



Deliverable 8.21 – WP8.9

OPERATIONAL IMPLEMENTATION OF THE ISOTOPE VRE, INCLUDING INFORMATION ON THE NETWORK OF ISOTOPE LABORATORY FACILITIES AND THE ACCESS RULES, AND THE ASSOCIATED USER GUIDE



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1 THE “ISOTOPE VRE” - WP 8 TASK 8.9

In the framework of the ITINERIS Project (Italian Integrated Environmental Research Infrastructures System), the main focus of the ITINERIS WP 8 Task 8.9 is the creation of the ISOTOPE Virtual Research Environment (VRE) dedicated to stable, unconventional stable, and radiogenic isotopes and embeds a national database on environmental isotope (which has been missing in Italy until now), along with a series of tools that enable users to produce models with the purpose of understanding the most important geo-environmental processes occurring throughout the Earth System.

Modelling geochemical data is fundamental in Environmental and Earth Science, and its interpretation requires visualization of increasingly large datasets. There are various software packages that help scientists to perform data analysis and modelling. Some of these are simple spreadsheet programs, such as MS Excel or Microcal Origin, while others are more complex, using programming languages, like R or Matlab. Moreover, often software and/or programming languages do not respond to the Open Science principles.

On the other hand, scientific database is a computerized, organized collection of related data, accessible for scientific inquiry and long-term stewardship. Scientific databases facilitate the integration of dissimilar data sets and allow data to be analysed in new ways, often across disciplines, making new types of scientific inquiry possible. These databases have proven the ability to organize and extract knowledge from huge scientific datasets. Significant data repositories in the Earth Sciences domain already exist, providing a large amount of scientific data, such as GEOROC¹ (Geochemistry of Rocks of the Oceans and Continents), EarthRef² (Earth Reference Data and Models), PANGAEA³, NOAA⁴ (National Oceanic and Atmospheric Administration), IsoBank⁵, IAEA⁶ (International Atomic Energy Agency), and GeoReM⁷.

¹ GEOROC – <https://georoc.eu/georoc/new-start.asp>

² EARTHREF – <https://earthref.org/>

³ PANGAEA – <https://www.pangaea.de/>

⁴ NOAA / NCEI – <https://www.ncei.noaa.gov/services/world-data-system>

⁵ ISOBANK – <https://isobank.tacc.utexas.edu/>

⁶ IAEA – <https://www.iaea.org/>

⁷ GeoREM – <http://georemo.mpch-mainz.gwdg.de/>

These repositories include several datasets contain all the geochemical information (major and trace element concentrations, as well as radiogenic, non-conventional stable, and stable isotopic compositions) related to a given sample, standard and/or geo-material. To store, organize, and manage large amounts of data in a structured way, and to facilitate the retrieval and manipulation of data through tables that have relationships with one another, a relational database – designed to stores and organizes data in a structured way (e.g., Harrington, 2009) – appears to be particularly well-suited.

1.1 The Virtual Research Environment and the D4Science e-Infrastructure

Open Science is a cultural movement based on transparency, sharing, inclusiveness, research integrity, collaboration, and cooperative work, promoting an enhancing approach to science. It represents a set of principles and practices that aim to make scientific research from all fields accessible to everyone for the benefits of scientists and society (Maedche et al., 2024). The effectiveness of the Open Science approach of a project can be enhanced by using a digital infrastructure like D4Science, which promotes collaboration and cooperative work with Virtual Research Environments (VREs) (Candela et al., 2023). In more detail, D4Science supports communities in collaborative activities providing a shared workspace for data exchange, social networking area for communication, data analytics platforms, computing resources for modelling as well as publishing platforms (e.g., catalogues). This infrastructure provides researchers and practitioners with a working environment, where Open Science practices are transparently promoted (Assante et al., 2019).

The ISOTOPE VRE implementation was carried out using the D4science e-Infrastructure (<https://www.d4science.org>, last access: 29/01/2025). D4science is an organization, hosted by the Istituto di Scienza e Tecnologie dell'Informazione “A. Faedo” of the National Research Council of Italy (ISTI, CNR), which offers a data infrastructure since the last 10 years. D4Science data infrastructure consists of a network of hardware and software resources (e.g., databases, services, machines) and is managed by a team of Information and Communication Technology (ICT) professionals and researchers having as main objective the infrastructure maintenance, updating, operation and support for users. The infrastructure relies on the *gCube* technology (https://gcube.wiki.gcube-system.org/gcube/About_gCube,

last access: 29/01/2025). *gCube* is an open-source software system specifically conceived for the construction and development of VREs (Assante et al., 2019a and b; Candela et al., 2013).

Currently, D4Science hosts about 26 different gateways (<https://services.d4science.org/thematic-gateways>, last access: 10/02/2025) and over 175 active VREs with a total of more than 25k active users worldwide. To support this ecosystem with high availability and resilience, the infrastructure is deployed across five geographically distributed sites, including the D4Science data centre in Pisa and three locations within GARR (the Italian National Research and Education Network), providing access to substantial computing resources: 11,700 CPU cores, 82 TB of RAM, and 1,720 TB of storage. The use of the D4Science infrastructure thus enhances the effectiveness of the Open Science approach, supporting collaborative science and the sharing of competences with the creation of VREs (Assante et al., 2019a).

The D4Science architecture comprises two primary layers: the hardware layer and the service layer. The hardware layer is structured as a dynamic pool of virtual machines that provide computational and storage capabilities. The service layer, on the other hand, encompasses e-infrastructure middleware, storage, and end-user services. The hardware layer is powered by an OpenStack installation, which facilitates the deployment of services in the upper layer by supplying the necessary computational and storage resources. The service layer (Figure 1) is composed of five integrated service frameworks.

The **Enabling Framework** provides foundational services essential for the operation of all other services and the VREs. It includes a resource registry for dynamically managing e-infrastructure resources, authentication and authorization services for access control, auditing services for usage tracking, and a VRE manager for deploying tailored VREs with selected applications.

The **Storage Framework** offers advanced, efficient, and on-demand digital data management. It supports various data formats, including files in distributed systems, metadata record collections, and time series in spatial databases, serving all other frameworks except the enabling framework.

The **Analytics Framework** provides tools for executing scientific methods with seamless access to the underlying computational cloud, enabling parallel computation and offering a wide array of pre-packaged statistical methods.

The **Collaborative Framework** underpins VREs with features like social networking, user management, shared workspaces, and WebUI access to the information cloud and analytics framework through dedicated analytics laboratory services. The Collaborative Framework is the core of the VRE concept, which promotes teamwork among users and offers a collaborative space to share digital objects. Indeed, the use of social networking enables opinion exchanges within the team working in a fast and traceable manner. The workspace provides shared access to data for the entire team, eliminating the need for costly data transfers. This ensures that experiments can be easily repeated multiple times and by different development teams without continuously moving data, while also facilitating the access to intermediate results and development progress.

Finally, the **Publishing Framework** facilitates the documentation and publication of research outputs such as datasets, notebooks, and processes. It promotes adherence to FAIR principles by enabling the production and sharing of richly described community-defined artifacts.

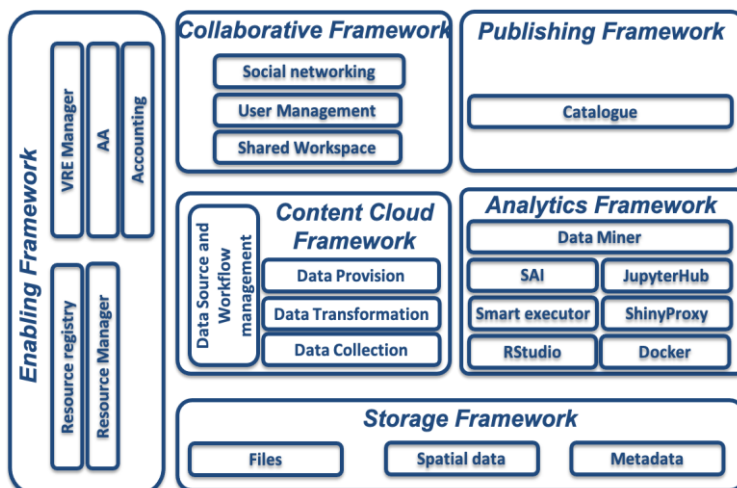


Figure 1. High-level architecture of the D4Science infrastructure.

These integrated frameworks collectively provide the infrastructure and tools necessary for the creation, management, and utilization of VREs. A VRE is an e-Science online environment favouring collaborations and shared solutions to answer specific scientific and/or management questions that require an ensemble of data, analysis tools, modelling solutions and graphical tools, in the spirit of the open science principles.

Virtual Research Environment, in fact, supports the principles of Open Science and data FAIRness (data which meet the principles of Findability, Accessibility, Interoperability, and Reusability) and aims to enhance collaboration among researchers and to find appropriate solutions and address specific scientific and/or management questions (Assante et al., 2019a, 2023). Virtual Research Environments are not “simple” repositories, because they require not only the collection and harmonization of data, but also the collection and development of analysis methods and tools, modelling solutions and graphical tools. Virtual Research Environments design and creation in general follow some simple steps that can be summarized as follows:

- identification of questions (and/or gaps) and stakeholders potentially interested in solving these by using the facilities provided by the VRE;
- collection and harmonization of validated datasets, modelling solutions, analysis and graphical tools;
- development of new data, knowledge and solutions to address specific scientific and/or management questions;
- definition and collection of the metadata to improve data FAIRness.

In this context, these D4Science enabled VREs will become tools supporting the whole research workflow.

As part of the Italian Integrated Environmental Research Infrastructures System (ITINERIS) Project, a comprehensive Italian Research Infrastructures (RDIs) hub in Environmental fields is under development and different multidisciplinary teams are working on the development of thematic VREs for topics including: (i) Critical Zone (CZ) VRE; (ii) Aquatic Biomass services (BIOMASS) VRE; (iii) Crops, Plants and Pests services (CPP VRE); (iv) Essential Variables (EV VRE); (v) Aerosol-biosphere (AERO VRE); (vi) Carbon Cycle services (CARBON VRE); (vii) Indicators and Impacts of Climate Change (CLIMA VRE); (viii) Downstream Effects of Environmental Change (DOWNSTREAM



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VRE); (ix) Isotope Database (ISOTOPE VRE). VREs are new eScience facilities that address scientifically and socially relevant topics, especially through the sharing of information and produced data. Research data and results products are managed and shared with the members of the VREs.

In the framework of ITINERIS Project, the scope of Task 8.9 is to build the Isotope Virtual Research Environment, which embeds a pioneering Italian isotope database dedicated to stable, non-conventional stable, radiogenic isotopes and a set of tools to analyse such data, that will go to fill the gap due to the absence of a complete isotope data collection. In Italy, there are several National Institutions, Universities, and Private Entities performing diverse isotope systematics through instrumentations able to guarantee high performances with high accuracy and producibility in isotope measurements. However, a meeting point between these institutions seems to be missing. In the light of this, the creation of the Italian Isotope Database fills this gap, providing to the scientific community isotopic data sharing set in a Virtual Research Environment (VRE) able to offer a series of powerful tools to understand and interpret environmental processes.

The aim of the ITINERIS ISOTOPE VRE is to provide stakeholders with data access and with a set of useful modelling and analysis tools allowing researchers and environmental managers to understand, analyse and interpret processes occurring in the Earth System. To realize this goal, we encapsulate all the functionalities in a web application hosted by the VRE. Using a web application, we can easily access all functionalities via a standard web browser regardless of a specific software platform.

1.2 The design of the ISOTOPE VRE

The design and development of a VRE dedicated to the isotopes is the fundamental part of the ITINERIS WP8, Task 8.9 project (funded by EU – Next Generation EU PNRR, Mission 4 “Education and Research” – Component 2: “From research to business” – Investment 3.1: “Fund for the realisation of an integrated system of research and innovation infrastructures”). Although other VREs developed in the framework of this project have some reference infrastructures (e.g., LifeWatch ERIC, ICOS ERIC, SIOS and eLTER RI for the Critical Zone VRE), the ISOTOPE VRE is not characterized by specific reference

infrastructure. Despite this, the ISOTOPE VRE – for the specific topics and aims – is strictly linked to other VREs developed in the field of the environment and earth science.

The main stakeholders of the ISOTOPE VRE were identified as environmental managers, together with the scientific community interested in the analysis and interpretation of the complex processes involved in the Earth system. In particular, the ISOTOPE VRE's team designed the VRE to respond to some of the needs of the researchers and to create a set of tools that could be also used by students involved in the environmental fields.

In general, the main sources (in terms of data) feeding ISOTOPE VRE are (i) existing data repositories in the Earth Sciences domain; (ii) the CNR-IGG laboratory facilities; (iii) the laboratory facilities across the Italian territory.

The ISOTOPE VRE contains different types of “products”, in terms of web application functionalities and features for creating and sharing computational documents, subset of the datasets and/or graphic representations. A brief synthesis is showed in the Table 1.

<i>Product</i>	<i>Software Platform</i>	<i>Type of feature/functionality</i>	<i>Description</i>
RDBMS	PostgreSQL	Software components	Permanent storage of the dataset in a relational database
REST APIs	Java / Jersey	Software components	Web services REST to interact through the database
Web user interface	Angular / Bootstrap	Software components	Graphic interface for end users
Data search and management	(in the web-application)	Capabilities	Customized queries and data export
Two end-member mixing	(in the web-application)	Capabilities	Tool for calculation and graphical visualization
Three end-member mixing	(in the web-application)	Capabilities	Tool for calculation and graphical visualization
Data plotting	(in the web-application)	Capabilities	Tool for graphical visualization
Ternary diagram	(in the web-application)	Capabilities	Tool for calculation and graphical visualization

Spider diagram	(in the web-application)	Capabilities	Tool for calculation and graphical visualization
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Table 1. Main types of products in terms of “products”, in terms of web application functionalities and features implemented and/or available in the ISOTOPE VRE.

1.3 Structure of Web Application Software

In the framework of Working Package 8.9 of the ITINERIS Project, the web application, named “Isotope Studio” (IS) has been developed. The main aims of IS are (i) collection of geochemical data which include stable, non-conventional, and radiogenic isotopes; (ii) provide the most common tools for data analyses and interpretation to the stakeholders; (iii) data sharing between all the institutions involved. The architecture of the application is based on three main layers (Figure 2):

- The “*First Layer*” is represented by a relational Database, designed to collect heterogeneous data, with the software aimed to manage DB connections and all “CRUD operations” (Create, Read, Update, Delete). PostgreSQL was chosen as relational database, which represents a powerful, open-source object-relational database system (RDBMS), based on SQL language. As the base language for developing database management, we opted for Java 11, because it was a stable version during the initial development of the web application and is compatible with the PostgreSQL driver used.

In a relational database, data are organized into one or more tables, each with a unique name and set of columns. Each row within a table represents a single record (e.g., a single information), while the columns specify the attributes or characteristics of that record. By structuring data in this way, even originally unstructured information can be systematically organized, enabling efficient querying, fast retrieval, and deeper insights through relationships between tables. This structured approach enhances data consistency, reduces redundancy, and allows for powerful analysis that would be difficult to achieve with unstructured data. A database management system (RDBMS) is used to manage relational databases. Key functions of an RDBMS include data storage, retrieval, manipulation, data security, and backup. The standard way to interact with a relational database is the Structured Query Language (SQL). SQL code statements are used for all operations that can be performed on a relational database: retrieving data, inserting new data and so on (e.g., *Date, 2015*). When creating a new relational database structure, the first step is to construct a data



model, which represents a precise, and complete definition of the data to store. The Entity-Relationship (E-R) data model follows these steps: (i) Identify and define the principal data objects (entities, relationships, and attributes); (ii) Diagram the data objects using the E-R approach; (iii) Translate the E-R data objects into relational constructs; (iv) Resolve the logical data model; and finally (v) Normalize the logical data model. The final product of data modelling is a fully defined database design encoded.

- The “*Second Layer*” is a web services API designed to allow automatic interactions with other applications in a “Service Oriented” perspective. The API is compliant with the constraints of the REST architectural style. See the paragraph “1.5 ISOTOPE STUDIO REST API Interface” for detailed information on the REST APIs released.

- The “*Third Layer*” is a one-page web interface providing end-users with a friendly, reactive, and powerful interface. This interface – developed with Angular 14.3.0 and Bootstrap – allows to easily access to the main functionalities of the application, as, for instance, data retrieving and elaboration, i.e., finding data directly within the application or saving dataset as spreadsheets (directly on their own machines or in the VRE’s workspace).

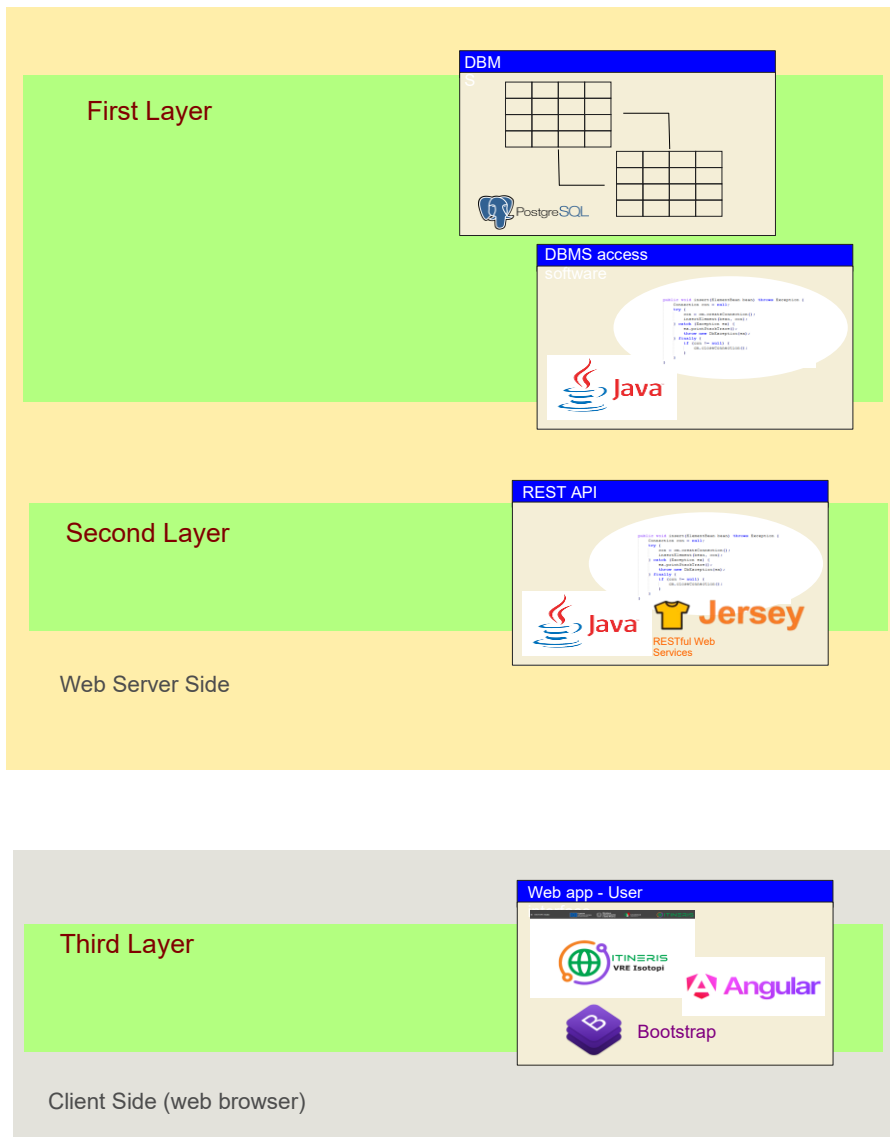


Figure 2. Simplified sketch of the software architecture with the technologies used for the implementation. The yellow box indicates the software that runs on the server side (back-end). The grey box indicates the software that runs on the web browser.

The web application was deployed in the cloud using Docker container technology. Docker is an open container platform designed “for developing, shipping, and running applications” (<https://docs.docker.com/get-started/docker-overview/>, last access: 04/02/2025), and is currently the most widely used solution for packaging web applications (Kim et al., 2022 and reference therein). By encapsulating applications and their dependencies into lightweight, portable containers, Docker ensures consistency across different environments, reducing compatibility issues. It abstracts the underlying infrastructure, enabling seamless deployment across cloud and on-premises systems. This approach accelerates software delivery, streamlines updates, and minimizes downtime, reducing the time between development and production deployment.

The Docker container of the web application is hosted in a dedicated folder in the ISOTOPE VRE’s workspace.

1.4 ITINERIS Isotope database (gathering data and interoperability)

Isotope Geochemistry examines the natural variations in the isotopic compositions of elements found in various Earth materials. Applications of stable (H, O, C, N, and S), noble gases (He, Ne, Ar, Kr, and Xe), non-conventional stable (B, Li, Fe, Cu, Zn, Mg, Ca, Si, Cl, Cr, Ni, Ge, Se, Mo, Hg, and Tl) and radiogenic (Pb, U, Th, Rb, Sr, Sm, Nd, K, and Ar) isotopes have proved valuable in a diversity of research areas, which include Earth System Science and inter-disciplinary, as well as multi-disciplinary studies involving Biology, Archaeology, Agronomy, Ecology, Medicine, food authenticity and traceability and many others. In Italy, several National Institutions, Universities, and Private Entities perform diverse isotope systematics through instrumentations that guarantee high performances with high accuracy and producibility in isotope measurements.

However, a meeting point between these institutions seems to be missing until now. In the light of this, the creation of the Italian Isotope Database, fills this gap, providing the scientific community isotopic data sharing set in a VRE that offers a series of powerful tools to understand and interpret environmental processes.

Gathering data is a critical aspect of ISOTOPE STUDIO software. To achieve this aim, data are collected, harmonized and integrated from several heterogeneous sources of data (and/or metadata), as external websites/applications or single tabular files (e.g., *.csv, *.xlsx)



uploaded and processed by our software. As regards the external repositories, our working group referred to the numerous repositories identified on this specific topic (e.g., GEOROC, PANGAEA, IAEA, and GeoReM). All the identified repositories have been contacted to create a synergistic link with the ITINERIS RI offering IS API to interact with data available in the Isotope VRE. Currently, GEOROC provides positive feedback to our requests, whereas as regards PANGAEA, we used the *pangaeR* R package (<https://cran.r-project.org/web/packages/pangaeR/pangaeR.pdf>, last access 04/11/2024) to perform queries and download data in csv format.

In ISOTOPE STUDIO the database was designed considering the need to store data expressed in a heterogeneous format, as different file types (e.g., spreadsheets, databases) and/or varied data formats. The harmonization of heterogeneous data was achieved by storing the "*sample*" as the fundamental information element in the database and managing other associated data (e.g., geographic data, descriptive data, chemical composition, isotopic ratios, authors) as "*attributes*" of the same sample. This approach ensures a flexible database structure, enabling the collection of data from any type of source. To collect the datasets from other sources, like other Research Institutes, Universities and/or other laboratories, we sent a request for receiving files with references (e.g., DOI) of the most significant works containing isotopic data. All the data derived from the indicated publications are reported in a specific template. The template has been implemented as a spreadsheet that can be managed using the most common spreadsheet app (e.g., open-source office software suite like OpenOffice and LibreOffice, or MS Excel Microsoft license). The template establishes a minimal set of mandatory fields: an identifier for the samples, the related matrices and a "marker" indicating that the file is composed according to the template rules. In addition, it contains a set of "desired" (not mandatory) information, for instance: geographic coordinates, referred DOI (if it is available), authors list, and so on. Some descriptive data can be added, depending on the type of information required for its completion. (e.g., temperature and pH in water data).

For each dataset, the minimal set of information collected allow to generate metadata. In general, metadata is defined as "the information that describes and explains data" (De Keyser, 2012). It provides context with details such as the source, type, owner, and relationships to other data sets. Generally, metadata are organized in a Metadata Catalogue,

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which enhances the FAIRness of the data and represents a powerful tool to concentrate and to make data easily findable and available to the broader scientific community from a unique access point.

Metadata creation involves several steps that allow for an accurate and structured data description, facilitating search, access, and use. This description includes the dataset title, a brief explanation of the data's representations, relevant keywords, the author or organization that created the data, and the creation and update dates. Geographic information may also be included. It is crucial to adhere to a recognized metadata standard, such as those established by the INSPIRE directive (for spatial data), the ISO 19139 schema (for geospatial data), and the Italian RNDT 2.0 guidelines. These standards define what information must be included and how it should be structured. Once the standard is selected, the various required fields must be filled in. This can be done manually or with the assistance of software that helps ensure the information is entered in the correct format. The required information varies depending on the standard but typically includes the title, description, unique identifier, coordinates (latitude and longitude), spatial reference system, data accuracy, completeness, reliability, availability, and usage rights of the data. Several tools are available for creating metadata, among the many *GeoNetwork* (for geospatial metadata), *DataCite Metadata Generator* (for metadata related to scientific publications), and *CKAN* (for managing and publishing open datasets). The choice of which tool to use is still being finalized.

Currently, a BibTex format file is generated in the Isotope Studio web-app to collect minimal reference information for each dataset retrieved from GEOROC and for the dataset coming from a direct upload. Metadata can be also uploaded without restrictions on the format. Furthermore, the metadata of the dataset collected in the database will become harvestable in the general ITINERIS catalogue.



Figure 3. Schematic representation of Metadata Catalogue.

Once created, the metadata must be published in a metadata catalogue (Figure 3). Currently, WP. 8.9 is awaiting the assignment of its own catalogue. In general, metadata is defined as “the information that describes and explains data”. It provides context with details such as the source, type, owner, and relationships to other data sets.

Data will be available in the ITINERIS ISOTOPE VRE and they will be FAIR - Findable, Accessible, Interoperable and Reusable. The under-development ITINERIS catalogue is designed to promote openness principles, as well as the Fairness, and interoperability among the various ITINERIS VREs. Existing vocabulary (Thesaurus) will be used for describing data and facilities. VRE members can participate in the VRE and contribute to the creation and editing of metadata.

In addition, as already mentioned, a key point of our software design is its capability to interoperate with other applications. This feature is achieved through the implementation of a set of REST APIs, which allow external applications to access several functionalities implemented in our software. These "functionalities" include not just retrieving data from our database, but also executing a set of tools for calculations and modelling implemented on our platform. The Mixing Process of two or three end-members is a good example of “functionality” exposed by REST API: external applications can get numeric results of a Mixing Process simply invoking the proper entry point of our REST API (see Di Giuseppe



et al., 2024). The first “client” of this REST API is the “*third layer*” (see previous paragraph) of our platform who make use of this interface for interact with the application’s server side.

Regarding interoperability, Isotope Studio is open to make use of external Web Service API evenly offered by external software. For instance, Isotope Studio is “client” of the REST API implemented by GEOROC (<https://georoc.eu>, last access 05/11/2024) to search and collect isotopic data from this site.

1.5 ISOTOPE STUDIO REST API Interface

REST (**R**epresentational **S**tate **T**ransfer) APIs are application programming interfaces of software architectural style for designing scalable and interoperable web services. They are widely used to allow communication between clients and servers via the HTTP protocol. REST is an architectural style, and an approach to communications that is usually used when developing Web Services. REST is lighter in terms of bandwidth usage, and easier to implement and scale with respect to another contender. RESTful Web Services have been implemented by using Jersey Library.

Isotope Studio has been developed considering the strong importance of a well-developed interoperability framework that allows to disseminate data with and to other service providers and applications in a “service-oriented” perspective. For this reason, the Isotope VRE and – in particular – the Isotope Studio web-application offers the possibility to use web services (REST API endpoints) to communicate between the user interface (front-end) and the server-side application (back-end).

All the API requests are performed with a “base URL” (that is represented by the name of the endpoint) and the format used for each request (as well as for the responses) is the JavaScript Object Notation (JSON) format. So, resources are represented by specific URLs.

In general, the API REST endpoints⁸ of the Isotope Studio web-application support the HTTP methods specified in the Table 2.

⁸ Endpoints are the access points to a REST API. Each endpoint is associated with a unique URL and represents a specific resource. Endpoints are generally organized based on the structure of resources and the operations that can be performed on them.



<i>Method</i>	<i>Description</i>
GET	Return the requested data. It retrieves information from a resource. Parameters, if any, are usually passed in the query string.
POST	Creates a new resource. Data are passed in the request body.
PUT	Updates an existing resource. Data are passed in the request body.
DELETE	Deletes a resource. The reference of the resource is passed usually in the query string.

Table 2. Main HTTP methods used by the API REST endpoints of the Isotope Studio web-application.

Through the RESTful API, external applications can retrieve data from the database by issuing simple HTTP calls.

An HTTP request uses a “status code” to relay the outcome of the request to the client, thus the status codes indicate the outcomes of the requests. Different status codes are used for various purposes throughout this document. These codes are described in detail by the HTTP specification and the most common status codes and their descriptions are listed below in the Table 3.

<i>Status code</i>	<i>Description</i>	<i>Notes</i>
200	OK	The request was successfully completed.
201	Created	New resources have been successfully created.
400	Bad Request	The request is malformed or contains invalid data.
401	Unauthorized	Authentication is required or it has failed.
403	Forbidden	The user does not have the necessary permissions to access the resource.
404	Not Found	The requested resource was not found.
500	Internal Server Error	An internal server error occurred. This error often denotes a syntax error in the request.

Table 3. Most common status codes and their descriptions.



Currently, the Isotope Studio web-application is still under development and – for this reason – also the REST APIs and the documentations will be improved. Following section is dedicated to the documentation of some of the main endpoints used, in particular, to search for, obtain data and to calculate a mixing process data. In particular, here REST API documentation, including definitions and examples of endpoint can be find.

<i>Endpoint</i>	<i>Method</i>	<i>Query string</i>	<i>Body</i>
/query-info	POST	(Not used in this method)	set of search criteria

This endpoint allows to extract data from the database according to rules defined by a set of search criteria. The search criteria allowed are:

<i>Parameters</i>	
Name	Description
Reference	the DOI (or a link) directly related to the dataset imported in the database
Authors	a list of authors (at least one author)
Keywords	a list of keywords (separated by a space) associated to the dataset
Publication year	the year of publication of the articles from which the datasets were extracted
Geographic information	latitude and longitude coordinates (CRS: WGS-84 - EPSG: 4326) of a rectangular boundary box
Matrix	the type of material (named “matrix”) of the sample source (e.g., water, air, minerals)

Search criteria are combined with logical operators. In particular, the logical operator “AND” can be used for the “intersection” among two or more criteria; while the logical operator “OR” for the “union” among two or more criteria. Despite this, these combinations can create a very complex data request, and the relative endpoint based on a GET method would result in a query string too long and difficult to manage. The endpoint based on POST method is used to bypass this problem and allow to use a set of search parameters in JSON format contained in the request body. A set of a search criteria is a JSON object like this:

```
{ "polygon": { ... }, "year": { ... }, "reference": { ... }, "authors": { ... }, "keywords": { ... }, "matrix": { ... } }
```



The order of the keywords is not relevant. Each keyword is the key of a specific JSON object; for instance, the keyword “polygon” is associated to JSON object with the coordinates of a geographic rectangle:

```
{ "polygon": {
    "operator": "AND | OR",
    "topLat": ... ,
    "topLon": ... ,
    "bottomLat": ... ,
    "bottomLon": ...
  }
}
```

<i>Endpoint</i>	<i>Method</i>	<i>Query string</i>	<i>Body</i>
/get-authors/{author-id}	GET	specific identifier or nothing in order to get the full author list	(Not used in this method)
/get-references/{reference-id}	GET	specific identifier or nothing in order to get the full reference list	(Not used in this method)
/get-years	GET	(Not used in this method)	(Not used in this method)

Other examples for data search are here described. In particular, the REST APIs interface can be also used to get other database content, for instance a list of authors or article references (e.g., DOI). These endpoints are based on the GET method and allow to filter the data on the base of a specific criteria (e.g., the authors or the publication year).

<i>Endpoint</i>	<i>Method</i>	<i>Query string</i>	<i>Body</i>
-----------------	---------------	---------------------	-------------



/mixing-model

POST

(Not used in this
method)

Mixing model input data

This endpoint is based on the POST method and can be used to perform analysis of the dataset selected from the database or uploaded in the web application. In particular, this endpoint allows to perform the calculation for a mixing model of two or three end-members directly through the REST API web service. Mixing model input data is a JSON object providing: the step increment to be applied on each iteration and the description of the end-members. Each end-member is described by the following parameters:

<i>Parameters</i>	
Name	Description
member	the member name / identifier
element	the chem. Element or isotope ratio
concentration	the numeric value of the element
concentration2	optional, required only when "element" indicates an isotope ratio

A detailed manual describing all the endpoints, as well as all the parameters, will be provided at the end of the development of the web application and REST APIs. The endpoint briefly described in this paragraph must be considered only a preliminary version (last access: 31/01/2025).

2 USER GUIDE ON THE ISOTOPE VRE

2.1 Access to the VRE

A specific section of the ITINERIS Project website is devoted to the ITINERIS Hub (<https://itineris.cnr.it/itineris-hub/>, last access: 30/01/2025). The ITINERIS Hub will be the unique access point to all the services, facilities, tools and datasets collected and provided by the Italian RIs in the environmental domains (Figure 4). The Hub is conceived as a sort of “unique comprehensive catalogue” where researchers will also publish the VREs metadata and users will be able to access the ITINERIS VREs Gateway.

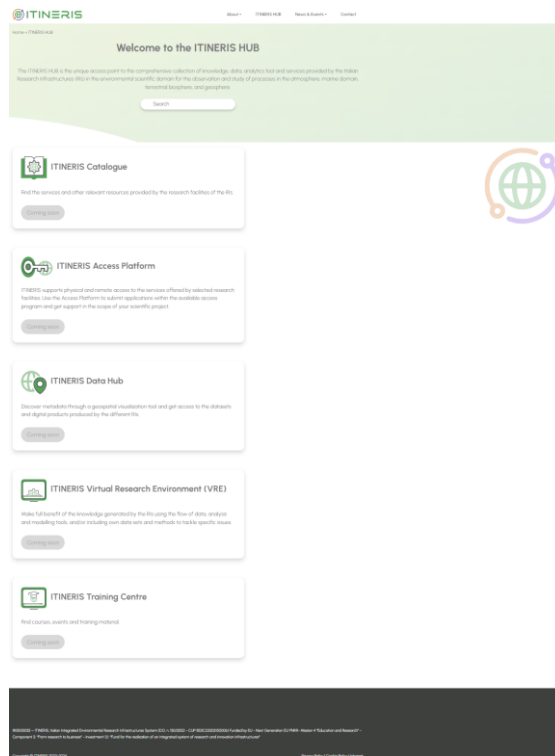


Figure 4. View of the screen of the ITINERIS Hub (<https://itineris.cnr.it/itineris-hub/>, last access: 30/01/2025).

The D4Science infrastructure allowed to create a unique Gateway to access multiple VREs: the ITINERIS VREs Gateway (<https://itineris.d4science.org/>, last access:

29/01/2025; Figure 5a). D4Science is equipped with an Identity and Access Management (IAM) system.

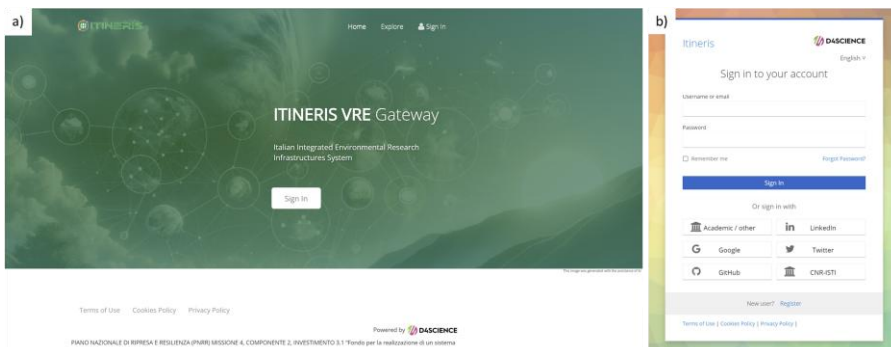


Figure 5. a) View of the screen of the ITINERIS VREs Gateway. b) View of the screen of the sign-in page where the user can insert the username and the password or select one of the different methods available for login. For the creation of a new D4Science account, the users can select the “Register” button and proceed.

After the login with the D4Science’s username and password or selecting another method for the login (by using existing accounts, e.g., ORCID, GitHub, Google, LinkedIn; Figure 5b), the VREs will be available and accessible. In particular, multiple teams of the ITINERIS WP8, with a high level of trans-disciplinarity, are working on the development of several thematic VREs [e.g., Critical Zone (CZ VRE); Aquatic Biomass services (BIOMASS VRE); Essential Variables (EV VRE); Aerosol-biosphere (AERO VRE); Carbon Cycle services (CARBON VRE); Indicators and Impacts of Climate Change (CLIMA VRE); Downstream Effects of Environmental Change (DOWNSTREAM VRE); Isotope Database (ISOTOPE VRE)].

Once the users have identified the VRE they are interested in, they can click the button “Request Access” (Figure 5b) and confirm the request after stating a motivation for accessing to the VRE (this represents a mandatory field). Each VRE has moderators and managers who can review the access requests. In general, in a brief time (typically within a few hours) the user receives a notification via email about the outcome of the request. Thus, the ITINERIS ISOTOPE VRE is accessible after the registration and the specific request to access the ISOTOPE VRE from the ITINERIS Gateway (Figure 6).



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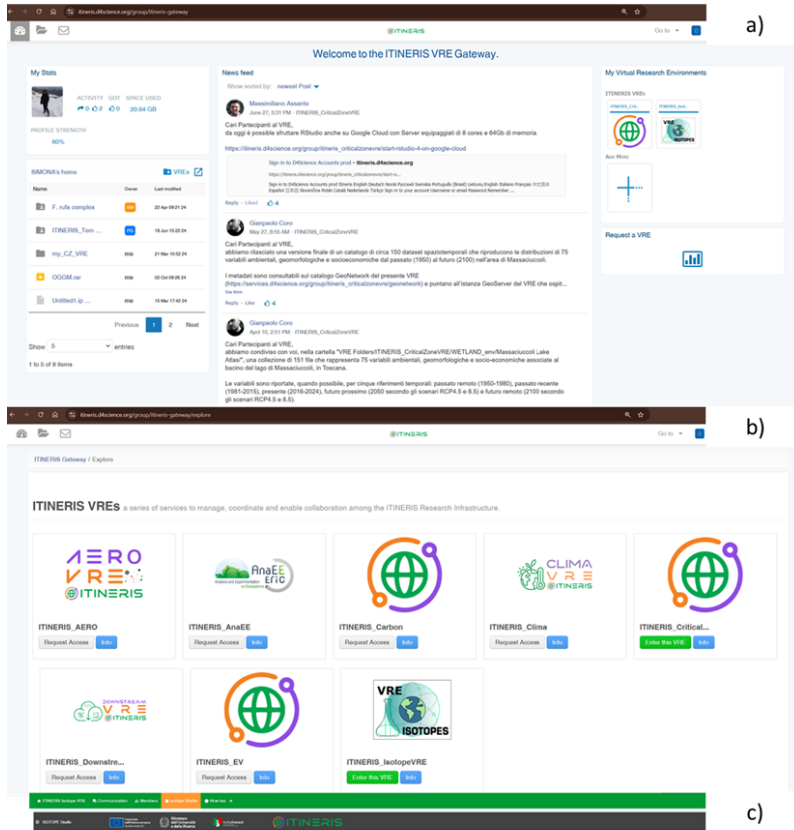


Figure 6. a) Panel on the top shows how the users can see their gateway after the login. On the left the panel “My Virtual Research Environments” allows to add one or more VRE(s) by clicking on the button “+” (“Add More”). b) By clicking on “Add More”, the users can start to see the VREs available. Once the users have identified the VRE they are interested in, they can click the grey button “Request Access” and confirm the request after stating a motivation for accessing to the VRE (this represents a mandatory field). c) Introductory screen of the ISOTOPE VRE.

2.2 Basic services of the ISOTOPE VRE: the workspace and the social network board

The primary services offered by the ISOTOPE VRE are a **workspace** with high computing capabilities, a shareable folder system, and a **social networking board system**. In particular, these basic elements are described below.

The VRE is equipped with an area for data collection with Collaborative Storage Framework and a collaborative workspace that promotes teamwork and offers the opportunity to share digital objects. In particular, the “**workspace**” is an exceptionally reliable, distributed, online file system that allows one to upload files, create private folders, share folders with specific colleagues, publish folders, share data, and directly publish data in a catalogue. The VRE users will find (named with the name of the user: “USER’s workspace”) a space named “**VRE Folders**” in their workspace, identified by a white star on the icon of the folder. Files and digital objects added or created in the VRE folders are automatically shared with the other VRE’s members. Users also can make use of a restricted area; folders and/or files in this area are private, unless the user shares them. To share folders and/or files, users must use the share option (Figure 7) and select the user(s) to share with and the adequate sharing policy (Figure 8). The selectable policies (“Permission”, Figure 7) are three: *Write Any* (all users can modify all files), *Read Only* (users other than the owner can only read files), and *Write Own* (all users can create files but only modify files they own). These three different options are also identified by different icons (Figure 8).

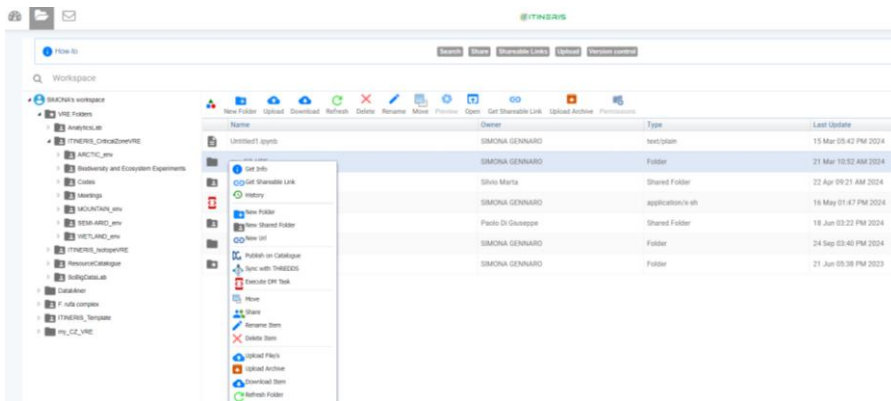


Figure 7. View of the workspace and of the drop-down menu available by right-clicking on a file or a folder in the private space.

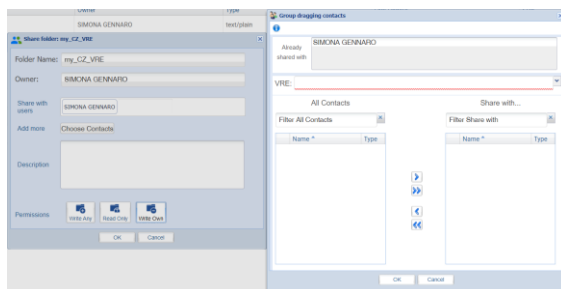


Figure 8. View of the “Share folder” window. At the bottom of this window, the user can select permissions. By clicking on “Choose Contacts” in the “Share folder” window, the user can access the window named “Group dragging contacts”, where the users can manage the selection of the contacts.

The **social networking board system** integrated into the VRE allows the exchange of messages between users. The board (also called “feed”; available by clicking on “Communication”, see the Figure 6c above) for open discussions allows to share updates, links and files from the VRE folders. It is also possible to use the “@” symbol to explicitly mention other participants, or a tag (“#”) to identify topics and keywords. Members of the VRE can also reply to a specific post or add a “Like” as reaction. VRE’s members can set specific options to receive notification (via email and/or on the ITINERIS VRE Gateway) for the social network board, the workspace, as well as for the catalogue.

2.3 Guide on the ISOTOPE STUDIO web application

Visualization and modelling of geochemical data are fundamental in all the fields of Geosciences, with data visualisation playing a crucial role in the interpretation of natural geo-environmental processes. In many cases, plotting geochemical data can be a slow and tedious process, often involving several steps that are prone to human error. To address these challenges, various software programs have been developed over time to assist students and researchers in performing specific geochemical models. Plotting operations can be carried out using different software packages, such as common spreadsheet programs, interpreted scientific programming languages (e.g., Matlab or R), or software dedicated to a typical research fields, such as PetroGraph (Petrelli et al., 2005) for igneous petrology, IsoplotR (Vermeesch, 2018) for geochronology, EQ3/6 version 8.0 (Worely and Jarek, 2003) for modelling geochemical interactions between aqueous solution, solids, and gases, and many

others. Currently, the Isotope Portal offers two main functions on the menu (Fig. 9): i) “*Database Querying*”, for searching relevant data; ii) “*Data Import*”, for uploading data in .xls or .csv formats. These functions allow the user to enter the web application module dedicated to the modelling (see paragraph 2.6 for the guide on the modelling tools offered in the Isotope VRE).

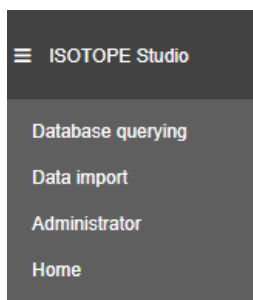


Figure 9. Introductory screen of Isotope Studio Database.

2.4 Data Querying

Data Querying allows users to select a dataset relative to a single or multiple publications by entering a DOI or author’s name (Fig. 10). Alternatively, users can choose data associated with a specific study area by entering geographic coordinates (if any; Fig. 11) or by using other parameters through a keyword filter. The dataset will then display all the data relevant to the search (Fig. 12). At this stage, the user can select the data they wish to use for modelling environmental processes.

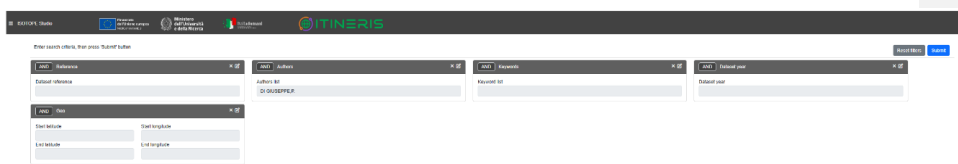


Figure 10. Screen of data querying by author.



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Figure 11. Screen of data querying based on a selection on a map. This system has been implemented by using OpenStreetMap (<https://www.openstreetmap.org/>, last access: 22/02/2025; WGS-84 coordinate system - EPSG 4326).

ISOTOPE ID	ISOTOPE NAME	ISOTOPE SYMBOL	ISOTOPE MASS	ISOTOPE ABUNDANCE	ISOTOPE HALF-LIFE	ISOTOPE DECAY MODE	ISOTOPE ENERGY	ISOTOPE PERIOD	ISOTOPE TYPE	ISOTOPE STATUS	ISOTOPE SOURCE	ISOTOPE REFERENCE	ISOTOPE DATE	ISOTOPE LOCATION	ISOTOPE COORDINATE	ISOTOPE PROJECT	ISOTOPE USER	ISOTOPE CREATED	ISOTOPE MODIFIED	
0001	Hydrogen	H	1.007825	99.985	12.320	Stable	0.000000	0.000000	Stable	Active	Hydrogen	1.007825	1911	Hydrogen	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0002	Deuterium	D	2.014102	0.015	12.320	Stable	0.000000	0.000000	Stable	Active	Deuterium	2.014102	1911	Deuterium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0003	Tritium	T	3.016049	0.000000	12.320	Radioactive	0.018808	12.320	Radioactive	Active	Tritium	3.016049	1911	Tritium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0004	Helium	He	3.016029	0.000000	12.320	Stable	0.000000	0.000000	Stable	Active	Helium	3.016029	1911	Helium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0005	Lithium	Li	6.941	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Lithium	6.941	1911	Lithium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0006	Beryllium	Be	9.012182	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Beryllium	9.012182	1911	Beryllium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0007	Boron	B	10.012738	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Boron	10.012738	1911	Boron	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0008	Carbon	C	12.010738	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Carbon	12.010738	1911	Carbon	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0009	Nitrogen	N	14.003074	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Nitrogen	14.003074	1911	Nitrogen	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0010	Oxygen	O	15.994915	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Oxygen	15.994915	1911	Oxygen	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0011	Fluorine	F	18.998403	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Fluorine	18.998403	1911	Fluorine	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0012	Neon	Ne	19.992479	0.000000	12.320	Stable	0.000000	0.000000	Stable	Active	Neon	19.992479	1911	Neon	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0013	Sodium	Na	22.989769	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Sodium	22.989769	1911	Sodium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0014	Magnesium	Mg	24.304688	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Magnesium	24.304688	1911	Magnesium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0015	Aluminum	Al	26.981538	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Aluminum	26.981538	1911	Aluminum	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0016	Silicon	Si	28.085583	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Silicon	28.085583	1911	Silicon	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0017	Phosphorus	P	30.973761	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Phosphorus	30.973761	1911	Phosphorus	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0018	Sulfur	S	32.065	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Sulfur	32.065	1911	Sulfur	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0019	Chlorine	Cl	35.453	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Chlorine	35.453	1911	Chlorine	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0020	Argon	Ar	39.948	0.000000	12.320	Stable	0.000000	0.000000	Stable	Active	Argon	39.948	1911	Argon	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0021	Potassium	K	39.0983	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Potassium	39.0983	1911	Potassium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0022	Calcium	Ca	40.078	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Calcium	40.078	1911	Calcium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0023	Scandium	Sc	44.955912	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Scandium	44.955912	1911	Scandium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0024	Titanium	Ti	47.88	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Titanium	47.88	1911	Titanium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0025	Vanadium	V	50.9415	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Vanadium	50.9415	1911	Vanadium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0026	Chromium	Cr	51.99616	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Chromium	51.99616	1911	Chromium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0027	Manganese	Mn	54.938044	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Manganese	54.938044	1911	Manganese	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0028	Iron	Fe	55.845	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Iron	55.845	1911	Iron	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0029	Cobalt	Co	58.933195	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Cobalt	58.933195	1911	Cobalt	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0030	Nickel	Ni	58.6934	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Nickel	58.6934	1911	Nickel	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0031	Copper	Cu	63.546	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Copper	63.546	1911	Copper	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0032	Zinc	Zn	65.38	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Zinc	65.38	1911	Zinc	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0033	Gallium	Ga	69.723	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Gallium	69.723	1911	Gallium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0034	Germanium	Ge	72.630	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Germanium	72.630	1911	Germanium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0035	Arsenic	As	74.9216	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Arsenic	74.9216	1911	Arsenic	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0036	Selenium	Se	78.9718	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Selenium	78.9718	1911	Selenium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0037	Bromine	Br	79.904	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Bromine	79.904	1911	Bromine	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0038	Krypton	Kr	83.80	0.000000	12.320	Stable	0.000000	0.000000	Stable	Active	Krypton	83.80	1911	Krypton	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0039	Rubidium	Rb	85.4678	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Rubidium	85.4678	1911	Rubidium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0040	Strontium	Sr	87.62	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Strontium	87.62	1911	Strontium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0041	Yttrium	Y	88.905848	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Yttrium	88.905848	1911	Yttrium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0042	Zirconium	Zr	91.224	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Zirconium	91.224	1911	Zirconium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0043	Niobium	Nb	92.90638	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Niobium	92.90638	1911	Niobium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0044	Molybdenum	Mo	95.94	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Molybdenum	95.94	1911	Molybdenum	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0045	Technetium	Tc	98.90625	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Technetium	98.90625	1911	Technetium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0046	Ruthenium	Ru	101.07	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Ruthenium	101.07	1911	Ruthenium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0047	Rhodium	Rh	102.9055	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Rhodium	102.9055	1911	Rhodium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0048	Palladium	Pd	106.42	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Palladium	106.42	1911	Palladium	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0049	Silver	Ag	107.8682	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Silver	107.8682	1911	Silver	40.7128	14.8797	1	1	2025-02-22	2025-02-22
0050	Cadmium	Cd	112.411	0.000000	12.320	Radioactive	0.000000	12.320	Radioactive	Active	Cadmium	112.411	1911	Cadmium	40.7128	14.8797	1	1	2025-0	

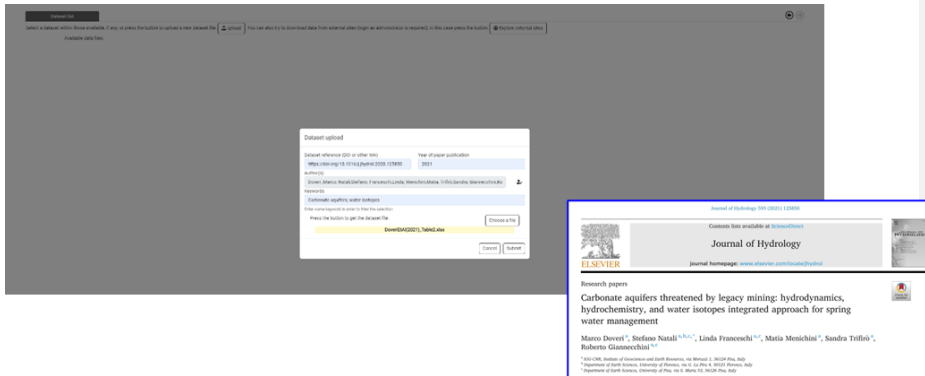


Figure 13. Example of data upload and related publications linked to them. On the right, the publication uploaded (Doveri et al. 2021).

Before uploading data, the user can select and specify the type of data to be submitted and review the information related to each data item. This includes “*sample field*” which provides a description of the sample’s location, “*chemical element*” which indicates any chemical element expressed as oxide (e.g., SiO₂), cation/anion (e.g., Ca²⁺), or trace element (e.g., Th, Rb, Sr). Additionally, also isotope can be selected as for ratio (e.g., ⁸⁷Sr/⁸⁶Sr) and delta value (e.g., δ¹¹B; Fig. 14a). A final summary of all information to selected dataset is then reported (Fig. 14b).



Currently, data can also be downloaded and viewed through links related to external websites. An example can be represented by GEOROC data repository (Fig. 15).

2.6 Data Modelling: examples and guide to the tools

The geochemical data already available can either be searched and selected through the application, or, if unpublished, directly imported by the user into the Isotope Studio database in *.xls or *.csv file formats, following the same procedure reported by Di Giuseppe et al. (2024) and briefly described above. Once the data are selected, the user can visualize them using three different types of plots commonly used in the field of Geosciences: i) binary plots, ii) ternary plots, and iii) normalized (spider) diagrams.

Binary Plot

A binary plot is a graphical representation of mixtures of two components. Binary diagrams are typically used to represent the composition of a combination of two components. The selected data can be plotted on X-Y axes using either linear or logarithmic (base 10) scaling. Each axis can display values for selected elements (major or trace), element and isotopic ratios (e.g., Rb/Sr or $\delta^{11}\text{B}$). In addition to element ratios, it is possible to add, subtract, and multiply values of different elements. Reverse operations ($1/x$ or $1/y$) can also be applied. Users can define a range of values (e.g., maximum and minimum) for the X and Y axes to zoom in on a specific area of the graph to display a specific distribution range of values, which is particularly useful when working with large datasets. An example of a binary plot is shown in Figures 16(a, b) and 17.



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a)

The screenshot shows the ITINERIS software interface with a data table. A context menu is open over the table, listing options: Plot data, Spider diagram, Ternary diagram, Mixing model, Crystallization mass balance, and Melting. The table has columns for ITINERIS_ID, LOCATION, MATRIX, MATRIX SUB-GROUPS, SAMPLE FIELD, SAMPLE NAME, YEAR OF PUBLICATION, B, Ca2+, Cl, Na+, Sr, and Zr.

ITINERIS_ID	LOCATION	MATRIX	MATRIX SUB-GROUPS	SAMPLE FIELD	SAMPLE NAME	YEAR OF PUBLICATION	B	Ca ²⁺	Cl	Na ⁺	Sr	Zr
19802	Campo di olio	Walls	Olivaria Phase	Cornia Plain	04.1	2000.0	5.26	543.0	2073.0	560.0	4.38	0.11
19801	Campo di olio	Walls	Olivaria Phase	Cornia Plain	05.1	2000.0	5.29	513.0	954.0	360.0	2.93	0.08
19802	Fucoli	Walls	Olivaria Phase	Cornia Plain	06.0	2000.0	4.5	923.0	2380.0	370.0	0.90	0.3
19803	Private wall	Walls	Olivaria Phase	Cornia Plain	08.0	2000.0	5.03	110.0	700.0	490.0	1.90	0.1
19804	Private wall	Walls	Olivaria Phase	Cornia Plain			4.97	402.0	1090.0	140.0	3.67	0.08
19802	Il Salice (wall 2)	Walls	Olivaria Phase	Cornia Plain			4.75	1043.0	3743.0	750.0	0.30	0.02
19806	Private wall	Walls	Olivaria Phase	Cornia Plain			5.24	1203.0	3021.0	630.0	10.01	0.08
19807	Private	Walls	Olivaria Phase	Cornia Plain			4.01	573.0	2013.0	770.0	3.03	0.1
19808	Farm. Pisciardi	Walls	Olivaria Phase	Cornia Plain			3.60	703.0	3217.0	1307.0	4.4	0.02
19809	Campo di Rio	Walls	Olivaria Phase	Cornia Plain			1.24	142.0	310.0	147.0	0.0	0.02
19805	Stazione Luciani	Walls	Olivaria Phase	Cornia Plain			0.36	110.0	730.0	320.0	0.0	0.4
19804	Prodotto di Montecorona	Walls	Olivaria Phase	Cornia Plain			1.44	483.0	2260.0	870.0	0.0	0.02

b)

The screenshot shows the 'Manage plotting series' dialog box. It allows users to choose X and Y axes, set operators, and define data series. The X-axis is set to 'B' and the Y-axis is set to 'delta118'. The X range is 0.17 and the Y range is -6.4. The data definition is '75 points to assign'. The series is named 'square' with a red color and 37 points. There is a checkbox for 'On mixing diagram'.

Manage plotting series

Choose X axis and Y axis

Operator X Axis: B Operator Y Axis: delta118

X logarithmic scale: 0.17 Y logarithmic scale: 6.36

Y range: -6.4

Data definition: 75 points to assign. Use button to add a new data series

Name: square Color: red #Points: 37

On mixing diagram

Close Reset all PLOT

Figure 16. a) Screen of selecting modeling; b) Manage plotting series command.

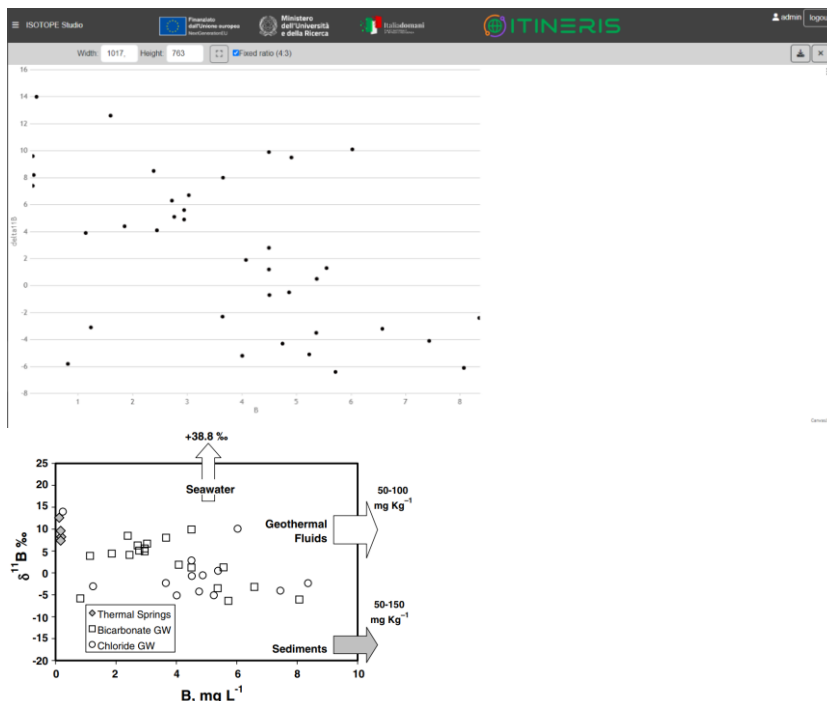


Figure 17. Representation of a binary plot containing the isotopes of B (expressed in delta per mil) on the Y-axis and the concentration of the same element on the X-axis. On the right, the same plot as shown in Pennisi et al (2006).

Ternary Plot

A ternary plot is a three-variable graph used to represent the composition of a mixture or system made up of three components. Ternary diagrams are typically displayed as equilateral triangles, with each apex representing one of the three components. The interior of the triangle represents all possible combinations of these components, and data points are plotted within this triangular space. Ternary diagrams are graphical representations of mixtures of three components, usually expressed as percentages that sum to 100%. The three corners of the triangle correspond to the pure compositions of each component. Each vertex can represent either a single element (e.g., Mg^{2+}) or the ratio/sum of elements (e.g., $HCO_3^- + CO_3^{2-}$). The three axes of the triangle connect the vertices and represent the relative



proportions of each component in the mixture, ranging from 0% (at the vertex) to 100% (at the opposite side). The selected data are normalized using the following formula:

$$(A_v/(A_v+B_v+C_v))*100$$

$$(B_v/(A_v+B_v+C_v))*100$$

$$(C_v/(A_v+B_v+C_v))*100$$

where A_v , B_v , and C_v are the values for each vertex.

Figure 18 reports an example of common ternary plot for water samples.

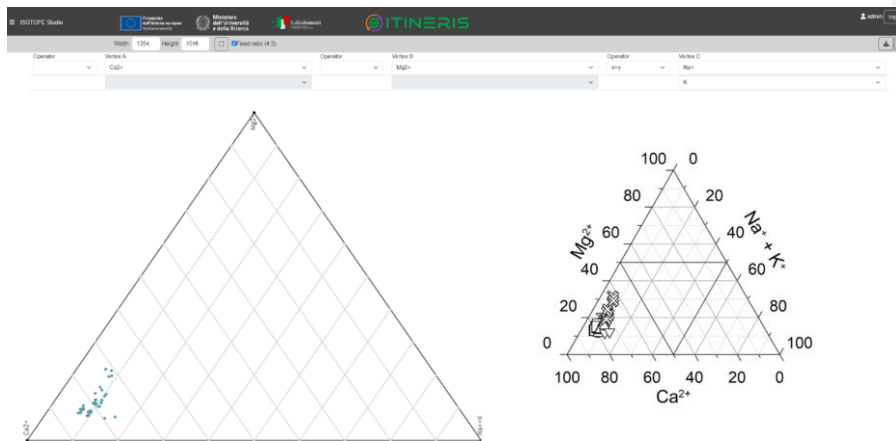


Figure 18. Representation of a ternary plot reporting water cations (Ca^{2+} , Mg^{2+} , and $Na+K+$). On the right, the ternary plot reported in Doveri et al (2021).

Normalized diagrams (Spider diagram)

It is quite common in the field of Geosciences to express compositional differences between studied samples and specific geochemical reservoirs (or end-members) using so-called spider diagrams (also known as multi-element diagrams; Fig. 19). Spider diagrams allow for the representation of the composition of one or more samples on a single graph. Typically, logarithmic diagrams are used, where elemental concentrations are 'normalized' (divided) by those of a selected standard, enabling the comparison of concentrations that may differ by several orders of magnitude. In this case, the user can choose to plot data on the Y-axis using either linear or logarithmic (base 10) scaling, while the X-axis displays only



the selected elements. Key options include selecting normalization values from a list of predefined reservoirs. Additionally, as Rare Earth Element (REE) spider plots are among the most common, these can also be displayed. Normalization values are referred to:

- average Upper Continental Crust (UCC; Taylor and McLennan, 1985;1995)
- average Middle Continental Crust (MCC; Rudnick and Gao, 2003)
- average Lower Continental Crust (LCC; Rudnick and Gao, 2003)
- Average CI Chondrite (McDonough and Sun, 1995)
- Average CI Chondrite (Sun and McDonough, 1989)
- Pyrolite (McDonough and Sun, 1995)
- Primitive Mantle (PM; Sun and McDonough, 1989)
- Primitive Mantle (PM; Palme and O'Neill, 2014)
- Normal MORB (N-MORB; Sun and McDonough, 1989)
- Enriched MORB (E-MORB; Sun and McDonough, 1989)
- OIB (Sun and McDonough, 1989)
- Global Subducted Sediments (GloSS I&II; Plank and Lannngmuir, 1998; Plank, 2014)

In addition, users have the opportunity of manually adding a normalization factor for each selected element.

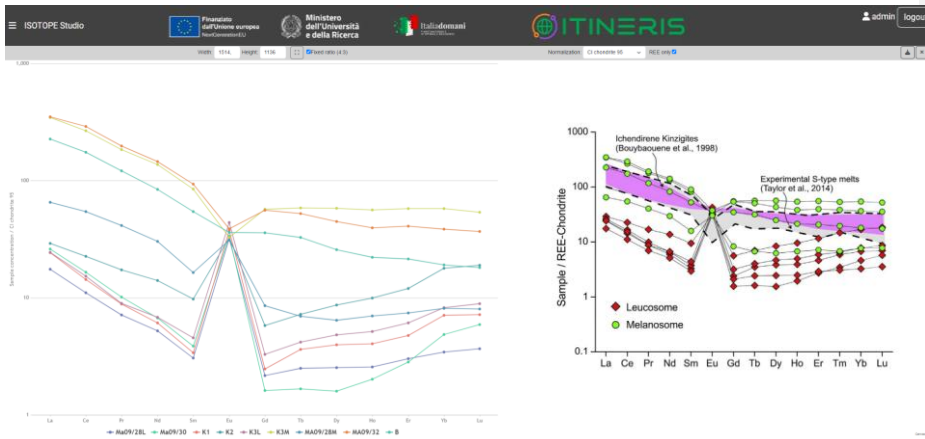


Figure 19. Representation on normalized (spider) diagram with trace element values normalized using average Chondrite values (McDonough and Sun, 1995). On the right, spider diagram reported in Rossetti et al (2020).



Mixing Modelling

Mixing model is widely used to improve process understanding throughout Earth and Environmental Science. The term “*Mixing Calculation*” refers to the computation of the proportions (mixing ratios) in which two or more selected end-members are mixed in a sample. The calculation of mixing ratios is a key task in diverse fields of Earth Science, which include marine and atmospheric science such hydrology, ecophysiology, biogeochemistry, and petrology.

Binary mixing can be considering as the simplest mixing model concerns a single tracer in two sources:

$$C_M = f(C_1 - C_2) + C_2 \quad (\text{Eq. 1})$$

in which C_1 , C_2 and C_M are the concentrations of an element in end-member 1, end-member 2, and in the mixed sample resulting from mixing between end-member 1 and 2, respectively; whereas f is the degree of mixing. This equation (1) can be applied to both major and trace elements.

For isotope compositions, the equation is expressed as:

$$I_M = I_1 (C_1/C_M) f_1 + I_2 (C_2/C_M) (1-f_1) \quad (\text{Eq. 2})$$

where, I_{C1} , I_{C2} , and I_{Cm} represent the isotopic ratios of any element in end-member 1, end-member 2, and in the mixed sample resulting from the mixing between end-members 1 and 2. Given:

$$C_M = f_1 C_1 + (1-f_1) C_2 \quad (\text{Eq. 3})$$

$$I_M = [I_1 C_1 f_1 + I_2 C_2 (1-f_1)] / [C_1 f_1 + C_2 (1-f_1)] \quad (\text{Eq. 4})$$

It is often the case that a third (or more) end-member contributes to mixing process. In this case, calculating the mixing fractions is still possible, although the modelling requires a second conservative parameter to solve the mixing equations. In a “three-component mixing” scenario using the mass balance approach, three different end-members, named 1, 2 and 3, are assumed to mix each together. This implies that:

$$f_1 + f_2 + f_3 = 1 \quad (\text{Eq. 5})$$

$$C_M = f_1 C_1 + f_2 C_2 + f_3 C_3 \quad (\text{Eq. 6})$$

$$I_M = I_1 C_1 f_1 + I_2 C_2 f_2 + I_3 C_3 f_3 / f_1 C_1 + f_2 C_2 + f_3 C_3 \quad (\text{Eq. 7})$$



To carry out typical mixing processes, users can select the desired samples and define two or more end-members (Fig. 20).

SAMPLE NAME	B	CA	CL	CS	FE	F	K	LI	MG	MN	NA	SR	SE	V
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MS	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0

Figure 20. Selected Data for modelling.

End member A

End member B

End member C

Element: Concentration:

Element: Concentration:

Element: Concentration:

Back to data | Clear cache | Show results | Submit

Element	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z
B	15.0	150.0	400.0	440.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
CA	150.0	1500.0	4000.0	4400.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0	100.0
CL	400.0	4000.0	40000.0	44000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0
CS	440.0	4400.0	44000.0	44000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0	1000.0
FE	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
F	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
K	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
LI	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MG	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
MN	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
NA	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
RE	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
SR	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0
V	10.0	100.0	1000.0	1000.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0	10.0

Figure 21 List of end-members selected for modelling and showing sample description (chemical elements and isotopes compositions) and r final results of the mixing modelling.

As illustrated in Figure 21, users can model the mixing process by selecting two or more end-members. The database offers several approaches for modeling the mixing process: i) element comparison (e.g., V vs. K), ii) element and/or element ratio (e.g., B vs. Nb/Ta), iii) element/element ratios and/or isotopes (e.g., B vs. $\delta^{11}\text{B}$), or iv) two isotope ratios (e.g., $^{87}\text{Sr}/^{86}\text{Sr}$ and $^{143}\text{Nd}/^{144}\text{Nd}$). When an isotope ratio or delta value is chosen, the database automatically retrieves the corresponding element concentration. If the concentration of a particular element is not available, the user has the option to manually input the value (Fig. 22).



Figure 22. Example of binary mixing, in which Sr concentration is added manually.

At this point, the user is presented with two options, both of which can be selected:

1. The user can choose to either plot the data on the mixing graph and export the graph or manually input data and plot it on the mixing graph. Additionally, it is possible to plot a single point within the graph, and the coordinates representing the mixing
2. percentage between end-members can be extracted (Fig. 23a-b).

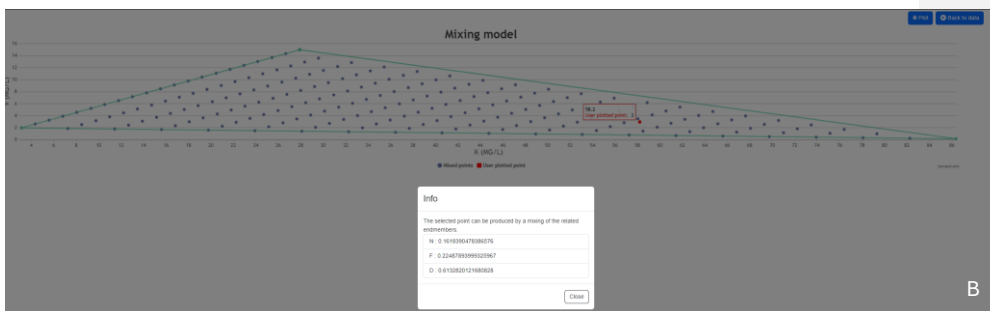
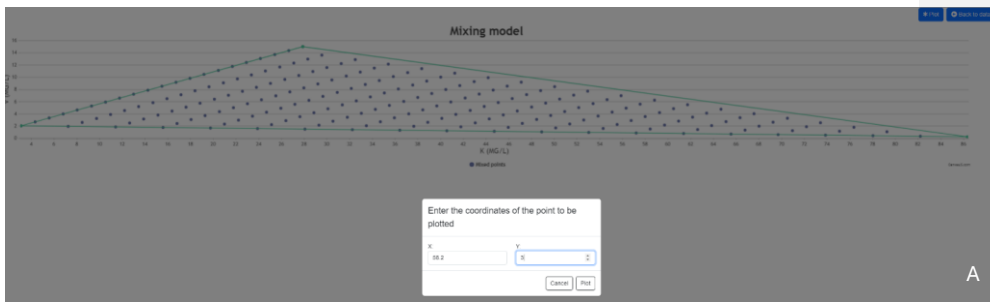


Figure 23. Example of scheme reporting a three-endmember mixing model results. Green lines are the mixing between end-members 1, 2, and 3 when f_1 , f_2 , or f_3 are zero, respectively. Grey points are all the possibilities of mixing values between end-members. A) A sample is plotted in the graph; B) Red square represents the plotted samples; the mixing percentages between the three end-members are also calculated.

3. The user can download the mixing results to an Excel sheet (.csv) for further customization and analysis (Fig. 24).



	A	B	C	D	E	F	G	H
1	N :V(MG/L)	F :V(MG/L)	D :V(MG/L)	MIX	N :K(MG/L)	F :K(MG/L)	D :K(MG/L)	MIX
2	0.00	1.00	0.00	2.00	0.00	1.00	0.00	3.10
3	0.00	1.00	0.00	2.00	0.00	1.00	0.00	3.10
4	0.00	1.00	0.00	2.00	0.00	1.00	0.00	3.10
5	0.00	0.95	0.05	1.91	0.00	0.95	0.05	7.27
6	0.00	0.90	0.10	1.82	0.00	0.90	0.10	11.43
7	0.00	0.85	0.15	1.73	0.00	0.85	0.15	15.60
8	0.00	0.80	0.20	1.64	0.00	0.80	0.20	19.76
9	0.00	0.75	0.25	1.55	0.00	0.75	0.25	23.93
10	0.00	0.70	0.30	1.46	0.00	0.70	0.30	28.09
11	0.00	0.65	0.35	1.37	0.00	0.65	0.35	32.26
12	0.00	0.60	0.40	1.28	0.00	0.60	0.40	36.42
13	0.00	0.55	0.45	1.19	0.00	0.55	0.45	40.59
14	0.00	0.50	0.50	1.10	0.00	0.50	0.50	44.75
15	0.00	0.45	0.55	1.01	0.00	0.45	0.55	48.92
16	0.00	0.40	0.60	0.92	0.00	0.40	0.60	53.08
17	0.00	0.35	0.65	0.83	0.00	0.35	0.65	57.25
18	0.00	0.30	0.70	0.74	0.00	0.30	0.70	61.41
19	0.00	0.25	0.75	0.65	0.00	0.25	0.75	65.58
20	0.00	0.20	0.80	0.56	0.00	0.20	0.80	69.74
21	0.00	0.15	0.85	0.47	0.00	0.15	0.85	73.91
22	0.00	0.10	0.90	0.38	0.00	0.10	0.90	78.07
23	0.00	0.05	0.95	0.29	0.00	0.05	0.95	82.24

Figure 24. Example of downloaded excel sheet containing the results of mixing calculations.

Two different examples of mixing modeling are shown below: i) two end-member (binary) mixing; ii) three end-member (ternary) mixing.

Two endmembers mixing

We conducted a groundwater mixing analysis using data from Wang et al. (2020). To replicate their groundwater mixing analysis, we selected the same two end-members represented by: i) BBM01 cold groundwater as end-member 1, characterized by a Sr concentration of 2559 $\mu\text{g/L}$ and an isotope composition of 0.70827; ii) The average of samples PC04 and PC05 as the deep groundwater end-member 2, with a Sr concentration of 456 $\mu\text{g/L}$ (average) and $87\text{Sr}/86\text{Sr} = 0.710092$ (calculated; Fig. 25). Wang et al. (2020) plotted a theoretical mixing line according to calculated $87\text{Sr}/86\text{Sr}$ versus Sr concentrations, where water samples from the hot springs clustered closely around the mixing line. This



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supports the proposed genesis, suggesting that the shallow reservoir is formed by mixing deep groundwater fluid with cold groundwater. The mixing ratios of cold groundwater in most shallow geothermal water samples range from 5% to 10%, except for one sample (BBDM02), which is mixed with approximately 35% cold groundwater (Fig. 25).

IDENTIFICAZIONE	IDROGEOLOGICA TIPO	SAMPLE LOCATION	SAMPLE NAME	SAMPLE TYPE	SAMPLE ANALYZE	STO. CONCENTR.	T	TOT. SODIO	GEN. SODIO (%)	STANCO (%)	NO. SODIO (%)	STANCO (%)	STO. SODIO (%)
BBDM01	NaCl	Quart	BBDM01	Flow Production/Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM02	NaCl	Quart	BBDM02	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM03	NaCl	Quart	BBDM03	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM04	NaCl	Quart	BBDM04	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM05	NaCl	Quart	BBDM05	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM06	NaCl	Quart	BBDM06	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM07	NaCl	Quart	BBDM07	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM08	NaCl	Quart	BBDM08	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM09	NaCl	Quart	BBDM09	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM10	NaCl	Quart	BBDM10	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM11	NaCl	Quart	BBDM11	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM12	NaCl	Quart	BBDM12	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM13	NaCl	Quart	BBDM13	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM14	NaCl	Quart	BBDM14	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM15	NaCl	Quart	BBDM15	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM16	NaCl	Quart	BBDM16	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM17	NaCl	Quart	BBDM17	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM18	NaCl	Quart	BBDM18	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM19	NaCl	Quart	BBDM19	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM20	NaCl	Quart	BBDM20	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM21	NaCl	Quart	BBDM21	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM22	NaCl	Quart	BBDM22	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM23	NaCl	Quart	BBDM23	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM24	NaCl	Quart	BBDM24	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM25	NaCl	Quart	BBDM25	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM26	NaCl	Quart	BBDM26	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM27	NaCl	Quart	BBDM27	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM28	NaCl	Quart	BBDM28	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM29	NaCl	Quart	BBDM29	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM30	NaCl	Quart	BBDM30	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM31	NaCl	Quart	BBDM31	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM32	NaCl	Quart	BBDM32	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM33	NaCl	Quart	BBDM33	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM34	NaCl	Quart	BBDM34	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM35	NaCl	Quart	BBDM35	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM36	NaCl	Quart	BBDM36	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM37	NaCl	Quart	BBDM37	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM38	NaCl	Quart	BBDM38	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM39	NaCl	Quart	BBDM39	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM40	NaCl	Quart	BBDM40	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM41	NaCl	Quart	BBDM41	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM42	NaCl	Quart	BBDM42	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM43	NaCl	Quart	BBDM43	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM44	NaCl	Quart	BBDM44	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM45	NaCl	Quart	BBDM45	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM46	NaCl	Quart	BBDM46	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM47	NaCl	Quart	BBDM47	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM48	NaCl	Quart	BBDM48	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM49	NaCl	Quart	BBDM49	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0
BBDM50	NaCl	Quart	BBDM50	Drilling water	4/2019	1.00	85.0	170.0	100.0	100.0	100.0	100.0	100.0

Figure 25. Selection of end-members for binary modelling.

We used equations 1 and 2 to model the mixing process between end-member 1 and end-member 2. All results are plotted in Figure 26. Our modeling and results align with those reported by Wang et al. (2020), where sample BBDM02 represents a mix of 35% cold groundwater and 65% deep geothermal water, while the remaining samples fall along the 5-10% cold groundwater mixing trend, confirming the reliability of our mixing modeling (Fig. 26).

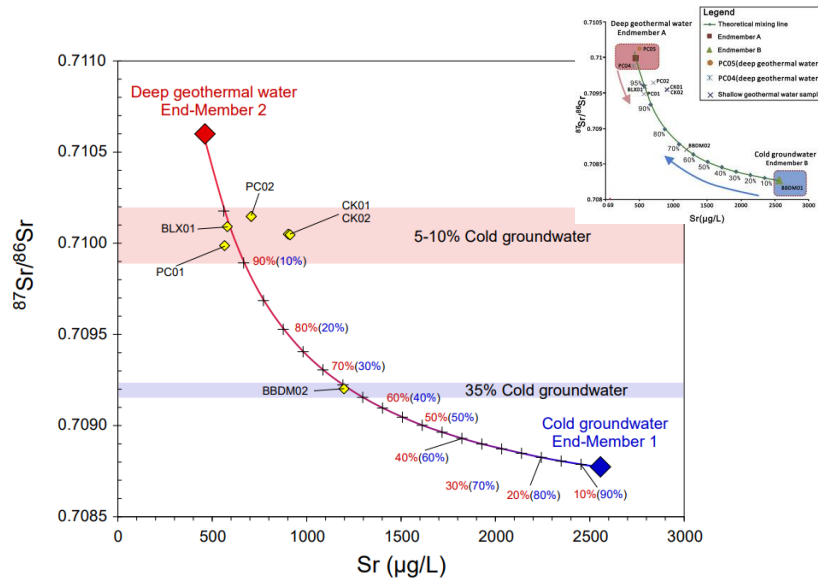


Figure 26. The $^{87}\text{Sr}/^{86}\text{Sr}$ vs Sr diagram using database results. Crosses indicate the increment of mixing (5%). The figure was created based on the results obtained from the mixing process and subsequently downloaded. On the right, the same figure reported by Wang et al. (2020).

Three end-members mixing

We conducted a three-end-member groundwater mixing analysis using data from Cuoco et al. (2021), who introduced a new geochemical method capable of quantifying and visualizing the dynamics of three-component mixing. We used our database to perform the same three-end-member mixing model and compared our results to those obtained by Cuoco et al. (2021) and the EMMA (End-Member Mixing Analysis) method that the authors described in their article (see Table 2 of Cuoco et al. 2021). As with the binary mixing, we selected the same end-members: i) N end-member, which is a groundwater hosted in volcanic deposits; ii) F end-member, representing a Ca-Mg-HCO₃ type groundwater hosted in carbonate units; iii) D end-member, which is dominated by Ca-HCO₃ but exhibits the highest concentrations of major ions, alkali, and alkaline earth elements, as well as trace elements, due to water-volcanic rock interactions. A modified and simplified Table, showing



the three end-members used in our mixing modeling, along with six water samples (#26, #20, #16, #17, #27, #25), is presented in Figure 27.

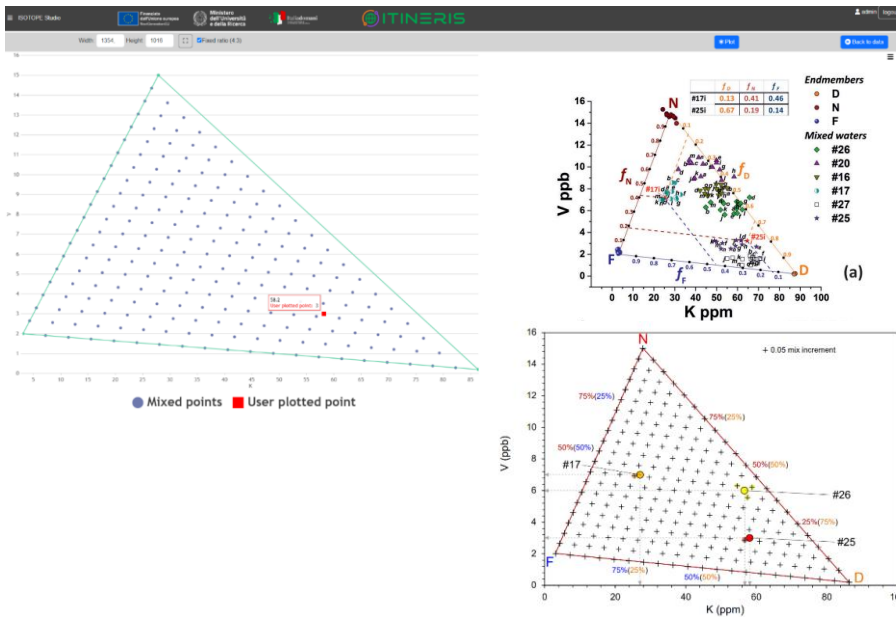


Figure 27. a) Example of scheme reporting a three-endmember mixing model results. Green lines are the mixing between end-members 1, 2, and 3 when f_1 , f_2 , or f_3 are zero, respectively. Grey points are all the possibilities of mixing values between end-members. A sample is plotted in the graph and represented by a red square. The mixing percentages between the three end-members are also calculated. B) V vs K diagram reported by Cuoco et al (2021). C) Re-drawn diagram using database results. Crosses indicate the increment of mixing (5%). Colored crosses indicate the mixing points closest to the selected samples and plotted in the diagram. Grey dotted lines indicate the X-Y coordinates (values of K and V) of selected samples.

Figure 27 presents the results from our modeling based on equations 3 and 4. To determine the exact position of selected samples within the mixing diagram, we used equation 8:

$$\begin{aligned} x_P &= f_A x_A + f_B x_B + f_C x_C \\ y_P &= f_A y_A + f_B y_B + f_C y_C \\ f_A + f_B + f_C &= 1 \end{aligned}$$

and solved the system as follow:

$$\begin{aligned} f_A &= (x_B y_C - x_C y_B - x_P y_C + x_C y_P + x_P y_B - x_B y_P) / (x_B y_C - x_C y_B - x_A y_C + x_C y_A + x_A y_B - x_B y_A) \\ f_B &= (x_P y_C - x_C y_P - x_A y_C + x_C y_A + x_A y_P - x_P y_A) / (x_B y_C - x_C y_B - x_A y_C + x_C y_A + x_A y_B - x_B y_A) \end{aligned}$$



$$f_C = 1 - f_A - f_B$$

The results obtained from the Isotope Studio database are shown in Table 4 and compared to those obtained by Cuoco et al. (2021) and the EMMA method. As shown, our results are comparable to those in the literature, confirming the validity of our method.

Sample	Results	N	F	D
#25	Isotope Studio	0.15	0.25	0.59
	Cuoco Et al. (2021)	0.16	0.24	0.60
	EMMA	0.16	0.24	0.58
#17	Isotope Studio	0.43	0.41	0.16
	Cuoco Et al. (2021)	0.44	0.41	0.15
	EMMA	0.44	0.41	0.15
#26	Isotope Studio	0.38	0.09	0.53
	Cuoco Et al. (2021)	0.41	0.08	0.51
	EMMA	0.41	0.05	0.53

Table 4. Summary results between literature and Isotope Studio database

2.7 Examples of future modelling implementation

Other types of modeling are currently under development. Some examples are briefly described in the following sections.

Schoeller-Berkaloff diagram

These diagrams are used to show the relative concentrations of anions and cations, typically expressed in milliequivalents per liter. Multiple samples from different wells can be plotted on a single diagram to identify similar patterns in the ratios of specific anions and cations. Water concentrations depend on both the groundwater geochemistry and the chemical composition of the aquifer rock material. With spider diagrams, the user can choose to plot data on the Y-axis using either linear or base-10 logarithmic scaling, while the X-axis displays only the selected elements. Elements, anions, and cations can be plotted using initial concentrations or converted to meq/L.



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Rayleigh Fractionation

Rayleigh fractionation represents an exponential relationship that describes the partitioning of isotopes between two reservoirs as one reservoir decreases in size. The equations used to model Rayleigh fractionation describe an isotope fractionation process when: i) material is continuously removed from a mixed system containing molecules of two or more isotopic species, ii) the fractionation accompanying the removal process at any instance is described by a fractionation factor (α), and iii) α remains constant throughout the process.



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3 INFORMATION ON THE NETWORK ON ISOTOPE LABORATORY FACILITIES

Specific information on each laboratory facilities are described in the Deliverables 8.11 (*“Report indicating the full Implementation of New Laboratory Facilities constituting the Italian Environmental Isotope Network”*) and 8.6 (*“Report on the Acquired Instrumentation to fill the Knowledge Gaps in the Construction of the CZ VRE Services”*) for new high-performance Field Emission Scanning Electron Microscope (FE-SEM), non-existent in Italy until now. A synthesis of laboratories implementation and aims is reported in figures 28-31, as presented during the *“Giornate di confronto sulla Paleoclimatologia in Italia”* meeting, held in Rome (19-20th September 2024).

All laboratory facilities have been acquired and installed in recent months at CNR-IGG in dedicated laboratories located in Pisa, Italy.

Laboratories are accessible upon request by the respective laboratory manager or designated reference personnel. These facilities can host students, PhD students and visiting researchers. Guests are required to document their activities in the laboratory logbooks and may engage in all phases of the analytical procedures. They receive thorough training, information, and guidance on the analytical protocols established by the researchers and collaborators at CNR-IGG, which encompass various chemical methodologies and analytical techniques. Furthermore, before to gaining access to the laboratories, guests will undergo a briefing on the hazards and potential risks related to the chemicals and laboratory procedures.



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ISTITUTO DI GEOSCIENZE E GEORISORSE (IGG) - PISA

STABLE ISOTOPE LABORATORY

REFERENCE PERSON: CHIARA BOSCHI
REFERENCE PERSON: ILARIA BANESCHI

Dual-Inlet (DI) and Continuous Flow (CF) analyses
High range of sample size (μg - to mg -level)
Reducing cost per sample
High-Precision elemental and isotopic analysis




Thermo Scientific 253 Plus 10 kV IRMS

CARBON CAPTURE STORAGE LABORATORY

REFERENCE PERSON: CHIARA BOSCHI
REFERENCE PERSON: ILARIA BANESCHI

Control and regulation of force, displacement, speed, deformation, temperature and temperature gradient
Configurable for EBSD Analysis
Measurement and monitoring of deformation without contact



NewTec Scientific MT1000

CARBONATE CLUMPED ISOTOPES SYSTEM

- TEMPERATURE OF CARBONATE MINERALS
- TEMPERATURE HISTORY OF SURFACE AND SUBSURFACE ENVIRONMENTS
- CO₂ MINERAL SEQUESTRATION
- BIOMINERALIZATION PROCESSES
- ALTERATION HISTORY OF METEORITES

CATHODOLUMINESCENCE

- GROWTH TEXTURES
- MINERAL ALTERATION
- MINERAL REPLACEMENT
- ELEMENT DISTRIBUTIONS
- STRUCTURAL STATES OF SOLIDS

Figure 28. Presentation of Stable Isotope Laboratory and Carbon Capture Storage Laboratory.

ISTITUTO DI GEOSCIENZE E GEORISORSE (IGG) - PISA

MASS SPECTROMETRY LA-ICP LABORATORY

REFERENCE PERSON: ALBERTO ZANETTI

Fast wide mass range data acquisition for applications such as laser ablation imaging and nanoparticle analysis
High sensitivity to probe micron sized trace element
High physical resolving power Time-of-Flight (TOF) mass spectrometer to give interference free analysis
Unique quad. cell, TOF option for the ultimate flexibility in removing interferences



Nu Vitesse Time of Flight (TOF) ICP-MS

FE-SEM LABORATORY

REFERENCE PERSON: ANDREA DINI

New generation EDS
WDS parallel beam with 5 crystals covering from Be to U
Micro-XRF source for light to heavy elements up to concentrations of a few tens of $\mu\text{g/g}$



The Zeiss Sigma 360 FE-SEM
ACQUIRED AS PART OF WP 8.1

IN SITU ANALYSES

- LU-Hf SYSTEMATICS
- Pb-U-Th SYSTEMATICS
- DEVELOPMENT OF NEW SYSTEMATICS IN THE FIELD OF STABLE ISOTOPES

MINERALOGICAL-GEOCHEMICAL MAPPING

- ORGANIC AND INORGANIC MATRICES
- CHARACTERISING THE CRITICAL ZONE
- CRYSTAL STRUCTURE ANALYSIS

Figure 29. Presentation of Mass Spectrometry LA-ICP Laboratory and FE-SEM Laboratory.



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ISTITUTO DI GEOSCIENZE E GEORISORSE (IGG) - PISA

ISOTOPE CHEMISTRY LABORATORY

REFERENCE PERSON: ELEONORA REGATTIERI

Sensitivities up to 800 molecules per CO₂ ion in Dual-Intet mode and 1000 molecules per ion in Continuous-Flow mode

Equipped with GasBench Plus system composed by TriPlus RSH SMART autosampler which offers exceptional precision, flexibility, and productivity in a robotic sample-handling solution




Thermo Scientific DELTA Q IRMS and GAS BENCH III

RADIOGENIC AND UNCONVENTIONAL STABLE ISOTOPES LAB

REFERENCE PERSON: SAMUELE AGOSTINI

Thermal stability of the quadrupole power
High Performance Analyses
Reduced re-runs in the daily workload with assured accuracy and repeatability



iCap Qnova series ICP-MS

PALEOCLIMATIC RECONSTRUCTIONS ENVIRONMENTAL RESEARCH

- ISOTOPE DETERMINATIONS OF AIR AND/OR CARBONATE CO₂
- CO₂ FROM DIC (DISSOLVED INORGANIC CARBONATE)
- ¹⁸O AND D ANALYSES FROM AQUEOUS SAMPLES

ELEMENTAL ANALYSES

- SETUP OF ISOTOPE SYSTEMATICS
- WASTEWATER AND SOIL ANALYSIS
- DRINKING WATER
- PETROCHEMICAL
- MINING/METALLURGY




Figure 30. Presentation of Isotope Chemistry Laboratory and Radiogenic and Radiogenic and Unconventional Stable Isotope Laboratory.

ISTITUTO DI GEOSCIENZE E GEORISORSE (IGG) - PISA

RADIOGENIC AND UNCONVENTIONAL STABLE ISOTOPES LAB

REFERENCE PERSON: SAMUELE AGOSTINI

-  SAMPLE PREPARATION
-  SAMPLE WEIGHTING
-  SAMPLE DIGESTION
-  CHEMICAL SEPARATION
-  MEASUREMENTS



Thermo Scientific NEOMA MS/MS MC-ICP-MS

- IN SITU ANALYSES
- INTERFERENCE SEPARATION



Neoma MS/MS MC-ICP-MS
Enabling the transformation of your workflow

- 11 Faraday Cup mobile detector array
- 10¹³ Ω Amplifier Technology
- Highest sensitivity and stability
- Superior Vacuum System
- Extra High Resolution (XHR) increasing the resolving power
- Retarding Potential Quadrupole (RPCQ) improving abundance sensitivity

Figure 31. Particularly of Neoma LA-MC-ICP-MS installed in the Radiogenic Unconventional Stable Isotope Laboratory



3.1 Analytical Techniques under development

Radiogenic and Unconventional Stable Isotope Laboratory

The methodologies already implemented in the Radiogenic and Unconventional Stable Isotope Laboratory, as well as those under development, are shown in Figure 31.

Here, we provide a brief overview of the isotopic methodologies developed and currently under development in relation to the ITINERIS project. Most importantly, these methodologies will be further advanced through the acquisition of new instrumentation (Figures 32-34).

Fe-Cu-Zn systematics: the distinct geochemical properties of Fe, Cu, Zn, make them applicable to a wide range of processes, rendering these elements powerful tools for fingerprinting metal sources or evaluating the biogeochemical reactions that influence their transport. They also provide valuable insights into both low- and high-temperature geological processes, such as hydrothermal fluid circulation, the different compartments of the critical zone, weathering of the continental and oceanic crust, material cycling through the crust and mantle, as well as biological and cosmochemical processes. For this reason, the Laboratory Team has developed methodologies for the separation of Fe from various matrices and the determination of Fe isotope ratios using a High-Resolution Multi-Collector Inductively Coupled Plasma Mass Spectrometer (HR-MC-ICPMS). The first official results were presented at the *Congresso della Società Geologica Italiana* (Di Giuseppe et al., 2024) through an oral presentation titled “*Iron isotope systematics and ore-forming processes: first results from the ophiolite-hosted, Tuscan Cu-Zn VMS deposits*”.

The chalcophile nature of Cu makes it ideal for deciphering metal-sulfide equilibria in iron meteorites, as well as the mineralizing conditions of sulfides. Applications for Zn include its tendency to partition into fluid phases at magmatic temperatures and its significant fractionation during biological uptake. Cu-Zn methodologies are in development, with plans for further advancements.

Li and Mg systematics: Lithium is one of the key elements for the green energy transition, mainly for rechargeable batteries production, while its isotopes provide a broad spectrum of scientific application. Li isotopes show different geochemical behaviours and significant fractionation between ^6Li and ^7Li due to their large mass difference. These characteristics

make Li isotopes highly suitable for a variety of applications including, paleo-weathering, paleo-CO₂ and paleo-climate reconstructions; water-rock interaction processes; geothermal exploration; crustal recycling in subduction zone; metasomatism; nuclear fusion reactor development. A method for lithium chemical purification from different matrices (rocks, sediments, waters, brines) and isotope measurement via MC-ICP-MS has recently been established in the laboratory and the results on several international standards were intercompared with those from another laboratory (BRGM, Orleans, France) to assess accuracy and reproducibility. The first official results were disclosed at the Congresso della Società Geologica Italiana (Salvadori et al., 2024) through an oral presentation titled “Potential sources of Li-rich fluids in Northern Apennines (Italy): first results on lithium distribution in pelitic rocks”.

With an additional step in the Li purification procedure, the extraction of a magnesium purified aliquot is possible. For this reason, the Mg isotope systematic is currently under development, with potential applications in studying weathering processes, soils characterization, meteorites classification, metasomatism and biogenic processes.

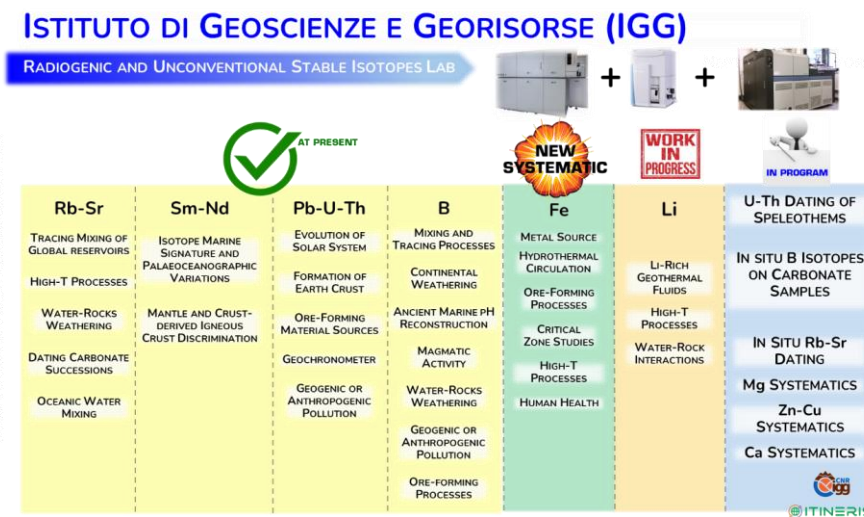


Figure 32. List of some common isotope methodologies. Yellow: isotope methodologies already implemented; Green: new isotopic systematics; Orange: isotope methodologies under development; Blue: future applications in program.



Figure 33. The new Laser Ablation (LA) - MC-ICP-MS Thermo Scientific Neoma was installed in January 2025.



Figure 34. The new iCAP Plus ICP-MS Thermo Scientific Neoma was installed in January 2025.

Isotope Chemistry Laboratory

In January 2025, the new system for C and O stable isotope analyses (Delta Q, Gas Bench plus with triplus RSH autosampler) was installed in the LCI laboratory of IGG (Fig. 36).

The method to analyze C and O isotope ratios in solid carbonates has been already settled. It involves precise weighing of the powdered sample, in the range of 0.15 or 0.6 mg depending on the method used, i.e. if sample dilution with He is activated or not. The powder is placed within borosilicate vials. Vials are then placed within the instrument's sample tray. The analysis involves a first phase, called flush, when the air within the vials is evacuated and replaced with He. Subsequently, a few drops of orthophosphoric acid are manually added to each vial to produce gaseous CO₂ from the CaCO₃ sample. This CO₂ is then sampled from the vial's head space by the instrument needle and transported to the Gas Bench within a flow of carrier gas (He). The He+CO₂ is then purified within the Gas Bench (by passing through two water traps and a gas chromatography column) and then inserted within the MS by an active open-split. Each analysis comprises three injections of reference CO₂ from a gas tank and seven injections of sample aliquots. Raw isotope ratios are calculated based on the isotope ratios of the CO₂ from the tank: Results are then calibrated (on a run basis) by using the values of standard materials of known isotope values (4 different standards, each measured five times with the same procedure used for the real samples. Mean error are around 0.05‰ for carbon and 0.08‰ for oxygen.

In the near future, we plan to set up the method to analyse the isotopic composition of dissolved inorganic carbon in water.



35

Figure 36. Delta Q, Gas Bench plus with triplus RSH autosampler installed at IGG-CNR.

LA-ICP-TOF-MS Laboratory

A new instrumentation consisting of an inductively-coupled-plasma mass-spectrometer with time-of-flight analyser (ICP-TOF-MS), model Vitesse (Nu-Ametek), and a latest-generation 193nm excimer laser system with fast-washout sample cell, model IRIDIA (Teledyne-Photon Machines), has been installed at IGG-CNR Pisa (Fig. 37). Testing is ongoing. The instrument is designed for semi-quantitative to quantitative 2D and possibly 3D mapping of trace, minor and major elements and isotope ratios in inorganic and organic materials through laser ablation (LA) sampling.



Figure 37. The LA-ICP-TOF-MS instrumentation installed at IGG-CNR in Pisa.

FE-SEM Laboratory

New high-performance Field Emission Scanning Electron Microscope (FE-SEM), non-existent in Italy until now, has been acquired and installed at CNR-IGG in a dedicated laboratory in Pisa (Fig. 38). The new FE-SEM was tested for a configuration strongly aimed at the chemical characterization of materials, from inorganic to organic, as well as a good/excellent system for imaging. For these reasons, the new FE-SEM was equipped with



three detectors/sources for micro analysis: i) new generation EDS (SDD) of 100 mm²; ii) WDS parallel beam with 5 crystals covering from Be to U and iii) Micro-XRF source for light to heavy elements up to concentrations of a few tens of µg/g.



Figure 38. The high-performance Field Emission Scanning Electron Microscope (FE-SEM) installed at IGG-CNR in Pisa.

Stable Isotope Laboratory

The new 253 plus Spectrometer was installed in the Stable Isotope Laboratory of IGG-CNR (Pisa) in February 2025 (Fig. 39). The spectrometer is interfaced with an IBEX instrument aimed at producing pure CO₂ gas from different types of carbonate minerals. This new configuration, the first in Italy, is devoted to CO₂ clumped isotopes, to define the temperature of mineral precipitation.

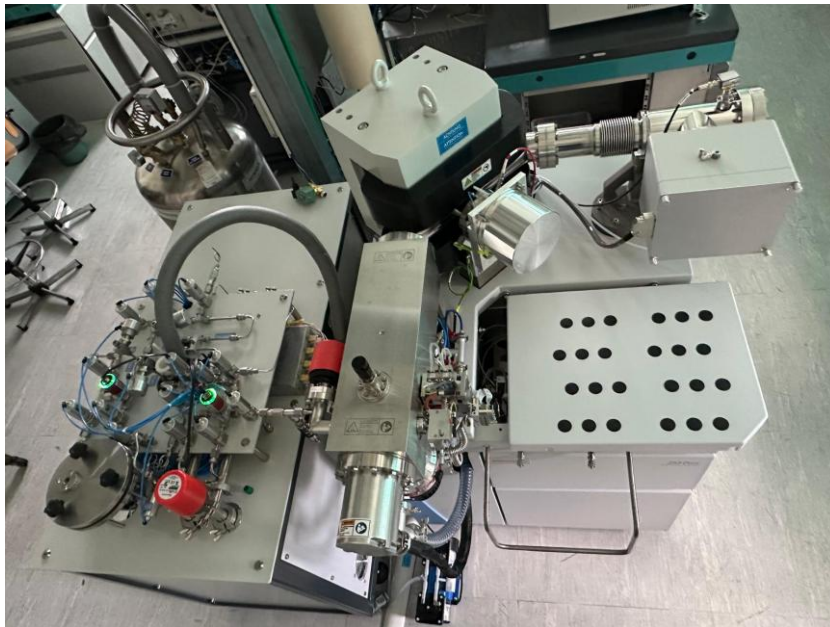


Figure 39. 253 plus Spectrometer (right) interfaced with Ibox instrument (left).

Carbon Capture Storage Laboratory

The NewTec Scientific MT1000 instrument was installed in the CCSLab at the IGG-CNR (Pisa) in November 2024 (Fig. 40). The instrument is made an optical microscope linked to a vacuum chamber with sample holder and reflective lighting. The instrument is devoted to acquiring images to define the real structure of minerals and materials and to understand the mineralogical process of formation and alteration. The instrument was calibrated with different test materials and preliminary results has been performed.



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Figure 40 The NewTec Scientific MT1000 instrument.

4 OBJECTIVES ACHIEVED AND CHALLENGES

As previously described, the VRE and, in particular, the Isotope Studio web application is capable not only of storing a significant amount of data but also of modelling it effectively. The calculations performed during the modelling processes (see Table 4) align perfectly with the models presented in the literature, confirming the validity of the work carried out so far.

However, it is important to highlight the challenges encountered up to this point. So far, only the GEOROC data repository has shared its RESTful APIs with us, enabling access to its dataset and allowing for external connections to directly download data. Other repositories, on the other hand, have either requested more time or have shown no interest in sharing their data. Another challenge concerns the responses received from researchers at various institutions. Despite repeated outreach since November 2023, the willingness to collaborate has been limited. A significant issue has been the hesitation to share unpublished data. Additionally, many researchers expressed concerns about the lack of a method for depositing data and obtaining a DOI, as is the case in other platforms such as GFZ or Zenodo. Recently, our institute has taken steps towards the creation of the Data Infrastructure Office, which will have, among other tasks, the responsibility of creating a data registry for IGG accredited on DataCite, and we will therefore be able to issue CNR-IGG DOIs. This registry will be operational by June 2025.

In response to this challenge, WP 8.9 proposed a temporary solution: to include, at least initially, data from already existing publications. However, due to time constraints and the significant workload required to catalogue and select the works published by Italian researchers, it was decided to ask researchers to fill out a template with the DOIs of the publications they considered most relevant to the themes addressed by ITINERIS. To gather this information, a survey was sent to directors, lab managers, and researchers from Italian research institutions and universities. Unfortunately, the response was limited. The main criticisms have been received because it was pointed out that the data already published and no longer unpublished were easily accessible online.



5 REFERENCES

Assante, M., Candela, L., Castelli, D., Cirillo, R., Coro, G., Frosini, L., Lelii, L., Mangiacrapa, F., Pagano, P., Panichi, G., Sinibaldi, F., 2019a. Enacting open science by D4Science. *Futur. Gener. Comput. Syst.*, 101: 555-563. <https://doi.org/10.1016/j.future.2019.05.063>

Assante, M., Candela, L., Castelli, D., Cirillo, R., Coro, G., Frosini, L., Lelii, L., Mangiacrapa, F., Marioli, V., Pagano, P., Panichi, G., Perciante, C., Sinibaldi, F., 2019b. The gcube system: Delivering virtual research environments as-a-service. *Future Generation Computer Systems* 95: 445–453. <https://doi.org/10.1016/j.future.2018.10.035>

Assante, M., Candela, L., Castelli, D., Cirillo, R., Coro, G., Dell'Amico, A., Frosini, L., Lelii, L., Lettere, M., Mangiacrapa, F., Pagano, P., Panichi, G., Piccioli, T., Sinibaldi, F., 2023. Virtual research environments co-creation: The D4Science experience. *Concurrency Computat. Pract. Exper.*, 35(18): e6925. <https://doi.org/10.1002/cpe.6925>

Candela, L., Castelli, D., Pagano, P., 2023. The D4Science Experience on Virtual Research Environments Development. *Computing in Science & Engineering* 25: 12–19. <https://doi.org/10.1109/MCSE.2023.3290433>

Candela, L., Castelli, D., Pagano, P., 2013. Virtual research environments: an overview and a research agenda. *Data Science Journal* 12: 75-81. <https://doi.org/10.2481/dsj.GRDI-013>

Cuoco, E., Viaroli, S., Darrah, TH., Paolucci, V., Mazza, R., Tedesco, D., 2021. A geometrical method for quantifying endmembers' fractions in three-component groundwater mixing. *Hydrological Processes* 35, 14409. <https://doi.org/10.1002/hyp.14409>

Date, C. J., 2015. *SQL and Relational Theory How to Write Accurate SQL Code*, 3rd Edition, O'Reilly Media, Inc. pp 523. ISBN: 978-1-491-94117-1

De Keyser, P., 2012. Metadata formats and indexing. *Indexing*, 143–166. <https://doi.org/10.1016/b978-1-84334-292-2.50008-8>

Di Giuseppe, P., Agostini, S., Rielli, A., Vezzoni, S., Dini, A. 2024. Iron isotope systematics and ore forming processes: first results from the ophiolite-hosted, Tuscan Cu-Zn VMS deposits. In: "Geology for a sustainable management of our Planet", Congresso



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SGI-SIMP, 2-5 Settembre 2024, Bari, Italia. Abstract a cura della Società Geologica Italiana, p. 1408. DOI: <https://doi.org/10.3301/ABSGI.2024.02>

Doveri, M., Natali, S., Franceschi, L., Menichini, M., Trifirò, S., Giannecchini, R., 2021. Carbonate aquifers threatened by legacy mining: hydrodynamics, hydrochemistry, and water isotopes integrated approach for spring water management. *Journal of Hydrology* 58, 125850 <https://doi.org/10.1016/j.jhydrol.2020.125850>

Harrington, J. L., 2009. *Relational Database Design and Implementation: Clearly Explained*, Morgan Kaufmann, Burlington, VT. Kim, B. S., Lee, S. H., Lee, Y. R., Park, Y. H., & Jeong, J., 2022. Design and Implementation of Cloud Docker Application Architecture Based on Machine Learning in Container Management for Smart Manufacturing. *Applied Sciences*, 12(13), 6737. <https://doi.org/10.3390/app12136737>

Maedche, A., Elshan, E., Höhle, H., Lehrer, C., Recker, J., Sunyaev, A., Sturm, B., Werth, O., 2024. Open Science. *Business & Information Systems Engineering* 66, 517-532. <https://doi.org/10.1007/s12599-024-00858-7>

Pennisi, M., Bianchini, G., Muti, A., Kloppmann, W., Gonfiantini, R., 2006. Behaviour of boron and strontium isotopes in groundwater–aquifer interactions in the Cornia Plain (Tuscany, Italy). *Applied Geochemistry* 21, 1169-1183. <https://doi.org/10.1016/j.apgeochem.2006.03.001>

Perrone, E., Di Giuseppe, P., Gennaro, S., Agostini, S., Trumpy, E., Baneschi, I., Boschi, C., Cornacchia, I., Pennisi, M., Regattieri, E., Rielli, A., Salvadori, M., Vezzoni, S., Provenzale, A. (2024). The ISOTOPE Virtual Research Environment (ITINERIS project, PNR). In: *Proceedings of the SGI-SIMP 2024 Conference, Bari, 03rd-09th September 2024 - “Geology for a sustainable management of our Planet”*, pp. 768. DOI: <https://doi.org/10.3301/ABSGI.2024.02>

Salvadori, M., Pennisi, M., D’Orazio, M., Dini A. 2024. Potential sources of Li-rich fluids in Northern Apennine (Italy): first results on lithium distribution in pelitic rocks. *Proceedings of the SGI-SIMP 2024 Conference, Bari, 03rd-09th September 2024 - “Geology for a sustainable management of our Planet”*, pp. 1174. DOI: <https://doi.org/10.3301/ABSGI.2024.02>



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dall'Unione europea
NextGenerationEU



Wang, C., Zheng, M., Zhang, X., Xing, E., Zhang, J., 2020. O, H, and Sr isotope evidence for origin and mixing processes of the Guidi geothermal system, Himalayas, China. *Geoscience Frontiers* 11, 1175-1187. <https://doi.org/10.1016/j.gsf.2019.09.013>

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