity of data used for forecasting extreme events. The use of isotopes in addition to volumetric water fluxes in hydrological models offers an alternative methodology to reduce model uncertainty, facilitate the selection of appropriate model structures and their parameters, and constrain dominant hydrological processes that are under a state of change. The need to restrict the loss of crucial ecologically sensitive systems, which are often highly complex, requires a multifaceted method integrating isotopes and hydrological modelling tools. These developments form the basis to explore a range of different nature based solutions and approaches to counteract the environmental consequences of a globally warmer climate.

This publication was designed to support beginner modellers or water managers and more advanced hydrologic modellers who may wish to learn about isotope-enabled modelling. Its development was supported by isotope hydrologists, data network specialists and modelling specialists from a range of different countries around the world. Examples of their isotope modelling applications have been provided to give context to the guidelines in this publication, where these examples highlight the versatility of isotopes across a range of different environmental and climate settings. Lessons from the application of isotope-enabled modelling techniques in each of the diverse climate and water settings are discussed.

This publication is an outcome of the coordinated research project, Isotope-enabled Models for Improved Estimates of Water Balance in Catchments, which was carried out by the IAEA between 2018 and 2023. Project participants from 13 countries used their unique modelling objectives and approaches. They shared their experience to develop a guideline on the best practice approach in isotope-enabled modelling. The IAEA officer responsible for this publication was Y. Vystavna of the Division of Physical and Chemical Sciences.

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1. INTRODUCTION

1.1.BACKGROUND

Climate change impacts freshwater systems and their management as was observed by projected temperature growth, sea level rise and precipitation variability [1]. Semi-arid and arid areas in many parts of the world are believed to be more vulnerable to the impacts of climate change on freshwater. Climate change affects both surface and groundwater resources and can lead to increased intensity and level of flooding in many parts of the world while simultaneously modifying drought patterns in other parts. These changes associated with climate change have significant ramifications on freshwater availability, sustainability, cost, and socio-economic aspects. Some areas are much more affected than others with one or more of the above consequences [1]. Global, regional, and local climate and water balance models are playing instrumental roles in understanding the extent and magnitude of these impacts on society and ecosystems. These models are used to estimate hydrological components such as evapotranspiration and streamflow and their variation in time and space. The stable isotopes in water molecule (^{18}O and ^{2}H) can be applied to identify the flow paths and residence times of water in a catchment and constrain the simulated water balance components (baseflow, soil water, groundwater and snowmelt contribution, etc). Global datasets of meteorological, hydrological, and physical variables become increasingly available and can facilitate the use of water balance models. Open datasets can improve an estimation of model parameter and fill the gaps in data where local measurements are limited or unavailable.

Separate tracing of the stable isotopologues of water (i.e., $^{1}H^{1}H^{16}O$,$^{1}H^{1}H^{18}O$, $^{1}H^{2}H^{16}O$) within ocean, atmosphere, land surface and coupled hydrological models, was first accomplished in the 1980s. Isotope-enabled models, which track the isotopic composition of water cycle components and simulate fractionation processes, have included atmospheric General Circulation Models (GCMs) [2-4], oceanic GCMs [5,6], regional climate models [7,8] and mesoscale hydrological models [9]. Recent trends in model development include fully coupled Climate System models [10,11] and Earth System Models (ESM) [12,13] as well as more efficient computational versions [14]. Isotope-enabled models have demonstrated high potential as validation tools, for sensitivity analysis, and inverse modelling of water cycling processes, as they benefit from additional mass balance constraints imposed by the physical-isotopic system. Applications have also included paleoclimate simulations to assist interpretation of isotope archives [15], study of convective precipitation and other complex climate processes [16,17], ecosystem water and carbon cycling [18], and hydrological processes [4,19-24]. Current trends in hydrological research at the catchment scale is for wider inclusion of isotopic tracers in an array of customized models of varying complexity at a range of scales, either designed to answer specific hydrologic problems or for testing current understanding of processes through calibration, validation, and model-data intercomparison.

Water balance modelling often involves the use of model parameters that are difficult to measure or estimate. It is common practice to apply model calibration, that selects the best combination of parameter values with the minimum difference between observed and simulated events. During model calibration, we may get the "right" answer for the "wrong" reason, whereby different combinations of parameter values may give the same "best" answer. This problem, known as equifinality [25], can be partly minimized using conservative tracers such as stable water isotopes that are used to evaluate different hydrological process simulations. Furthermore, the use of isotopes offers means to restrict optimization and parameters searching procedures to eliminate implausible model results and parameters combination. The IAEA has been exploring the practice of its Global Network of Isotopes in Precipitation (GNIP) and Global Network of Isotopes in Rivers (GNIR) data in different hydrological and climate models for application that can be used to support the water resources management in basins around the globe.

1.2.OBJECTIVE

The guideline was developed based on the results of the Coordinated Research Project F31005 – "Isotope enabled models for improved estimates of water balance in catchments" that gathered participants from 13 countries with different modelling objectives and approaches. In this guideline, project participants shared their unique experience on model selection, modelling objectives, data collection and modelling procedure. The IAEA, through the development of the collaboration in water resource management and isotopic application is advancing the best practice approach in isotope-enabled modelling to provide a consistent process and improve interpretation and suitability of the isotope-enabled modelling results. The purpose of the technical document is to provide a guidance on the best practice in isotope-enabled modelling for water resource management that covers different steps of modelling such as setting modelling objectives, identifying data sources and collecting data, provision of quality assurance of the data and understanding its limitations, model selection, different calibration approaches, and performance criteria.

1.3.SCOPE

The main scope of this technical document is to contribute to the improvement of hydrological modelling by using stable isotopes in water that can provide an additional means of water balance simulation, model calibration, and validation procedures. This in turn will improve model capabilities to forecast impacts of climate and other changes on freshwater availability and sustainability as well as isotope-based assessment and management of water resources in Member States of the IAEA.

The purpose of most hydrology surface-groundwater interactions and hydrochemistry modelling is related to providing information in support of decision making for some water management policy. Isotope-enabled hydrological models can provide the following information for decision makers in water resource management:

- Knowledge of the catchment runoff and water quality, and how these components vary in time and space, particularly under changing climate: seasonal, inter-annual, and inter-decadal.
- Estimation of the contributions of individual hydrological compartments in catchment (groundwater, surface runoff, etc.) to water availability in the catchment or even a much larger region, such as transboundary basins.
- Calculation of how hydrological components in the catchment and water availability altered over time in response to changes in the catchment, such as streamflow damming land-use, land management and climate changes.

In certain cases, with a high-quality and dense network of long-term flow gauges, hydrological observations can be used to estimate water sources and flow paths through the streamflow hydrograph separation. However, there are limitations to hydrometric process inferences in term of sub-surface water flow paths and transit time, which can only be resolved with additional tracer information. The more common situation is where short-term gauging stations, variable quality data, and gaps in spatial coverage take place. In this case, hydrological information can be projected using isotope-enabled hydrological models to estimate:

- Hydrological flow components (surface runoff, interflow and baseflow) for ungauged catchments.
- Water balance in ungauged catchments.
- Surface water – groundwater interaction, groundwater recharge, river baseflow and evapotranspiration.
- Estimate transit and residence times of waters as a link to water quality and biogeochemical catchment processes.

Isotope-enabled hydrological models can be used to forecast hydrological changes for some immediate future period (typically for an annual and multi-annual periods), trained on existing observations in the catchment. Isotope-enabled models can be used to assess land use or vegetation cover change in the catchment and simulate the flows that could occur under a variety of scenarios including past, present, and future modifications in the catchment. This may comprise assessment of a catchment setting that may be non-stationary in the observed records or simulated conditions. An additional advantage of isotope-enabled models is that they can be used to assess the potential impact of climate change on flows from both gauged and ungauged catchments. Although the estimation of magnitude of these impacts for ungauged catchment will be uncertain, isotopes provide a relevant means to constrain the modelled processes.

Among several challenges of implementing isotope enabled hydrological models is a lack of a well-designed guideline. This is particularly important considering the limited number of experts who are engaged in embedding isotope capability in water balance simulation. This guideline will be instrumental in describing basic approaches to be followed in efforts to model isotope enabled water balance models. Best practice isotope-enabled hydrological modelling can be described as a workflow of steps and actions taken to ensure that development, implementation, and application of isotope-enabled hydrological modelling corresponds to the planned purpose and achieves the optimal outcome. We consider that the recommended best practice can be highly dependent on data availability, time, budget, plus human and other resources. Hence, we developed a guideline in a generic way with the focus on the minimum standard isotope-enabled hydrological modelling workflow, available models, and case studies derived from the IAEA CRP, which included global catchments and a wide range of data availability. The modelling results are also subject to interpretation, which can be influenced by the overall state of knowledge and available technology. However, the knowledge and technology in modelling is progressively advancing over time with growing availability of machine learning tools, new remote sensing data sources coming online, and new computing hardware and software.

It is our belief that isotope-enabled hydrological models can offer more information than traditional hydrologic models alone, in that they provide critical information on flow paths, residence times, surface water-groundwater interactions, and water storage within catchments. This guideline is intended to support isotope-enabled hydrological model application with the objective of providing water managers, consultants, and research scientists with information on the use of isotope-enabled hydrological models, including model selection (fit for purpose), requirements, and guidelines for adequate calibration and validation of the model. The CRP focus was on regional or global water balance estimation, which guided the selection and availability of potential models and model inputs discussed here within. The practices proposed in this technical document are flexible enough and can accommodate variations that allow for continuous advancement the state of knowledge and technology in the hydrological modelling.

1.4.STRUCTURE

This publication discusses the different steps of the hydrological modelling that uses environmental isotopes, comparing advantages and disadvantages of isotope-enabled modelling. It also shows real examples of isotope-enabled model applications in different countries. The publication includes a general overview of procedures related to isotope-enabled hydrological modelling (Chapter 2) in terms of i) setting modelling objectives, ii) data collection, iii) selecting and setting-up of models, iv) calibration and validation, v) sensitivity analysis, vi) data management and accessibility. Additionally, the results of the diverse isotope-enabled model applications in 10 countries located in different geographic areas and climate zones are presented (Chapter 3). Discussions and future directions are presented in Chapter 4. The overall aim is to enable the reader to investigate hydrological modelling options using environmental isotopes and select the best approach towards isotope-enabled hydrological modelling for the purpose at hand.

2. OVERVIEW OF PROCEDURES FOR ISOTOPE-ENABLED HYDROLOGICAL MODELLING

2.1.PROBLEM STATEMENT AND SETTING MODELLING OBJECTIVES

The aim of the hydrological model is to resolve a specific task, which may include predictions into the future or for sites with no or limited data as well as improving understanding of the system being modelled [26,27]. This task then is the primary factor in deciding the appropriate model simplifications and assumptions and determining the characteristics of the mathematical model and associated code [28]. In this respect, the development of isotope-enabled hydrologic models has to be generic enough to address a wide range of applications and be transferable to different conditions where the model may be applied.

The modelling task (or problem statement) to be addressed has to be clearly articulated at the start of the project to guide the selection of the model and subsequent interpretation of modelling results. If a suitable model is not available, then consideration has to be given to invest in the modification of existing models or to develop new models to suit the task at hand. As water management decisions often involve more than one goal, it is important to identify all goals or objectives of the model at the start of the project and to list the objectives into different categories, according to their priority: primary, secondary objectives and so on. It is also worthwhile to reflect additional objectives and goals that can be raised in future. Guidance on model selection criteria is provided in Section 2.6.

2.2.BUILDING A MODEL

The choice of the isotope-enabled hydrological model will vary based on the purpose of the modelling, e.g., to understand the water balance of a catchment, seasonal low flow characteristics for an in-stream environmental need, to assess surface water-groundwater interaction, or to estimate overall catchment water yield on an average annual basis. When selecting a model, its predictive capacity and ability to fit the typical catchment response time are important. However, it is also important to consider the modelling time step and spatial discretization at which the intended hydrological processes are to be simulated. Moreover, certain processes, such as e.g., runoff generation, cannot be simulated at a coarse spatial resolution. Additional factors that should be considered are the modeler's preference and knowledge in using certain models, the aim of the modelling task, the time that is necessary to develop and apply a model, and the required level of accuracy. An issue in hydrological studies is determining which model is best applied to a specific catchment with certain hydrological conditions[26]. Section 2.6 provides further considerations for model selection.

Modelling steps usually follow the scientific method, where a question is asked, a hypothesis is constructed and tested, and then accepted or rejected. If rejected, the testing process is repeated with a revised hypothesis [28]. In general, the hydrologic models follow the same main steps (Fig. 1). When the purpose is clear, then the conceptual model can be built to describe the hydrological settings in the system and the components that should be simulated. Then various mathematical models can be applied to define individual hydrological processes in the catchment and the computer codes that exist in various computer languages selected (e.g., Fortran, C, Java, Python). These models should be calibrated/validated against available field-observed data; only once this is successfully complete, then they can be used to predict the hydrologic response to various external forces [29].

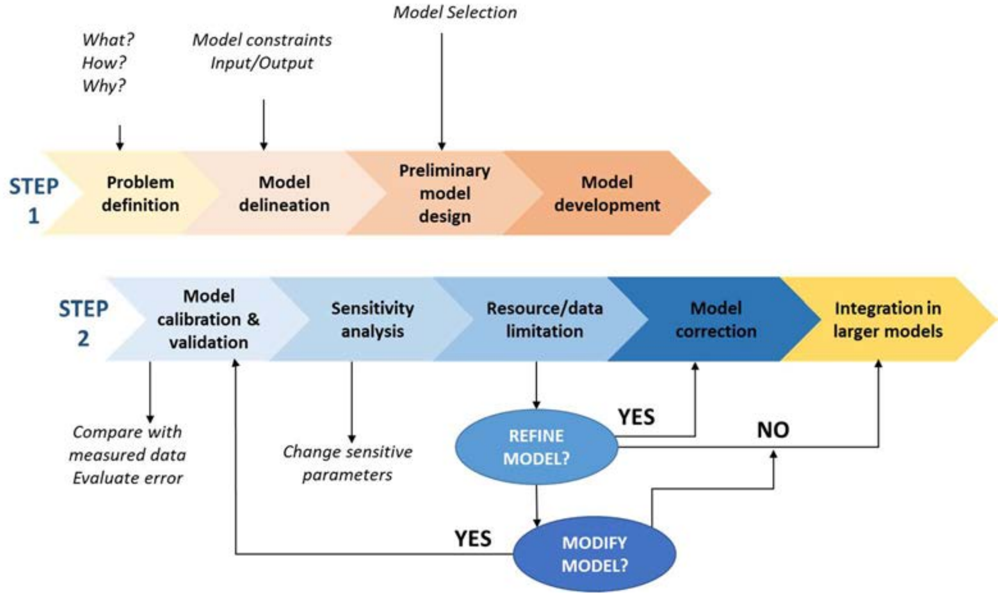


FIG. 1. Workflow of model selection and application. Refinements would be considered adding additional data (extending validation timeseries), whereas any change to parameters or structure would require recalibration.

Detail on the models available that are fit for purpose is provided in the Section 2.4.

2.3.DATA COLLECTION

Data collection is fundamental to drive and evaluate hydrological models. To describe the processes of streamflow formation [30,31], the precipitation amount (rainfall and snow) and other meteorological variables (e.g., air temperature, relative humidity, wind speed, radiation) are required as input to the model. The discharge data are generally used for model calibration and validation [30]. Spatially distributed models further require data on catchment properties such as land cover, soils and hydrogeology. More recently additional data on e.g., soil moisture and groundwater levels provide further insight into catchment behaviour and can help with model evaluation [32].

The data frequency depends on the model time step and purpose of the model application. Most hydrometric data is measured automatically (e.g., automatic weather stations, data loggers and sensors) at a sub-hourly scale satisfying rainfall-runoff modelling purposes. The data quality in form of gaps, outliers, errors, and non-stationarity is of crucial importance and should be carefully evaluated at the onset of a model application. Data gaps need to be filled and different methods exist to interpolate and extrapolate data time series even over longer time periods. Most recently, machine learning methods were used to fill data gaps, as were remotely sensed and global data sets [33,34].

Table 1 summarizes the minimum input data requirements for isotope-enabled modelling (in addition to the hydrologic and climatic data).

Often, isotope-enabled rainfall-runoff models use stable isotopes to evaluate these models, in addition to hydrometeorological data [35]. The data requirement includes stable isotopes (deuterium and/or oxygen-18) in precipitation and discharge, and may also use additional data on, e.g., soil water or groundwater isotope composition. Isotope data should be associated to the corresponding flux/volume data, but isotope tracers are commonly measured at a much lower frequency (daily to monthly) compared to the sub-hourly measured hydrometeorological data. Regarding precipitation isotope data, which is used as model inputs, the mismatch in data frequency requires adjusting data to precipitation measurements and model time step, particularly when using integrated models [36]. High frequency data can be obtained using automatic water samplers. The combination with isotope-enabled climate models [37] can also help to increase the precipitation input frequency [38].

Regarding streamflow isotopes data, which are used to evaluate the model, data frequency should ideally fit the characteristic response time of the catchment. River samples are usually collected manually on the back of routine water monitoring programs but can also be automated using water samplers. In-situ stable isotope measurements at sub-hourly frequency progressed over the last decade [39] but remain expensive and not feasible to operate at remote sites.

TABLE 1. MINIMUM RECOMMENDED DATA REQUIREMENTS FOR ISOTOPE-ENABLED MODELLING.

What to sample (minimum) →	δ_Q **Streamflow**	δ_P **Precipitation**	δ_{GW} **Groundwater**
Open Source(s)	GNIR	GNIP	Upon request to the Agency
Where to Sample	Outlet, major tributaries, subbasin (confluences) Co-located with gauging station to have corresponding hydrometric records	Match model input of precipitation time-series, co-located with meteostations. Depends on spatial discretization of model (lumped = 1, discretized >1)	Locate borehole/wells and collect screen depth, stratigraphy. Sample at different screen/well depths.
When/ How often	Minimum requirement to capture rising limb, falling limb and baseflow. Hydrograph analysis. Sampling frequency should be based on transit time in basin.	Monthly or less (event). Need continuous timeseries to drive the model (Δt dependent)	Yearly or less if seasonal variation.
Purpose of data	Calibration/validation	Input data to drive the model	Calibration/Validation (groundwater); Verification (surface water)

Additional data such as groundwater isotope composition, which can help with model evaluation, can be collected at a yearly/seasonal frequency. Main stem rivers should be sampled at the outlet, co-located with flow gauging station(s). Strategic sampling of basin tributaries that significantly impact the hydrograph shape or timing should occur above river confluences, to capture the unique signature of tributary inflows (Fig. 2).

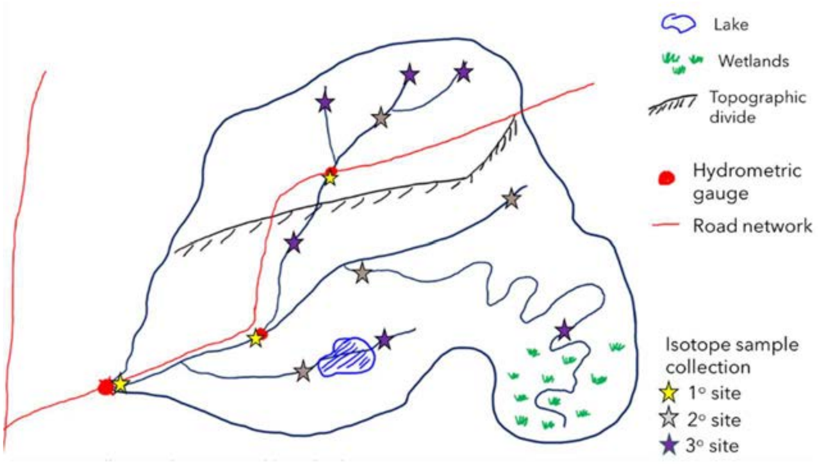


FIG. 2. *Isotope in streamflow sampling program designed to support minimum modelling efforts (1^0 sampling) to more detailed mixing model analyses (2^0) and headwater basin analyses (3^0).*

The number of sites sampled across the basin will likely depend on cost (availability of funding) and purpose of sampling. A tiered approach to sampling could be envisioned in Fig. 2, where primary (1°, yellow stars) samples are the most important (co-located with hydrometric gauging sites), secondary (2°, grey stars) samples emphasize tributary inflows for mixing model separations, and tertiary (3°, purple stars) sites afford more detailed headwater to downstream longitudinal profiling. Users should be cautious about relying on data from laboratories that have not participated in IAEA laboratory intercomparisons, as isotope data could be subject to errors if not properly compared to a standard.

2.4.CALIBRATION AND VALIDATION

Calibration is maybe the most important step in the modelling process, because it helps establish the legitimacy of numerical models and potential fitness for forecasting or long-term project simulations. Calibration can be described as a process of systematic adjustment of model parameter’s values and selection of a parameters set which provides the ‘best estimate’ of the water balance in a catchment, relative to observed data. As applied to hydrological models, validation means confirmation that results of the model calibration are robust, or acceptable for the planned purpose outside of the calibration period or conditions [40,41].

Model fit with isotope-enabled hydrological models is evaluated with the same performance statistics available to any hydrological model, such as the Kling-Gupta efficiency (KGE), the Nash-Sutcliffe efficiency (NSE and its logarithmic version lnNSE), the Root Mean Squared Error (RMSE), etc. More detailed information on performance metric selection in sections 2.4.3 and 2.4.4.

2.4.1. Calibration and Validation Approach

In catchments where there may not be sufficient data available (common for isotope-enabled applications), it is common to conduct calibration and validation over shorter periods within the full record. What is crucial is to ensure a range of wet and dry conditions are represented within each dataset for robust model calibration and validation. It is common in research studies to split the observed data sets into sequential calibration (two-thirds or one-half of the data) and validation (one-third or one-half of the data) preceding the study, to establish the model performance under these sets of conditions. This may be problematic in catchments with shorter records and decadal wet and dry cycles and may result in satisfactory performance for the calibration/validation data set but unsatisfactory results for the validation/calibration data set. Alternative approaches are to calibrate the water balance or runoff model to all available data (for catchments with very short records) and to show that the performance of the model is satisfactory over different data sets at the period when observed data is available. Alternatively, non-sequential calibration and validation years can be selected, should there be sufficient periods of record, ensuring both wet and dry periods are captured within both the calibration and validation data sets. Commonly, a flow time series is required from several catchments or sub-catchments within the model domain to conduct a spatial (versus temporal) calibration and validation from two or more stream flow gauges. While not all models are able to do this, an optimization procedure is able to disaggregate the missing data.

2.4.2. Calibration Best Practice

The efficiency of the calibration process can be maximized through defining and documenting the calibration and validation approach before beginning a modelling project. At the same time, it helps to avoid the temptation to “overfit” the model to noise in the observational data. We advocate a FAIR Principles (Findable, Accessible, Interoperable, Reusable) based approach to model development, that includes documenting and ensuring reproducibility of any calibration strategy [42]. A calibration strategy should therefore *a priori* outline and document in an accessible manner: (i) places where model calibration and validation will be done; (ii) acceptable and viable ranges for each model parameter value; (iii) identified constraints, dependencies, or relations among parameter values; (iv) calibration and validation periods at each place and (v) expected or calculated uncertainty in observations introduced by measurement uncertainty.

Additionally, a metric selection rational and application for calibration and validation performance should be documented. It may be beneficial also to select and justify a manual or an automated calibration strategy and document how a hybrid strategy of progressive manual and automated calibration was implemented. In case an automated or hybrid optimization strategy is used, the following additional details should be defined to ensure the transparency of the used methodology:

- Algorithms to be used for optimization of parameter values.
- Rationale for metric selection.
- Objective function(s) that will be applied to test the calibration procedure.
- To encourage fitting to different parts of the flow regime, weightings that may be applied in computation of objective functions.
- The set of model parameters that will be optimised through calibration procedure.
- Constraints on the allowable range of values for each parameter in the set used in modelling.
- Variables included in the multi-objective calibration (i.e., using two isotopes and/or additional tracers).

Ideally, the calibration approach should be known preceding the start of the calibration process. It is also appropriate for the calibration strategy to be reviewed and revised during the calibration. Guidance on isotope-enabled model calibration decisions, processes, and approaches across a variety of catchment sizes, geographic domains and data requirements can be found in the literature [43-45].

2.4.3. Calibration and Validation Efficiency Criteria

To evaluate model performance for different aspects of the simulated hydrograph and compare the results to previously reported values, goodness-of-fit or efficiency criteria are applied [46-48]. Frequently used efficiency criteria include: NSE in standard squared form, the relative volume error (PBIAS), KGE and RMSE. While the NSE has been widely applied in hydrological modelling, applications that assess overall model performance may be mis-represented as the NSE tends to over-emphasize peak flows due to the calculation of the mean square differences between simulated and observed streamflow [49,50]. As a result, other more balanced criteria such as the KGE [51] or a combination of criteria, such as lnNSE (commonly used to evaluate model performance at low flows) together with PBIAS and RMSE, can be used to evaluate model performance for high, median, and low values of the calibration target. While the above-mentioned efficiency criteria are commonly applied to an objective function evaluating the overall agreement between observed and simulated streamflow, we recommend the use of KGE or RMSE when fitting/evaluating objective functions using isotope data [45]. See Section 2.4.5 on performance metric selection. Isotope-enabled model evaluation can also be related to isotope mixing for flow component proportioning, reach mixing to quantify different sub-basin contributions, evaluation of simulated evapotranspiration using isotope fractionation, timing of flow and residence time, amongst other applications. Application examples are shown in the Chapter 3. As a result, it is important to ensure that the general trends within these applications are assessed while minimizing the effects of measurement errors within the isotope data.

The efficiency criteria for evaluating models can be performance ratings based on monthly time steps [48] (Table 2). The isotope data is often negative values, meaning that lnNSE or logarithmic form of KGE cannot be used.

TABLE 2. EFFICIENCY CRITERIA TO EVALUATE THE AGREEMENT BETWEEN MONTHLY OBSERVED AND SIMULATED STREAMFLOW

Performance Rating	NSE	PBIAS	KGE*
Very good	$0.75 < \text{NSE} \leq 1.00$	$\text{PBIAS} < \pm 10$	$0.60 < \text{KGE} \leq 1.00$
Good	$0.65 < \text{NSE} \leq 0.75$	$\pm 10 < \text{PBIAS} \leq \pm 15$	$0.50 < \text{KGE} \leq 0.60$
Satisfactory	$0.50 < \text{NSE} \leq 0.65$	$\pm 15 < \text{PBIAS} \leq \pm 25$	$0.30 < \text{KGE} \leq 0.50$
Unsatisfactory	$\text{NSE} \leq 0.50$	$\text{PBIAS} \geq \pm 55$	$\text{KGE} \leq 0.30$
Evaluation threshold^	$\text{NSE} = 0$	n/a	$\text{KGE} = -0.41$

*Based on [51], non-modified KGE formulation as outlined by [50].

^Minimum value of evaluation criteria that represents an improvement above the long-term mean.

When rating performance and evaluating objective functions for daily time steps, the efficiency criteria class usually shifts to one below (i.e., $0.65<NSE\leq 0.75$, 'Good'). Note that basin scale, region of application (data availability) and model type will impact benchmark efficiency criteria, meaning the larger the basin the more likely it is to have lower model performance.

2.4.4. Calibration Methodologies

At locations where hydrologic and isotopic data are available and streamflow or runoff estimates are required, several options for model calibration strategies are available to the modeller:

(a) Single objective calibration.
The calibration of a single model performance metric to derive the optimal solution (parameter) set for a single model variable (e.g., streamflow) over the calibration period.

(b) Multi-criteria calibration.
Involves the calibration of one or more model variables, which means the user has to first decide what is to be calibrated (e.g., streamflow and one or more tracers). This involves calibration of different model variables either separately or combined using a hybrid performance metric (combination of a series of model evaluation metrics). The methodology of calibration, however, does not significantly differ from that of single objective calibration, other than perhaps the selection of model performance metrics or derivation of a hybrid metric for minimization/maximization.

(c) Multi-objective calibration.

Like multi-criteria calibration, this involves the calibration of one or more model variables, which means the user has to first decide what is to be calibrated (e.g., streamflow and one or more tracers). Unlike multi-criteria calibration, however, multi-objective optimization considers the entire solution space for all variables in tandem and selects a set of "optimal" solutions (i.e., non-dominated) that represent equally satisfactory outcomes for the models' performance. No one optimal solution is defined using this method, but instead the modeler has control over the optimal solution they select, which represents a trade-off among the variables being optimized. For example, the best streamflow simulation in a hydrologic model likely does not correspond to the same parameter set used to derive the 'best' isotope ($\delta^{18}O$ or $\delta^{2}H$) simulation. In this case, the optimal model performance resides in strong outcomes for both variables – selected by the user and guided by the model application or intended use.

Similar to the hydrological models, the models used with application of isotopes may be calibrated independently for each catchment. Here, independent parameter sets will be obtained for each catchment, or a joint calibration may be applied. During the joint calibration, all models are calibrated with regional parameters to fit to the gauge records from two or more gauges. A single set of model parameters will be produced for all modelled catchments used to fit the flows at all the gauges within that group. It is the most common procedure for regional or global water balance modelling due to the computational demands and memory required for input (including parameters) datasets.

Calibration of the model normally involves running the model may (thousand) times or trials, testing different values of parameter within the parameter space (defined by upper and lower parameters boundaries), with the aim of improving the fit of the model to the calibration data and to reduce the generation of implausible parameter values. This is best done through automated methods and scripting using calibration algorithms such as Ostrich and the Non-dominated Sorting Genetic Algorithm (NSGA-II). Automated calibration can be facilitated by user input, however, in a variety of ways:

- Manual definition of starting values and ranges of parameters, requiring distinct knowledge of the model and catchment.
- Definition of optimization seed values or starting points and number of trials required to reach an optimal (set of) outcome(s).
- Using a hybrid approach of semi- automated optimisation phases, combined with manually implemented or defined trials of parameter sets.

2.4.5. On performance metric selection

Model evaluation during calibration and validation is only as good as the metrics selected to evaluate the model by. Meaning, if a single performance metric is used, the model outcome will likely be insufficient or non-robust across a variety of catchment responses and climatic conditions. If metric selection includes a variety of summative (streamflow performance), and formative (i.e., flow path and storage or tracer-based variables), then the model is likely to be more robust. It is noted that robustness is not always the desired fitness for purpose; in flood forecasting applications, it is likely that only peak flow generation is important, in which case it is likely that a single performance metric measuring only the models' ability to simulate peak flow or peak flow efficiency is needed.

The literature includes much guidance on performance metric selection and outcomes for model calibration [52,53]. Metric selection should be based on the (1) intended application of the model outcome, (2) non-stationarity or seasonality of the model output, (3) type of model output being calibrated, and (4) data availability and comprehensiveness of the data record, both regionally and temporally.

2.4.6. Determining Fitness for Purpose

It may never be obvious when a model is "fully or adequately calibrated", however there are several guidance documents in existence that suggest normal ranges of acceptable calibration based on performance metric choice [54], including on the use or inclusion of soft data in model calibration [55]. Generally, it is important to approach calibration with rigour and to establish a satisfactory level of confidence in the model's performance for the task at hand – what we call its "fitness for purpose". This does not mean the model has perform adequately across all possible performance measures. For example, if you are applying the model for long term average streamflow simulation, it is not necessarily a requirement that the model accurately reproduce the annual peak flow magnitude (though timing may be more important). Consider both the intended application and performance metrics selected for model evaluation.

When a model is deemed calibrated, it can be used to conduct predictive simulations. For example, these simulations can be used to derive the system response to future events in different climate change scenarios, or also for the risk assessment of contaminant transport (nuclear wastes, pesticides, etc). The predictions' quality will depend on how well the model is calibrated and on proper establishment of mathematical and numerical models applied. It should be considered that because of the nonlinearity of natural hydrologic systems and simplifications in the models, the predictions could produce unrealistic results. The calibrated model should not be used to forecast the system where the available field-observed data frequency is two-times shorter than the period of model calibration [28].

2.5.SENSITIVITY AND UNCERTAINTY ANALYSIS

There are various earth science models that incorporate the behaviour of water isotopes, such as global atmospheric general circulation models, regional climate models, cloud-resolving models, land surface models, river models, horizontal two-dimensional models, and Lagrangian models [56]. In all of them, the contribution of the water isotope ratio to the model is affected by both the behaviour of the water cycle and the behaviour of the water isotope itself. Although water isotopes are passive tracers and their abundance does not change the water cycle, water isotope ratios can change when the water cycle changes, especially when water phase changes are involved. For example, the sensitivity of water vapor isotope ratios to changes in evaporation efficiency, a parameter of atmospheric convective precipitation processes, is particularly pronounced in the tropics, especially in the mid-troposphere over oceanic continents [57]. There are an infinite number of such parameters influencing both the water cycle and water isotope ratio, and it is common practice to constrain such parameters that are sensitive to both the water cycle and water isotope behaviour with observed water isotope ratios [58]. On the other hand, there are several parameters in models that incorporate water isotopes that are only sensitive to water isotope ratios. For example, the equilibrium fractionation factor, which is the basis of the physical properties of water isotopes, is not always known with certainty, and its sensitivity on the isotopic results is sometimes variable. As for the parameters related to kinetic fractionation, the kinetic fractionation parameters depending on the intensity of evaporation and affect the water isotope ratios of water vapor and precipitation, and the sensitivity due to the way they are handled is often a major issue. When studying the water cycle and transport using water isotope models, it is important to use parameters that are well understood in the laboratory, i.e., the sensitivity to the water isotopes themselves can be assumed as small as possible.

In general, the sensitivities of numerical earth science models can be divided into two categories: sensitivities due to differences in initial conditions and sensitivities due to differences in boundary conditions; the same is true for all water isotope models. In this case, there are sensitivities due to initial and boundary conditions of water isotope ratios themselves, such as water vapor isotope ratios and precipitation isotope ratios, and sensitivities due to initial and boundary conditions of other physical quantities, such as temperature and water vapor content. It is important and useful to analyse each of these sensitivity factors when interpreting water isotope model results.

Uncertainty in groundwater models stems from several factors related to simplification of hydrological processes in the model. Thus, when the modeler selects a particular code, he/she indirectly makes assumptions about the set of hydrologic processes important to the modelling objective. This is because the selection of a code in effect reduces all processes to only those included in the code. Uncertainty can only be reduced, never eliminated, and the modelers have to consider the uncertainties that influence modelling results and a healthy scepticism of modelling output [28].

A typical order of importance of uncertainty sources includes: (i) input data in the model, including parameters, constants, and used data sets; (ii) assumptions and simplifications used in the modelling; (iii) the scientific evidence that is underlying the model; (iv) stochastic uncertainty (this is addressed under “variability” below) and (v) uncertainty sources such as numerical approximations and undetected software bugs. It should be noted that uncertainty sources should be considered early in the modelling process and then re-examined once the model has been calibrated, validated and applied for scenario runs.

Equifinality and the existence of different model parameter sets that result in equal model performance in environmental modelling is now widely accepted [59]. Therefore, optimization with the goal of finding a single optimal solution can only be justified in exceptional cases. Once equifinality is accepted, two main methods have been pursued to explicitly estimate parametric model uncertainty (following [60] and subsequent discussions): Generalized Likelihood Uncertainty Estimation (GLUE) and variants [59,61], and Bayesian statistics [62].

The GLUE method could be considered a particular case of the formal Bayesian approach; however, the difference lies in the statistical error model and that the sometimes “subjective” expert criterion of acceptability can be used as prior information [2]. Nonetheless, specifying a statistical error model is not always possible if data errors are present [63]. Furthermore, data and model structural uncertainty, in additional to parameter uncertainty, play an important role on the credibility of model simulation results [64,65]. Therefore, the modeler is left with the choice of two approaches that most importantly warrant a quantitative estimate of model parameter uncertainty, which is a cornerstone of good modelling practice [66].

2.6.MODEL SELECTION

The World Meteorological Organization (WMO) published several reports [67,68] where the following factors and relevant criteria should be considered when selecting a model:

- Objectives of the modelling that can include hydrological forecasting, assessing anthropogenic impact on the natural hydrological regime, or assessment of the climate change impact.
- The type of system that will be modelled, such as small catchment, river reach, reservoir, or large river basin.
- The hydrological element(s) that plan to be modelled, for example runoff, daily average discharges, monthly average discharges, water quality, and floods.
- The climatic and physiographic setting of the modelled system.
- Data that are available for modelling including the information on its origin, type and quality.
- Hydrological complexity should be considered.

Generally, the ability of the model to be updated conveniently, based on current hydrometeorological conditions, should be considered together with other issues such as: (i) a level of expertise in modelling; (ii) whether the model is going to be used on its own, or if it is going to be used in combination with other models. The core governing principle in model selection should be based on not having more parameters requiring calibration than the available data can support. It can help to minimise problems of spurious results and false calibrations.

2.7.DATA MANAGEMENT AND ACCESSIBILITY

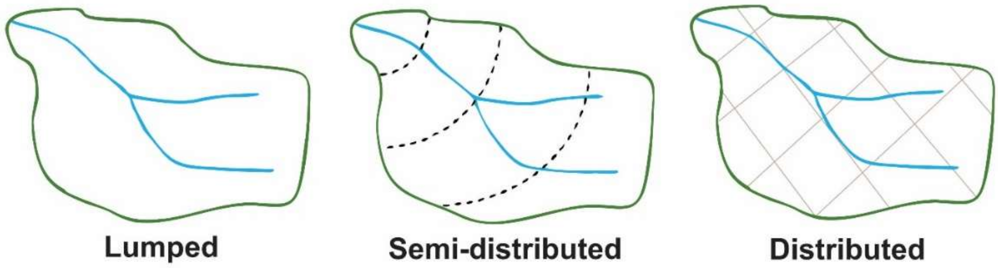
Researchers and funders are highlighting the importance of data, publications, and software sharing for the public use [69]. To begin to achieve this accessibility to data and communication between researchers, the enunciation of the FAIR principles was critical. FAIR is a set of guiding principles to make data findable (F), accessible (A), interoperable (I), and reusable (R) [42].

These principles provide guidance for management and stewardship of scientific data relevant to all stakeholders. Also, these principles have been extended to software and other academic output [70]. With a model that has been made based on the FAIR, it is possible to re-design the experiments done by the authors of that model. An additional option can be to develop novel research by applying the model to different locations, with diverse input data and/or settings. For the FAIR-based model, not only the software and required data need to be available, but models should be also properly documented and have well-defined interfaces [70].

3. APPLICATIONS OF ISOTOPE-ENABLED HYDROLOGICAL MODELS

This section discusses the characteristics of different isotope-enabled model types, along with a broad evaluation of the strengths and limitations of each approach used by the participants (Table 3).

The CRP´s participants used both lumped models that considers individual catchments as a single unit and distributed models that sub-divides each catchment in smaller cells. A lumped hydrological model generally averages spatial settings related to rainfall-runoff response for the whole area of the analysed catchment. Distributed model subdivides a catchment area based on a particular grid size to capture this spatial and temporal variability [71]. Another type, a semi-distributed model that is a variation of the lumped method where catchment is divided into smaller sub-catchment and for example, runoff amount is estimated based on streamflow from each of these sub-catchments. Fig. 3 highlights the difference between these models.



a) b) c)

FIG 3. Comparison between the three examples of model spatial discretization. a) Lumped Model, b) Semi-Distributed Model and c) Distributed Model (adapted from [71]*).*

TABLE 3. SUMMARY OF MODEL FRAMEWORKS USED IN CASE STUDY APPLICATIONS TO PERFORM ISOTOPE-ENABLED WATER BALANCE MODELLING.

Model	**Type**	**Δt**	**Δx**	**Spatial Disc.**	**Main dynamics**	**Tested basin**	**GUI/Platform**	**Reference**
IsoWATFLOOD	Int	Hourly, daily or monthly	50 km^2 and up	Distributed	Plant physiology, soil hydrology	Nelson & Mackenzie Rivers, Canada	No. Fortran. Windows	[19]
STARRtropics	Int	Hourly, daily	10 m to 1 km^2	Distributed	Water and solute balance, eco-hydrological water partitioning	San Carlos Basin, Costa Rica	No. Python. Windows/ Linux	[72,73]
Lake model	EMMA	Monthly	Various	Lumped	Water balance, isotopes	Chad Lake, Fitri Lake, Plešné Lake	No. Excel or Python	[74]
IsoMATSIRO/ IsoTRIP	Int	Hourly	1 km to 100 km	Distributed	Plant physiology, soil hydrology,	Global	No. Fortran. Linux	[37]
JAMS/ J2000iso	EMMA	Daily	Various	Distributed (HRU)	Process-based ecohydrological model	Berg River, South Africa	Yes. Java. Windows/ Linux	[75] http://jams.uni-jena.de/
MODFLOW/ MT3DMS	ADT	Hourly, daily, monthly	Various	Distributed	Water and solute transport, geochemical	Quenquen, Grande River	Yes. Fortran. Windows/ Linux	https://www.usgs.gov/software/mt3d-usgs-groundwater-solute-transport-simulator-modflow

Int=integrated water and isotope fluxes, EMMA=end-member mixing analysis, ADT=advection-dispersion transport only (not specific to isotopes)

3.1.ARGENTINE REPUBLIC

FIG 4. Los Padres Lake

Short statement: Application of stable isotopes to estimate water exchange processes in a shallow lake.

Challenge. Pampean shallow lakes have an important role in the balancing of physical and biological systems among several ecosystem services. However, key hydrological properties, such as evaporation loss and water residence time estimations are remained unknown. For this study [76], it was considered as a study area Los Padres Lake, which is a representative freshwater ecosystem and despite being located within a natural reserve area, it is embedded in a fruit-horticultural belt. The aim of this study was to calculate evaporation losses and the water residence time in this temperate shallow lake using the water isotope mass balance approach.

Approach. Groundwater, lake and stream samples were collected for δ^2H and δ^{18}O analysis. Water level fluctuations were recorded with data loggers and water samples were collected monthly for one year. Groundwater discharge estimations were calculated based on an automated digital filter technique. Isotopic rainwater composition was obtained from the GNIP sample collector. Stable isotopes were analysed by at the Hydrogeochemical and Isotopic Hydrology Laboratory (Universidad Nacional de Mar del Plata). Lake water balance was characterized using an isotope mass balance model, that estimates E/I (fraction of inflow water evaporated from a lake). The isotope-based lake water residence time (τ) was estimated using the Gibson et al [77] formula.

Lesson learned. The analysis of E/I ratios showed that water balance in the lake was mainly regulated by changes in water flow rather than changes in evaporation. A mean residence time was calculated. Long-term monitoring would enable the estimation of the changes in lake hydrological properties over time and facilitate the evaluation of the lake water cycle. Data resulting from this study have multiple impacts as the lake is within the area of agricultural watershed but also used for recreational activities.

3.2.AUSTRALIA

FIG 5. Tully River, Queensland, Australia

Short statement: Isotope-enabled hydrological modelling of the catchment water budget improves our ability to manage the demands on water resources of seasonal catchments better.

Challenge. Catchments in Northern Australia experience seasonal changes in rainfall that result in very distinct wet and dry season flow patterns, with implications for water resource allocation. This project uses two contrasting catchments, one largely forested (Tully River catchment) and another heavily impacted by agricultural activities (Barron River catchment), to compare water budget modelling results and their implications on water resource management.

Approach. Data collection for both catchments to represent physiographic variability and upstream to downstream linkages was conducted for 12 or 13 sampling locations given their size (1684 – 2188 km^2). Streams and lakes were sampled for stable water isotopes water quality parameters (e.g., pH, conductivity, turbidity, dissolved oxygen). Rainwater and groundwater were also sampled for the 2 years from November 2018 to end-October 2020.

Lessons Learned. As both catchments are close to the sea and have an elevation range of approximately 800-1000 m above sea level, this results in a clear elevation and distance effect on the isotopic composition of rainfall. Rainfall over both catchments is more depleted at high elevation locations and those further inland. There is a clear effect of rainfall seasonality on the stable water isotope composition for the rainfall and streamflow samples, seen more clearly for the Barron River catchment than the Tully River catchment. For rainfall, dry season rainfall tends to have more enriched $\delta^{18}O$ composition as compared with wet season rainfall samples which tend to be more depleted in both $\delta^{18}O$ and $\delta^{2}H$. Our results show a distinguishable isotope signature for different water budget components for both catchments with lake samples showing a more evaporative signature than stream samples. Isotopic compositions also show a distinct seasonal variability for the different source waters. Evaporation being an important process for isotopic variability especially for lake samples which have lower d-excess values compared to streamflow entering the sampled lakes. The future direction of this work is to invest in setting up a physical isotope-hydrologic model (e.g., isoWATFLOOD).

3.3.CANADA

FIG. 6. Odei River, tributary of the Nelson River and typical of northern Canadian Boreal Rivers

Short statement. Coupled physical water-isotope modelling is applied within the Nelson River basin (1.1M km^2) and Mackenzie River basin (1.7M km^2) of Canada. These basins collectively represent about 1/3 of Canada's landmass and both contribute to Arctic Ocean drainage. Both basins are undergoing rapidly accelerated climate change which is affecting water supply. Isotope-enabled modelling is being used to identify process representation and surface-subsurface hydrologic partitioning to constrain future long-term water balance simulation.

Challenge. The main challenge within this region is a lack of data when reliant on hydrometric or water balance methods alone. Isotopes offer a means to calibrate models in ungauged basins. This region is also highly seasonal with many cold regions processes. The size of the region is also a significant challenge here, with spatial scales and timesteps for modelling that are meaningful hydrologically.

Approach. A combination of analytical water-isotope balance modelling and physical coupled isotope-hydrologic modelling (isoWATFLOOD) was applied to identify significant water balance components, regional controls on the water balance, and to improve hydrologic model calibration [19,24, 45].

Lessons Learned. Modelling highlighted significant regional differences in water balance controls and runoff generation mechanisms at a continental scale, and facilitate partitioning of E/I, T/ET and water yield (runoff) for subbasins across Canada. Physical modelling complimented the analytical modelling by providing more detailed timeseries records of flow and isotopes. The isotope data were useful for improving and validating the model performance and calibration. Isotopes were found to improve calibration in large regions with process-based models over results calibrated to streamflow only [24,45].

3.4.CHAD, REPUBLIC OF AND FRENCH REPUBLIC

FIG 7. Lake Chad

Short statement. In the Sahelian area, Lake Chad represents a permanent access to surface water resource but undergoes significant seasonal and interannual surface changes (2500 – 25000 km^2) in response to climatic variability [78]. As an example, the shrinkage of the lake during the 1970-1990 period corresponded to the decrease in rainfall observed in the entire Sahel region [79], but a detailed understanding of the variability of Lake Chad requires knowledge of the response of flows to the respective roles of climate change and human activities. In addition, the lake Chad catchment contains several smaller lakes, such as the Lake Fitri, which has a behaviour very similar to Lake Chad at a smaller scale. The dramatic fluctuations in the extension of Lake Chad over the past decades have demonstrated the very high vulnerability of this crucial ecosystem for nearly 47 million people. High population growth, combined with the uncertainties of climate change, makes water resources vulnerable. In this context, the development of sustainable surface and groundwater management is crucial.

Challenge. Understanding the Lake Chad and Lake Fitri responses to climate variations requires the combination of catchment and lake models. In the Lake Chad basin, the Chari-Logone River basin (600000 km^2) represents the main water inflow to the lake. Regarding the Lake Fitri, the Batha River basin (90000 km^2) in the main inflow. In both situations, the main challenges are the lack of hydro-climatic data to characterize the water flows and their variations in these huge catchments.

Approach. The calibration of a lake model combining water, isotope and chemical mass affords more precise estimation of the water balance components of Lake Chad and their variability [74]. This approach will be applied to Lake Fitri. Regarding the application of a catchment model, previous studies on the Chari-Logone basin provided detail knowledge of the hydro-climatic and geochemical flux variabilities [79,80]. Additionally, stable isotope data were collected on a monthly basis between January 2013 and November 2016, with the objective of applying an isotope-enabled rainfall-runoff model.

Lessons learned. The combination of water, isotope, and chemical mass balance in a lake model was found to be the most effective way to evaluate the water balance components of Lake Chad and their variability [74]. For this purpose, monthly sampling of the lake and its tributary are sufficient and need to be combined with water level measurements and lake bathymetry. Regarding the application of an isotope-enabled rainfall-runoff model on the lake catchments, the main difficulty is to propose a quantitative interpretation of the isotopic signature of evaporative fractionation in terms of the magnitude of large-scale evaporation fluxes.

3.5.CZECH REPUBLIC

FIG 8. Plešné Lake, Czech Republic

Short statement. Lake catchments in the boreal forest of the Šumava National Park experienced a bark beetle (*Ips typographus*) infestation and strong deforestation

Challenge. Vegetation cover influences hydrological cycle through the interception of precipitation, changes in evapotranspiration that affects water dynamics, storage, and mixing. In deforested sites typically lack canopy interception and may subsequently have reduced transpiration, resulting in an accelerated hydrological cycle. This study focused on assessment of hydrological processes and their difference in forested and deforested catchments using isotope water balance modelling.

Approach. Isotope-enabled hydrological modelling was done in mountain headwater catchments (Czech Republic, Šumava National Park). The aim was to test the hypothesis that stable isotopes of water can trace hydrological variations derived after the deforestation. Sampling of precipitation, tributaries, lake profile and outflow were organized in forested and deforested catchments with similar conditions in 3 weeks interval in 2016-2021. Together with stable isotopes of water, basic hydrological and hydro chemical measurements were done.

Lessons Learned. Results of stable isotopes in water analysis showed that run-off in forested and deforested catchments has differences in hydrological processes. This is found to be attributed to distinct vegetation characteristics in the catchment. In the forested catchment isotopically enriched throughfall contributes to run-off in streams. This explains a higher storage capacity of intercepted precipitation and the ability of the mature spruce forest to intercept moisture. Higher throughfall amounts can lead to a larger evaporation signal as found in the streams of forested catchment, particularly, during warm periods of the year with a larger contribution of rainfall. In the deforested catchment, the larger contribution of isotopically lighter water during the winter relates to changes in ground snow cover formation and snow melt. Stable isotope data also indicated that evaporation, transpiration, and the mean transit time of water did not differ significantly between forested and deforested catchments [81]. Stable isotopes of water added interesting and hydrologically relevant information related to the effects of forest disturbance on catchment water partitioning that would otherwise have been difficult to obtain.

3.6.COSTA RICA, REPUBLIC OF

FIG 9. Rainforest in the San Lorencito experimental catchment in the Republic of Costa Rica

Short statement. The complex, tropical San Carlos catchment (2560km^2) in the Republic of Costa Rica with limited data availability lacks basic information on water quantity and quality. Tracer-aided hydrological modelling with STARR$_{\text{tropics}}$ (**S**patially-distributed **T**racer-**A**ided **R**ainfall **R**unoff) helped to better understand the spatial and temporal dynamics of flows and tracer mixing, storage and transport to establish more robust water balances.

Challenge. Tracers can be used to bridge the gap from water quantity to quality using concepts of water age distributions. However, the latter mostly requires modelling enabled to simulate tracer transport additionally to flows and if models developed at smaller catchment scales can perform in larger catchments where management decisions are most pressing. The class of tracer-aided hydrological models can help to reduce uncertainties of water balances and water and tracer flux estimates but comes at the expense of increased model parameters. Such a trade-off should be carefully evaluated to determine if the model is useful under the current data availability for the study site.

Approach. The modified spatially distributed and tracer aided STARR$_{\text{tropics}}$ model by Dehaspe et al. [66] and Correa et al. [73] was upscaled from previous applications at the 3.2 km^2 San Lorencito headwater rainforest sub-catchment to the full 2560km^2 tropical San Carlos catchment. The much more heterogeneous San Carlos catchment required modifications to the model time step (from hourly to daily) and grid (from 10m to 1km), as well as to the input data setup in form of 4 land cover classes represented by Leaf-Area-Index (LAI) for water partitioning and flux simulations. The spatially variable meteorological input to drive STARR$_{\text{tropics}}$ used an observation-based bias-corrected output from the regional isotope-enabled climate model IsoRSM by Yoshimura et al. [82]. Therefore, STARR$_{\text{tropics}}$ was run continuously from 1981 to 2020 simulating flows, water balances and tracer transport evaluated against 4 streamflow gauges in a split sample mode and monthly isotope measurements at 46 streams [83].

Lessons learned. The incorporation of isotopes into the hydrological model STARR$_{\text{tropics}}$ helped to constrain simulations for a more robust estimation of grid-based water balances that can be communicated to local decision makers. Independent model evaluation in form of soil and groundwater isotopes resulted crucial to constrain simulations. Model improvements can be achieved through better spatially distributed model input data.

3.7.ETHIOPIA, FEDERAL DEMOCRATIC REPUBLIC OF


a) b)

FIG 10. a) Irrigated Area and b) Modjo River, Federal Democratic Republic of Ethiopia

Short statement: Application of stable isotopes to minimize the inherent uncertainties of conventional groundwater recharge estimation.

Challenge. Proper estimation of groundwater recharge has a paramount importance to assess a groundwater potential of an area. Unfortunately, there is no method which gives best estimation in all climatic, topographic and geologic setting. It is commonly a trial-and-error approach to find a more realistic way of estimating groundwater recharge particularly in a complex environment. This research will try to evaluate existing methodologies for recharge estimation from different sources including primary data in selected watershed in the upper Awash basin including Addis Ababa and compare it with recharge estimation using the new technique, “Isotope enabled water balance modelling” to come up with a more realistic recharge estimation.

The main purpose of this research is to enhance the reliability of groundwater recharge estimation using isotope enabled water balance modelling under a changing climate so it can be used to design a proper and sound groundwater management plan.

Approach. Conventional groundwater recharge estimation using wets pass model and hydrograph separation is conducted. To apply these method thematic maps of the upper Awash basin has been prepared, processed and evaluated, river discharge data was processed and then the recharge estimation has been validated by comparison with previous studies. Moreover, as a parallel study the water quality change through time was evaluated using trend analysis by comparing two periods sampling with previous analysis results. The first group of samples for isotope analysis has been collected and analysed.

Lessons Learned. Samples taken from ground water shows depletion while the lake water and river water show slight evaporation. Groundwater recharge estimate using wets pass mode is about 125 mm which accounts 12.5 percent of the basin rainfall. Groundwater recharge estimated using hydrograph separation in one of the main tributaries was found to be 36 mm indicating, baseflow separation a less viable option because of the deep groundwater resulting and deep circulation. Groundwater recharge estimated using SWAT also 115 mm. Sulphate, chloride and nitrate are observed increasing from time to time particularly in major urban centre and rural area where intensive irrigation is practiced. IsoWATFLOOD will be used in the future.

3.8.JAPAN

FIG 11. Kinu River in 2015, Joso City, Japan

Short statement. This study showed that isotopic information had the potential to improve estimates of detailed global water balance by constraining isotope-enabled models with cutting-edge satellite-based vapor isotopic measurements. Furthermore, such isotopic information may help to improve the accuracy of weather prediction.

Challenge. The accuracy of weather prediction has been continuously improved, but there are many disasters occurring all over the world. Japan is one of the flood-prone countries. Stable water isotopes have been regarded as a good tool to help our understanding of various types of hydrological processes, but how much the isotopes could contribute to disaster prevention was rather unknown.

Approach. Isotope-enabled atmospheric general circulation model coupled with an isotope-enabled land surface model (Iso-MATSIRO) and an isotope-enabled hydrological model (Iso-TRIP) was used. Data assimilation method developed by Yoshimura et al (2014) was applied to constrain hydrological processes of the model with the satellite-based vapor isotope observation data.

Lessons Learned. Data assimilation of satellite-based mid-tropospheric vapor isotope information was tested. In Toride et al. (2021), it was confirmed that the wind speed, specific humidity, and temperature fields in the middle troposphere improved by more than 10% in ideal experiments when additional water isotope ratios were assimilated. Following this idealized work, Tada et al. (2021) conducted data assimilation experiments with the actual observed data obtained from April 1 to April 30, 2013. The results confirmed that the isotopic information has the potential of constraining the atmospheric hydrologic cycle, and it even contributed to improving weather prediction accuracy. With expansion of this approach, it may help to improve the prediction accuracy of heavy precipitation events, like the one occurred in 2015 in Japan, a.k.a. Kinu River flood event (Fig. 11).

3.9.SOUTH AFRICA, REPUBLIC OF

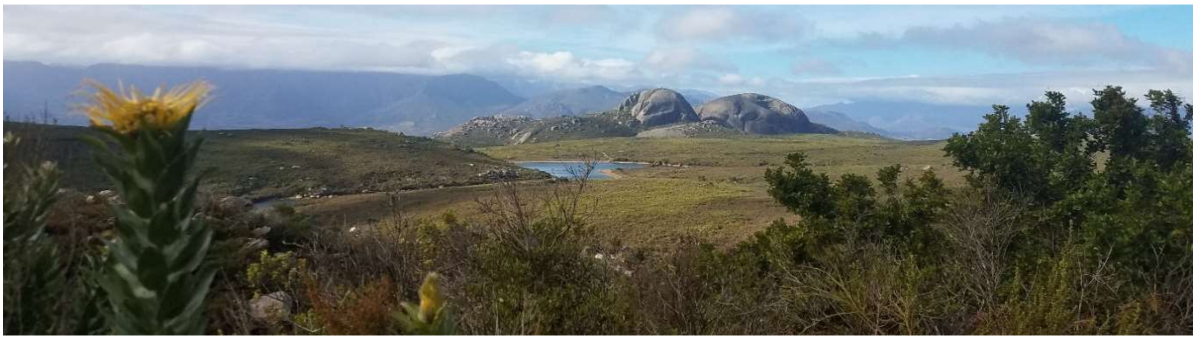


FIG 12. Berg River catchment in the Western Cape of the Republic of South Africa

Short statement. The Berg River catchment in the Western Cape of the Republic of South Africa experienced a severe drought between 2015-2018

Challenge. Centralized water supply systems which rely mainly on surface water reservoirs are vulnerable to climate variability. These issues are pronounced in semi-arid Mediterranean South Africa here precipitation follows a winter distribution, but water demands are highest during summer. Precipitation shortfalls therefore affect the ability of reservoirs to meet domestic, industrial, and agricultural requirements, as well as environmental flows.

Approach. This study focused on validating the simulated hydrological processes and the flow component separation ability of the distributed JAMS/J2000iso rainfall-runoff model of the Berg River catchment, which forms the basis of a future climate vulnerability assessment. While JAMS/J2000iso simulates small scale processes and flow dynamics at a hillslope scale, its groundwater and aquifer properties are more conceptual which affects 'plausible' model parameter combinations. Sampling of rain, stream, groundwater isotopes were taken between the periods 2020 to 2021 on a weekly basis and aggregated. A binary mixing model was used to determine the fractional water content of surface runoff and baseflow in the lower reaches and used for comparison purposes with the simulated flow components. The choice of 'plausible' model parameters relied on selecting parameters which gave a similar flow component breakdown using the fractional contribution of each of the water isotopes.

Lessons Learned. The isotope results illustrate a strong groundwater dominance in the hydrological flows for the catchment, accounting for around 70 % of the daily flows. Likewise, the most 'optimal' model solution favoured a strong groundwater dominance of around 50 %. Developments are still ongoing which allow for linking the isotope fractional water content with the simulated flow components within the model, to allow the automated calibration procedure to narrow search into more 'plausible' model parameter combinations. As climate change drives key stresses in the hydrological system, influencing conceptual rainfall-runoff relationships, the use of isotopes provides a means to reduce the uncertainty of simulated hydrological flows, especially in semi-arid/arid environments or small catchments where the signal to noise ratio is much higher and solutions tend towards 'implausible' scenarios.

3.10. VIET NAM, SOCIALIST REPUBLIC OF

FIG 13. Red River in Hanoi

Short statement. The Red River delta, especially Hanoi capital is already considered an area ‘at risk’ due to large scale infrastructure development and groundwater.

Challenge. The degree of interactions between the river and aquifers depends on many factors including the spatial heterogeneity of clay distribution and the large temporal fluctuations in the hydraulic heads of groundwater and river levels due to climate factors and pumping. Therefore, previous work has shown mixed results in the degree of this interaction.

Moreover, sustainable use of water resources in Hanoi requires solutions to manage irrigation and drinking water demands more effectively on surface water and groundwater resources. This requires a comprehensive understanding of the connection between these water resources.

In this project, the connection between surface and groundwater resources will be explored using isotopes to help resolve the challenge of spatio-temporal variability. These isotopic observations will then be used to better quantify the water balance in the delta using the IAEA Water Balance (IWBMIso).

Approach. The stable isotopes of water were used to identify the seasonal variations in groundwater and surface water interactions. Hydraulic head data from monitoring system was included to highlight hydraulic gradient directions and potential seasonal reversal. But it is only through the coupled use with stable isotopes that we can then quantify these exchanges for the catchment budget modelling. In this project we concentrate on the groundwater interactions with the Red River [84,85]. The project objectives include: (a) Identify areas of high connectivity with river water in temporal and spatial scale by using oxygen-18 and deuterium; (b) quantify the contribution and mean traveling time of baseflow using the isotope model.

Lesson learned. In the dry season groundwater in both Holocene and Pleistocene aquifers and water in the Red River has the same isotopic composition. It seems that Holocene and Pleistocene aquifers in that region were interconnected in the dry season and discharge to the Red River, and in the rainy season the river was recharged to groundwater. The results of this study are useful for the local water resources managers in terms of better management for groundwater abstraction to reduce potential contamination of groundwater from surface water to supply Ha Noi.

4. DISCUSSIONS AND FUTURE DIRECTIONS

The presented study showcases applications with improved water balance estimates, but also enhanced hydrological process simulations through the combined use of stable water isotopes and hydrological models. This information is relevant for water resource managers, decision makers and for policy creation. These guidelines aim to provide model users with the necessary information needed in the design of new isotope enabled hydrological models or new modelling approaches, provide supporting information for the presented example model applications, but are not restrictive in terms of how the field may progress. Additionally, we recognize that as isotope hydrology and hydrological modelling fields are quite diverse, these guidelines aim to bridge and provide information needed by both intended users.

Many of the previously described issues in relation to isotope-enabled hydrological modelling can be summarized under the three categories of i) model, (ii) data, and iii) training issues. The latter challenges also provide ample opportunity for future research directions and here we only briefly highlight those where we see the most potential:

4.1.MODEL ISSUES

Arguably all models are uncertain, and we therefore highlight the five main types of uncertainties, which are: 1) input data and 2) boundary conditions, 3) model structural, 4) model parameter selection, 5) uncertainty of data used for calibration and numerical uncertainty. We do not go as far as recommending a specific uncertainty quantification method, but we would very much want to highlight that uncertainty needs to be considered and transparently reported in any modelling study. Related to the uncertainty issue of hydrological modelling is the opportunity to reduce uncertainties by incorporating isotopes into the model evaluation procedure (Table 4).

TABLE 4. SIMPLE TESTS TO EVALUATE THE EFFECTIVENESS OF ISOTOPE DATA IN AIDING HYDROLOGIC SIMULATION.

Simple test	What to look for	Why	Evaluate
MWL	Compare data to local precipitation to GMWL in $\delta^{18}O$-$\delta^{2}H$ space	LMWL offset from GMWL informs humidity and air mass circulation processes	Signature of local precipitation processes
d-excess and LEL	Compare data to MWL in $\delta^{18}O$-$\delta^{2}H$ space Evaluate offset and data scattering along an evaporation line	Is there an evaporation signal or not? Is it seasonally varying?	Offset (slope) Variability
End member analysis	Evaluate data scattering along a mixing line in $\delta^{18}O$-$\delta^{2}H$ space. Identify endmembers and their variability.	Do they change through time and/or space? Is there the potential to evaluate mixing?	Mixing in catchment
$d_P \rightarrow d_Q$	Timeseries plot of both	Is there damping (mixing)? What is the offset?	Transfer function

The latter additional information to streamflow for model evaluation can help increase the robustness of model simulations in terms of both model accuracy and fidelity (or process representation). However, there is a need to standardize such model tests through a formal protocol that could involve a benchmark high-quality catchment data set, a model structure benchmark, both approved and taken up at a community level. A community level effort could even lead to developing open access modular code similar to the community climate and land surface models.

As a means of addressing modelling uncertainty, a series of simple tests can be run on preliminary isotope data to assess the degree to which isotope data may assist, or complement, the environmental modelling. These are outlined in Table 4.

4.2. DATA ISSUES

There is a clear need for more longer-term and higher frequency stable isotope data sets from catchments with different climate and geomorphic properties for comparative studies that enable to learn about catchment functioning and learn about catchment functions so that models can be tailed to catchment behavior. However, model testing can go beyond the more common rainfall-runoff data to include additional isotope data that characterize source waters such as soil, plant and groundwaters. Such multi-component data sets will provide a much more stringent model test in the future. Additionally, to the worth of data for model evaluation, we need spatially distributed data for large-scale catchment applications, particularly where spatial and topographical gradients exist. Likewise, the temporal resolution of the collected datasets needs to be considered, given the desired research questions, but also which anticipated model will be used. Ideally higher resolution datasets should be used for highly dynamic systems or for detailed process understanding, while lower temporal resolution data can form the basis for larger regional water management requirements. More detailed datasets are required for catchments which are under a state of change, but also for pristine catchments to ensure baseline comparisons are available. To fill such a gap, the use of isotope-enabled climate models could be promoted as hydrological model input if uncertainties are manageable.

4.3.TRAINING ISSUES

Many isotope-enabled models (see case studies) already exist and could be taken up by users for a more widespread application using the best-practice presented here. However, the isotope components add an additional layer of complexity to hydrological modelling that often requires expert programming knowledge in combination with a background in isotope hydrology. Even if model codes that do not include a graphical user-interface are well documented (which they are most often not), such research tools need training, which can be a time-consuming task. In the example application studies the isotope enabling considers improving model robustness but vary based on whether the isotope fluxes were simulated or whether the isotopes were solely used for evaluation. Training on isotope enabled hydrological modelling therefore is dependent on the end user (policy/water management/researchers) and their anticipated skills and background. We recognize that these isotope enabling applications can vary widely for different model codes (such as Fortran vs. Java), but the development of these approaches can be more easily achieved with models which are modular and isotope components can be easily combined with pre-existing model structure. Nonetheless, we recommend facilitating open access to codes and tools to maintain different versions in platforms such as e.g., GitHub. Model documentation and even training material in the form of e.g., video tutorials would be an asset for a more transparent and user-friendly experience of isotope-enabled hydrological models. Additionally, training workshops which keep users up to date with the latest isotope-enabled model developments are needed to expand the field and ensure the appropriate use of these tools.

While forecasting under enhanced global warming is a current priority within the field of hydrological modelling, which has seen the increased use of data driven approaches and machine learning, the progression of isotope-enabled models supports better process representation of models with the intention that these models will then still provide relevant predictions given the anticipated climate change. Additionally, the progression of different isotope enabled modelling approaches provides a good methodology to support already existing hydrological models with more physical constraints. While these guidelines have supported a range of different applications, we are looking to test these approaches under climate extremes and develop new tools focused at promoting enhanced performance for forecasting but also testing these models in ungauged catchments, formulating the best means to collect isotope support data and what the limitations of these approaches might be.

REFERENCES

[1] IPCC 2022: Climate Change 2021. The Physical Science Basis. Contribution of Working Group I to the Sixth Assesment Report of the Intergovernmental Panel on Climate Change. Cambridge University Press. In Press (2021).

[2] MATHIEU, R., et al., Simulation of stable water isotope variations by the GENESIS GCM for modern conditions. J. Geophys. Res. 107(D4) (2002) 4037.

[3] TINDALL, J.C., VALDES, P.J., SIME, L.C., Stable water isotopes in HadCM3: Isotopic signature of El Niño-Southern Oscillation and the tropical amount effect. J. Geophys. Res. 114 (2009) D04111.

[4] RISI, C., BONY, S., VIMEUX, F., JOUZEL, J., Water-stable isotopes in the LMDZ4 general circulation model: Model evaluation for present-day and past climates and applications to climatic interpretations of tropical isotopic records. J. Geophys. Res. 115 (2010) D12118.

[5] SCHMIDT, G.A., LEGRANDE, A.N., HOFFMANN, G., Water isotope expressions of intrinsic and forced variability in a coupled ocean-atmosphere model. J. Geophys. Res. 112 (2007) D10103.

[6] DANABASOGLU, G., et al., The CCSM4 ocean component. J. Clim. 25(5) (2012) 1361-1389.

[7] NOONE, D. C., STURM, C., Comprehensive Dynamical Models of Global and Regional Water Isotope Distributions. In J. B. West,G. J. Bowen, T. E. Dawson, K. P Tu (Eds.), Isoscapes 195–219. Netherlands: Springer (2010).

[8] DOMINGUEZ, F., MIGUEZ-MACHO, G., HU, H., WRF with water vapor tracers: A study of moisture sources for the North American Monsoon. J. Hydrometeorol. 17(7) (2016) 1915–1927.

[9] SODEMANN, H., WERNLI, H., SCHWIERZ, C., Sources of water vapour contributing to the Elbe flood in August 2002—A tagging study in a mesoscale model. Q. J. R. Meteorol. Soc. 135(638) (2009) 205–223.

[10] ROCHE, D.M., $\delta^{18}O$ water isotope in the iLOVECLIM model (version 1.0)—Part I: Implementation and verification. Geosci. Model Dev. 6(5) (2013) 1481–1491.

[11] FIELD, R. D., et al., Evaluating climate model performance in the tropics with retrievals of water isotopic composition from Aura TES. Geophys. Res. Lett. 41 (2014) 6030–6036.

[12] ZHU, J., LIU, Z., BRADY, E. C., OTTO-BLIESNER, B. L., MARCOTT, S. A., ZHANG, J., et al. Investigating the direct meltwater effect in terrestrial oxygen-isotope paleoclimate records using an isotope-enabled Earth system model. Geophys. Res. Lett. 44 (12) (2017b). 501–12, 510.

[13] BRADY, E., et al., The connected isotopic water cycle in the Community Earth System Model version 1. J. Adv. Model. Earth Syst. 11 (2019) 2547–2566.

[14] DEE, S., NOONE, D., BUENNING, N., EMILE-GEAY, J., ZHOU, Y., SPEEDY-IER: A fast atmospheric GCM with water isotope physics. J. Geophys. Res.: Atmos. 120 (2015) 73–91.

[15] GUAN, J., et al., Understanding the temporal slope of the temperature-water isotope relation during the deglaciation using isoCAM3: The slope equation. J. Geophys. Res.: Atmos. 121 (2016) 10342–10354.

[16] RUSSON, T., TUDHOPE, A.W., HEGERL, G.C., COLLINS, M., TINDALL, J., Inter-annual tropical Pacific climate variability in an isotope enabled CGCM: Implications for interpreting coral stable oxygen isotope records of ENSO. Climate of the Past 9(4) (2013) 1543–1557.

[17] HU, J., EMILE-GEAY, J., NUSBAUMER, J., NOONE, D., Impact of convective activity on precipitation δ18O in isotope-enabled general circulation models. J. Geophys. Res.: Atmos. 123 (2018) 13595–13610.

[18] ZHANG, S., WEN, X., WANG, J., YU, G., SUN, X., The use of stable isotopes to partition evapotranspiration fluxes into evaporation and transpiration. Acta Ecol. Sin. 30 (2010) 201-209.

[19] STADNYK, T.A., DELAVAU, C.J., KOUWEN, N., EDWARDS, T.W.D., Towards hydrological model calibration and validation: simulation of stable water isotopes using the isoWATFLOOD model. Hydrol. Process. 27 (2013) 3791–3810.

[20] SMITH, A., DELAVAU, C., STADNYK, T., Identification of geographical influences and flow regime characteristics using regional water isotope surveys in the lower Nelson River, Canada, Canadian Water Res. J. 40 (2015) 23-35.

[21] SMITH, A., WELCH, C., STADNYK, T., Assessment of a lumped coupled flow-isotope model in data scarce Boreal catchments. Hydrol. Process. 30(21) (2016) 3871–3884.

[22] BELACHEW, D.L. et al., 2016., IAEA Isotope-enabled coupled catchment–lake water balance model, IWBMIso: description and validation. Isot. Env. Health Stud. 4-5(52) (2016) 427-444.

[23] SPRENGER, M., et al., Measuring and modelling stable isotopes of mobile and bulk soil water. Vadose Zone J. 17 (2018) 170149.

[24] STADNYK, T.A., HOLMES, T., On the value of isotope-enabled hydrologic model calibration. Hydrol. Sciences J. 9(65) (2020) 1525-1538.

[25] KUPPEL, S., et al., EcH2O-iso 1.0: water isotopes and age tracking in a process-based, distributed ecohydrological model. Geosci. Model Dev. 11(2018) 3045–3069.

[26] BEVEN, K.J., Rainfall-runoff modelling: a primer. Wiley-Blackwell (2001).

[27] WAINWRIGHT, J., MULLIGAN, M. (2nd ed) Environmental modelling: finding simplicity in complexity, Wiley, 496 pp (2013)

[28] ANDERSON, M.P., WOESSNER W.W., HUNT, R.J., Chapter 1 – Introduction. p. 3-25. In Anderson Mary P., et al. (Eds.) Applied Groundwater Modelling (Second Edition). Academic Press (2015).

[29] YU, Z., Hydrology, floods and droughts | Modelling and Prediction, Editor(s): Gerald R. North, John Pyle, Fuqing Zhang, Encyclopedia of Atmospheric Sciences (Second Edition) Academic Press (2015) 217-223.

[30] BEVEN, K.J., Rainfall-runoff modelling: The primer, 2nd edn. Chichester: Wiley-Blackwell (2012).

[31] BIRKEL, C., CORREA BARAHONA A., Rainfall-Runoff Modelling: A Brief Overview, Reference Module in Earth Systems and Environmental Sciences. Elsevier (2019).

[32] SON, K., SIVAPALAN, M., Improving model structure and reducing parameter uncertainty in conceptual water balance models through the use of auxiliary data. Water Resour. Res. 43 (2007) W01415.

[33] ZAMBRANO-BIGIARINI, M., NAUDITT, A., BIRKEL, C., VERBIST, K., RIBBE, L. Temporal and spatial evaluation of satellite-based rainfall estimates across the complex topographical and climatic gradients of Chile. Hydrol. Earth Syst. Sci. 21 (2017) 1295–1320.

[34] PIETRONIRO, A., PROWSE, T.D., Applications of remote sensing in hydrology. Hydrol. Process. 16 (2002) 1537–1541.

[35] BIRKEL, C., SOULSBY, C., Advancing tracer-aided rainfall–runoff modelling: A review of progress, problems and unrealised potential. Hydrol. Process. 29 (2015) 5227–5240.

[36] BIRKEL, C., SOULSBY, C., TETZLAFF, D., Modelling catchment-scale water storage dynamics: reconciling dynamic storage with tracer-inferred passive storage. Hydrol. Process. 25 (2011) 3924 – 3933.

[37] YOSHIMURA, K., et al. Iso-MATSIRO, a land surface model that incorporates stable water isotopes. Glob. Planet. Change 51 (1–2) (2006) 90-107.

[38] GALLART, F., et al., Investigating young water fractions in a small Mediterranean mountain catchment: Both precipitation forcing and sampling frequency matter. Hydrol. Process. 34 (2020) 3618–3634.

[39] von FREYBERG, J., STUDER, B., KIRCHNER, W., A lab in the field: high-frequency analysis of water quality and stable isotopes in stream water and precipitation. Hydrol. Earth Syst. Sci. 21 (2017)1721–1739.

[40] REFSGAARD, J.C., HENRIKSEN, H.J., Modelling Guidelines—Terminology and Guiding Principles. Adv. Water Resour. 27 (2004) 71-82.

[41] ORESKES, N., SHRADER-FRECHETTE, K., BELITZ, K., Verification, validation, and confirmation of numerical models in the Earth sciences. Science 4, 263 (5147) 1994641-6.

[42] WILKINSON, M.D., et al., The FAIR Guiding Principles for scientific data management and stewardship. Sci. Data 3 (2016) 1–9.

[43] TUNALEY, C., TETZLAFF, D., BIRKEL, C., SOULSBY, C., Using high-resolution isotope data and alternative calibration strategies for a tracer-aided runoff model in a nested catchment. Hydrol. Process. 31 (22) (2017) 3962-3978.

[44] WANG, J., et al. What is the best time to take stream isotope samples for event-based model calibration? J. Hydrol. 577 (2019) 123950.

[45] HOLMES, T., STADNYK, T. A., KIM, S. J., ASADZADEH, M., Regional calibration with isotope tracers using a spatially distributed model: A Comparison of Methods. Water Resour. Res. 56(9) (2020) e2020WR027447.

[46] KUNDZEWICZ, Z.W., KRYSANOVA, V., BENESTAD, R. E., HOV, Ø., PINIEWSKI, M., OTTO, I.M., Uncertainty in climate change impacts on water resources. Environ. Sci. Policy 79 (2018) 1-8.

[47] LEGATES, D.R., MCCABE, G. J., Evaluating the use of ‘goodness-of-fit’ Measures in hydrologic and hydroclimatic model validation. Water Resour. Res. 35 (1) (1999) 233-241.

[48] MORIASI, D.N., ARNOLD, J.G., VAN LIEW, M. W., BINGNER, R.L., HARMEL, R.D., VEITH, T.L., Model Evaluation Guidelines for Systematic Quantification of Accuracy in Watershed Simulations. Trans ASABE 50(3) (2007) 885-900.

[49] KRAUSE, P., BOYLE, D.P., BÄSE, F., Comparison of different efficiency criteria for hydrological model assessment. Adv. Geosci. 5 (2005) 89-97.

[50] KNOBEN, W.J.M., FREER, J.E., WOODS, R.A., Technical note: Inherent benchmark or not? Comparing Nash–Sutcliffe and Kling–Gupta efficiency scores. Hydrology and Earth System Sciences. 23(10) (2019) 4323-4331.

[51] GUPTA, H.V., KLING, H., YILMAZ, K. K., MARTINEZ, G. F., Decomposition of the mean squared error and NSE performance criteria: Implications for improving hydrological modelling. J. Hydrol. 377 (2009) 80-91.

[52] BAJRACHARYA, A., AWOYE, H., STADNYK, T., ASADZADEH, M., Time Variant Sensitivity Analysis of Hydrological Model Parameters in a Cold Region Using Flow Signatures. Water 12 (2020) 961.

[53] LILHARE, R., POKORNY, S., DÉRY, S.J., STADNYK, T.A., KOENIG, K.A., Sensitivity analysis and uncertainty assessment in water budgets simulated by the variable infiltration capacity model for Canadian subarctic watersheds. Hydrol. Process. 34 (9) (2020) 2057-2075.

[54] MORIASI, D.N., GITAU, M.W., DAGGUPATI, P., PAI, N., Hydrologic and Water Quality Models: Performance Measures and Evaluation Criteria. American Society of Agricultural and Biological Engineers (ASABE) St. Joseph (2015)1763-1785.

[55] SEIBERT, J., MCDONNELL, J. J., On the dialog between experimentalist and modeler in catchment hydrology: Use of soft data for multicriteria model calibration, Water Resour. Res. 38(11) (2002) 1241.

[56] YOSHIMURA, K., Stable water isotopes in climatology, meteorology, and hydrology: A review. J. Meteorol. Soc. Japan 93 (2015) 513-533.

[57] YOSHIMURA, K., et al., Comparison of an isotopic atmospheric general circulation model with new quasi-global satellite measurements of water vapor isotopologues. J. Geophys. Res. 116 (2011) D19118.

[58] RISI, C., MULLER, C., BLOSSEY, P., Rain evaporation, snow melt, and entrainment at the heart of water vapor isotopic variations in the tropical troposphere, according to large-eddy simulations and a two-column model. J. Adv. Model. Earth Syst. 13 (2021) e2020MS002381.

[59] BEVEN, K.J., BINLEY, A.M., The future of distributed models: Model calibration and uncertainty prediction. Hydrol. Process. 6 (1992) 279–298.

[60] VRUGT, J.A., TER BRAAK, C.F.F., GUPTA, H.V., ROBINSON, B.A., Equifinality of formal (DREAM) and informal (GLUE) Bayesian approaches in hydrologic modelling? Stochastic Environmental Research and Risk Assessment 23 (2008) 1011–1026.

[61] BEVEN, K., BINLEY, A., GLUE: 20years on. Hydrol. Process. 28 (2014) 5897–5918.

[62] THIEMANN, M., et al., Bayesian recursive parameter estimation for hydrologic models. Water Resour. Res. 37 (10) (2001) 2521-2535.

[63] BEVEN, K.J., WESTERBERG, I., On red herrings and real herrings: Disinformation and information in hydrological inference. Hydrol. Process. 25 (2011) 1676–1680.

[64] KAVETSKI, D., KUCZERA, G., FRANKS, S.W., Bayesian analysis of input uncertainty in hydrological modelling: 1. Theory. Water Resour. Res. 42 (2006) W03407.

[65] RENARD, B., KAVETSKI, D., KUCZERA, G., THYER, M., FRANKS, S.W., Understanding predictive uncertainty in hydrologic modelling: The challenge of identifying input and structural errors. Water Resour. Res. 46 (2010) W05521.

[66] PAPPENBERGER, F., BEVEN, K.J., Ignorance is bliss: Or seven reasons not to use uncertainty analysis. Water Resour. Res. 42 (2006) W05302.

[67] WMO 2008: Guide to Hydrological Practices. Volume I: Hydrology – From Measurement to Hydrological Information. Published in 2008 and updated in 2020. World Meteorological Organization, Geneva, Switzerland.

[68] WMO 2009: Guide to Hydrological Practices. Volume II: Management of Water Resources and Applications of Hydrological Practices. Published in 2009 and updated in 2020. World Meteorological Organization, Geneva, Switzerland.

[69] HALL, D. K., et al. The role of declining snow cover in the desiccation of the Great Salt Lake, Utah, using MODIS data. Remote Sens. Environ. 252 (2021) 112106.

[70] HUT, R., et al., The eWaterCycle platform for Open and FAIR Hydrological collaboration (2021). 10.5194/gmd-2021-344.

[71] BRIRHET, H., BENAABIDATE, L., Comparison of two hydrological models (lumped and distributed) over a pilot area of the Issen watershed in the Souss Basin, Morocco. European Scientific Journal ESJ 12 (18) (2016) 347.

[72] DEHASPE, J., et al., Spatially distributed tracer-aided modelling to explore water and isotope transport, storage and mixing in a pristine, humid tropical catchment. Hydrol. Process. 32 (2018) 3206–3224.

[73] CORREA, A., et al., Modelling non-stationary water ages in a tropical rainforest: A preliminary spatially distributed assessment. Hydrol. Process. 20 (2020) 1– 18.

[74] BOUCHEZ C., et al., Hydrological, chemical, and isotopic budgets of Lake Chad: a quantitative assessment of evaporation, transpiration and infiltration fluxes. Hydrol. Earth Syst. Sci. 20 (4) (2016) 1599–1619.

[75] WATSON, A., et al., Predicting and preparing for a changing climate: implications for hydrological extremes and water resource management. Proceeding of the 9th International Conference on Water Resources and Environment Research (presentation 3b3) (2022) 153–157.

[76] QUIROZ LONDOÑO, O.M., et al., Water exchange processes estimation in a temperate shallow lake based on water stable isotope analysis. Isot. Environ. Health. S. 56 (5-6) (2020) 465-479.

[77] GIBSON, J.J., et al., Progress in isotope tracer hydrology in Canada. Hydrol. Process. 19 (2005) 303-327.

[78] LEMOALLE, J., et al., Recent changes in Lake Chad: Observations, simulations and management options (1973–2011). Glob. Planet. Change 80–81 (2012) 247– 254.

[79] MAHAMAT NOUR, A., et al, (2019). Geochemistry of the Lake Chad Tributaries Under Strongly Varying Hydro-climatic Conditions. Aquatic Geochem. 26 (2020) 3–29.

[80] MAHAMAT NOUR, et al., Rainfall-discharge relationship and water balance over the past 60 years within the Chari-Logone sub-basins, Lake Chad basin. J. Hydrol. Regional Studies 35 (2021) 100824.

[81] VYSTAVNA, Y., et al., Isotopic response of run-off to forest disturbance in small mountain catchments. Hydrol. Process. 32 (24) (2018) 3650-3661.

[82] YOSHIMURA, K., KANAMITSU, M., DETTINGER, M., Regional downscaling for stable water isotopes: A case study of an atmospheric river event. J. Geophys. Res. 115 (2010) D18114.

[83] BIRKEL, C., et al., Headwaters drive streamflow and lowland tracer export in a large-scale humid tropical catchment. Hydrol. Process. 34 (2020) 3824– 3841.

[84] THANH, T. N., et al., Methodology of determining effective porosity and longitudinal dispersivity of aquifer and the application to field tracer injection test in Southern Hanoi, Vietnam. Vietnam Journal of Earth Sciences 39 (1) (2017) 58–75.

[85] HUY, T. D., et al., Inverse analysis for transmissivity and the Red Riverbed’s leakage factor for Pleistocene aquifer in Sen Chieu, Hanoi by pumping test under the river water level fluctuation. Vietnam Journal of Earth Sciences 40(1) (2018) 26–38.

GLOSSARY

Benchmarking – a quantitative indicator (or combination of indicators) that allows comparison with models with a similar purpose to a standard set of data, observations or expected results.

Calibration – the process of adjusting or tuning model parameters defined within physical (or conceptual) equations in a water balance model such that the outcome of the model provides the best match to the output, or calibration, data (e.g., streamflow, isotopes timeseries).

d-excess – deuterium excess, or the offset between the δ^2H and $\delta^{18}O$ values defined by the equation $\delta^2H - 8\ \delta^{18}O$. The d-excess defines the relative influence of evaporation and humidity on the isotopic composition of the region and surface or meteoric waters.

End-member mixing analysis (EMMA) – is a mathematical approach that decomposes mixed constituent concentrations (or amounts) with respect to the flux contribution of by its end-members' isotopic ratio. It assumes that each discretised water body or "storage" has a distinct isotopic composition, and their dynamical flow and mixing are explicitly calculated in all times and space in the model domain.

FAIR – Findable, Accessible, Interoperable and Reusable, principles of conduct for code and model application development requiring that code/models.

GNIP – Global Network for Isotopes in Precipitation, representing a collection of meteoric waters analysed for $\delta^{18}O$, δ^2H (and other analytes) from around the world. These samples from GMWL, which is the flux weighted average of all meteoric waters around the world.

GNIR – Global Network for Isotopes in large Rivers, representing a collection of river samples analysed for $\delta^{18}O$, δ^2H (and other analytes of interest) from some of the world's largest rivers.

Isotope-enabled models – a classification of climate and hydrologic models that integrate utilize stable isotopes of water (mass) and water flux calculations as a coupled water/energy balance. Typically, this means specifically $\delta^{18}O$ and δ^2H tracers, as a means of tracking flow paths through the water (energy) cycle.

Model efficiency criteria – mathematical measures used to assess how well a model is able to reproduce measured observation

Model robustness – a degree of how well a model reproduces reality. Robust model has two meanings: goodness in model fidelity and model accuracy. A model's fidelity indicates how reasonable the model expresses the physical and biogeochemical processes. A model's accuracy indicates how well the model reproduces specific performance metrics.

Multi-criteria calibration – when calibration is conducted on two or more parameters within a model domain

Multi-objective optimization – the process of calibrating a model by requiring it to satisfy two or more numerical objectives relating to different model outcomes or variables. It is considered an optimization (rather than calibration) as there is not typically one unique solution, but rather a series of more (or less) desirable solutions representing a trade off in the decision space of the different variables (i.e., pareto front).

LEL – local evaporation line, derived from the regression around evaporated surface waters. In seasonal environments, it is advisable to flux-weight evaporation by the evaporative loss or flux. The LEL defines the degree of evaporation relative to meteoric waters using the difference in the slope between the GMWL and LEL.

Pareto front – a set of non-dominated solutions from a multi-objective optimization representing different, equally as good, model outcomes.

Sensitivity – quantifying or exploring the impact of altering one variable or input of a model on the model outcome, or output.

Uncertainty – refer to unknowns in a model and/or natural domain that result in errors, or deviations in predicting the actual behaviour and response of a system; they are largely classified as either *aleatory* or *epistemic*. Aleatory uncertainties are those associated with assuming constant statistical properties of a system (in a highly non-stationary natural world), whereas epistemic uncertainties are those arising from a lack of knowledge about a system or its behaviour. Sources of model's uncertainty are often classified into five types: input, structure, parameters, numerical, and output.

(i) *Input uncertainty* is one propagated from a model's initial and boundary conditions, and the model's forcing data and spatial discretization, for example.
(ii) *Model structural* uncertainty is often generated due to inappropriate expression of the actual processes (e.g., over- simplification)., or lack of physical representation of earth system processes.
(iii) *Parameter uncertainty* arises due to defining parameters that have unmeasurable properties or values (i.e., conceptual representations of processes). The reasonable ranges of such parameters are often determined, and the model's results vary depending on the range of values chosen for these of the parameters.
(iv) *Numeric uncertainty* is generated because of numerical solver choice (approximations of analytical solutions), and numerical approximation and the computational algorithms.
(v) *Output uncertainty* arises from the variability inherent in observations (errors) is generated because the model is calibrated with the observation data with inherent error influencing the accuracy of the model calibration or performance evaluation.

Validation – the process of comparing summative model output (e.g., streamflow, isotopes) to a distinct set of data not used in model calibration, which tests the robustness of the model in simulating the natural environment.

Verification – the process of comparing formative model output (e.g., upstream flow paths and storages) to a distinct set of data not used in model calibration, which tests the robustness of the model in simulating the natural environmental processes.

ABBREVIATIONS

GNIP	Global Network of Isotopes in Precipitation
GNIR	Global Network of Isotopes in Rivers
GLUE	Generalized Likelihood Uncertainty Estimation
GUI	Graphical User Interface
IAEA	International Atomic Energy Agency
FAIR	Findable, Accessible, Interoperable and Reusable
KGE	Kling- Gupta Efficiency
LEL	Local evaporation line
MWL	Meteoric water line
NSE	Nash-Sutcliffe Efficiency
PBIAS	Percentage bias

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