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François Renard, V. Mora, Pierre Horgue, J.M. Kerloch. THYRSIS: A QGIS plugin for hydrogeological modelling. *Computers & Geosciences*, 2024, 187, pp.105580. 10.1016/j.cageo.2024.105580. hal-04593298

HAL Id: hal-04593298

<https://ut3-toulouseinp.hal.science/hal-04593298v1>

Submitted on 29 May 2024

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Research paper

THYRSIS: A QGIS plugin for hydrogeological modelling

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ARTICLE INFO

Keywords:

Hydrogeology
Modelling
Simulation
Groundwater
Vadose zone
QGIS
OpenFOAM
PorousMultiphaseFOAM
SpatialLite

ABSTRACT

THYRSIS is a new opensource QGIS extension dedicated to hydrogeological modelling of flow and transport at multiple scales, from local to regional. Based on SpatialLite databases and time-dependent mesh layers, it is fully integrated into QGIS and allows the building of hydrogeological models. The modelling is based on 1D unsaturated vertical columns, coupled with a 2D horizontal groundwater model. Groundwater flow models can be imported or directly created with THYRSIS using the OpenFOAM cfMesh or GMSH mesh builders. Simulations are performed with the OpenFOAM porousMultiphaseFoam solvers, and the results are displayed in QGIS through the mesh layers. THYRSIS can handle several types of water or solute input in multiple zones, which can be defined at the surface or underground. Water or solute input can also be defined over the whole study area and directly in the groundwater body, ignoring the unsaturated zone. THYRSIS can therefore simulate the effect of heterogeneous, transient infiltration and reproduce variations in piezometric levels, or the transport of matter in the subsurface, from the ground to groundwater outlets, in order to estimate groundwater concentrations. Numerous functionalities are proposed such as uncertainty management, as well as the calculation and display of isolines and mass balance, time-potential or time-concentration graphs.

1. Introduction

Geographic Information Systems (GISs) are increasingly used in the scientific community, particularly in environmental studies (Rosas-Chavoya et al., 2022) because they provide an ideal means for processing and displaying spatially distributed data. Although GISs were originally designed to represent two-dimensional data, their use has been extended in recent years to the representation of 3D surface objects such as buildings and urban areas, but they are not yet adapted to the representation of 3D subsurface data. Nevertheless, several efforts have been made to use GISs for hydrological and hydrogeological modelling, primarily to prepare and process data and measurements for numerical modelling and simulation tools (Gogu et al., 2001; Martin et al., 2005; Strassberg et al., 2007; Bhatt et al., 2014; Rossetto et al., 2018, 2022). These efforts mainly concern hydrological processing due to variables of interest traditionally well managed by GIS.

Coupling a GIS with numerical hydrogeological modelling is more complicated because of the need to handle mesh generation and time-dependent mesh results. The most advanced applications in this field appear to be the PIHMgis framework (Bhatt et al., 2014) and the FREEWAT platform (Rossetto et al., 2018; De Filippis et al., 2020). These two softwares are available as QGIS (QGIS, 2024) plugins and offer a fully comprehensive interface allowing the integration of a

large amount of data and parameters to perform hydrological model simulations in relation to geology, soils, topography, land cover and use, as well as meteorological data and initial conditions. PIHMgis is based on the PIHM finite volume hydrological model (Qu and Duffy, 2007; Kumar, 2009) and the simulation results are stored in a shared geodatabase or in NetCDF files. FREEWAT is based on the MODFLOW family of finite difference groundwater modelling codes (Harbaugh, 2005; Niswonger et al., 2006; Hanson et al., 2014; Zheng et al., 1999; Bedekar et al., 2016), and simulation results are exploited through the generation of raster files at specific time steps.

Although these models are theoretically capable of simulating flow and transport in three dimensions, including the unsaturated zone (Kollet et al., 2010), large-scale studies require computation times which are virtually prohibitive due to the high non-linearity of Richardson-Richards' equation (Richardson, 1922; Richards, 1931). As a result, the unsaturated zone is often neglected or meshed very coarsely (De Filippis et al., 2020). These difficulties may be overcome by a 1D+2D approach, in which the unsaturated zone is modelled by 1D vertical columns, while the saturated zone is simplified into a two-dimensional problem by considering the Dupuit-Forchheimer hypothesis (Dupuit, 1863; Forchheimer, 1886). The coupling between the unsaturated columns and the saturated zone can be carried out iteratively or

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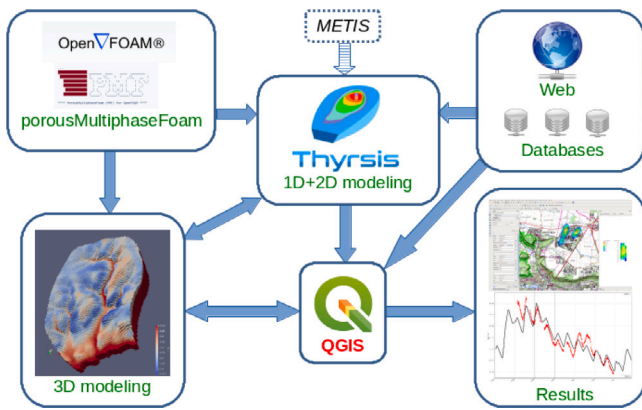


Fig. 1. THYRSIS plugin in relation to QGIS, hydrogeological modelling softwares and databases.

non-iteratively (Brandhorst et al., 2021), the latter method generally proving less accurate but more efficient in terms of calculation time (Zheng et al., 1999).

Comparisons between 3D and 1D+2D models were carried out as part of a study on the calibration of model parameters (Latour et al., 2023). It appears that the permeability fields estimated by inversion are almost identical, but the numerical cost of a 3D inversion is much higher. Similarly, the piezometric levels resulting from transient infiltration are well reproduced by each of the models, with a much lower numerical cost in a 1D+2D approach.

THYRSIS is a free and opensource QGIS plugin that implements this 1D+2D approach, with non-iterative coupling. Extensive integration into QGIS is achieved through the development of a time-dependent mesh layer manager. It is the French acronym of “Transport Hydrogéologique Rapide Simulé en zone Insaturée et Saturée”, which can be translated as “Rapid Simulated Hydrogeological Transport in Unsaturated and Saturated zones”.

In this paper we present the main features and development choices of THYRSIS in Section 2. Section 3 is devoted to the illustration of several representative case studies, with a paragraph comparing the results obtained with two different codes for cross validation.

2. THYRSIS architecture

THYRSIS is developed in Python-3 and currently compatible with QGIS-3.22 and later versions. Fig. 1 illustrates the role of the THYRSIS plugin in relation to QGIS, hydrogeological modelling softwares and databases.

2.1. Mesh layers

The THYRSIS plugin is based on a Python meshlayer module which implements the notion of value field defined on a mesh and integrates the temporal dependency of the results. To provide a powerful rendering solution, this module relies on the use of graphics acceleration via the OpenGL API (OpenGL, 2024) and on the use of the Python NumPy module (NumPy, 2024) which ensures the contiguity of data in memory. It allows an efficient display of data at nodes and at cell centres, as well as the setting up of continuous or categorized scales and the generation of isolines.

The meshlayer module implements two types of data provider, which define how data contained in files or databases should be displayed in QGIS layers: (i) a data provider for non-time-dependent data, to display steady-state fields related to the steady-state groundwater model (hydraulic head, permeability, Darcy velocities, etc.) and (ii) a data provider for time-dependent result fields. Time-dependent

providers are able to read NumPy simulation files with results computed at nodes or at cell centres.

This design makes it possible to obtain a fluid and interactive visualization of simulation results with millions of nodes.

Note that QGIS has implemented support of QgsMeshLayer (QgsMeshLayer, 2024) since the 2019 QGIS-3.4 version, thus offering an alternative to the meshlayer module developed for THYRSIS but which would require the development of many additional features, particularly for managing unit changes, writing in scientific mode, or displaying in logarithmic scale, features offered by THYRSIS.

2.2. Data management

The data needed by THYRSIS to perform hydrogeological modelling are managed by Spatialite databases (Gaia, 2024) and organized into three categories : (i) a general database containing all data related to the characterization of sites, such as points of interest, piezometric levels, chemical measurements, geological descriptions, etc., (ii) mesh and model databases storing information related to the steady-state groundwater model (mesh description, hydraulic head and permeability fields, topographic and bedrock elevation, etc.), (iii) computing databases created for specific simulations.

Simulation results are not stored in databases but kept in NumPy files. This straightforward solution guarantees excellent display performance for discretization of several million nodes and several thousand dates.

2.3. Modelling softwares

The currently implemented modelling softwares are METIS (Goblet, 1989) and the OpenFOAM porousMultiphaseFoam (PMF) solvers (Horgue et al., 2015, 2022). Other simulation codes could be integrated by taking advantage of the object-oriented design of the plugin.

2.3.1. METIS

METIS (Goblet, 1989) is a finite element code that simulates flow, mass and heat transport mechanisms in porous or fractured aquifers. It has been developed in FORTRAN over the last 30 years and has been used in several studies (Renard and Tognelli, 2016; Robineau et al., 2018; Mattei et al., 2020). METIS uses an internal simple mesh description and most results are generated at nodes except for saturation or Darcy velocities which are computed at cell centres. Although METIS can handle 1D to 3D simulations, 3D performance is limited by the non-parallel design. As METIS is not an opensource software, it is not provided by default with the plugin.

2.3.2. PorousMultiphaseFoam (PMF)

PorousMultiphaseFoam (Horgue et al., 2015, 2022) is an opensource OpenFOAM toolbox dedicated to the solution of multiphase flow equations (generalized Darcy’s law) or groundwater flow (Richardson-Richards’ equation). It makes use of the OpenFOAM finite volume platform, showing good parallel efficiency with automatic discretization on unstructured three-dimensional grids. Recent developments have been carried out to enable simulation of a wide range of real cases, with fast water flows and solute transfers in realistic hydrological configurations with variable boundary conditions (Horgue et al., 2022). Like METIS, porousMultiphaseFoam implements Newton’s method, which can be combined with Picard’s method, to significantly improve the convergence speed. The 2D solvers have been recently developed to replace METIS and are therefore well adapted to the THYRSIS approach. Validation of the porousMultiphaseFoam solvers was performed by extensive comparison with METIS results (Horgue et al., 2022). As porousMultiphaseFoam is an opensource software, it is provided by default with the plugin and sources can be modified and improved by users.

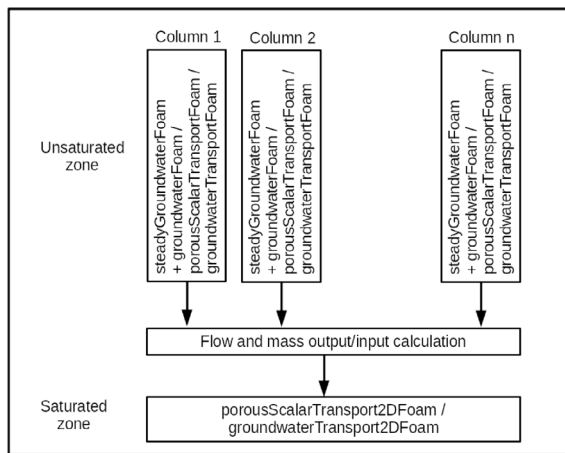


Fig. 2. Schematic view of the 1D+2D THYRSIS approach with the porousMultiphaseFoam solvers used at each stage.

2.4. Modelling approach

To reduce computational costs and produce simulation results in a very short time, THYRSIS breaks down the hydrogeological modelling process into 1D vertical simulations of unsaturated columns, coupled with 2D simulations of the water table (Fig. 2). This approach is based on the construction of steady-state groundwater flow models, which are stored in SpatialLite databases and can be selected for use in transient flow and transport simulations.

2.4.1. Steady state groundwater flow

Steady-state groundwater flow models can be built with THYRSIS by creating a “mesh project” and (i) interactively defining a domain and then meshing it, (ii) defining a permeability field and the characteristic parameters of the subsurface, as explained below.

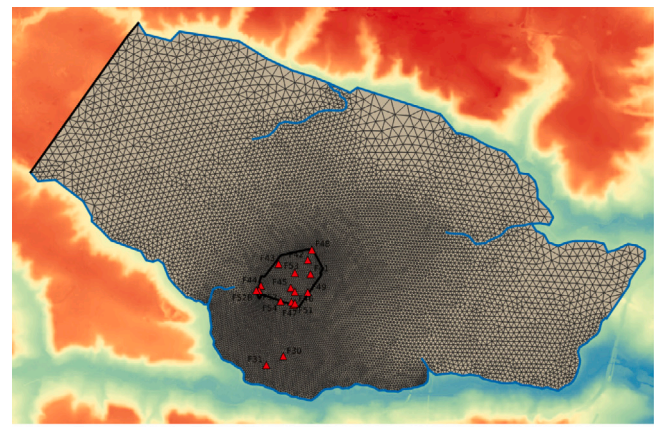
2D meshing. 2D meshing can be performed with the GMSH mesh builder (Geuzaine and Remacle, 2009) or the OpenFOAM cfMesh toolbox (Juretic, 2015), both being licensed under GPL and used as external softwares. GMSH is a finite element 3D meshing software, distributed with a complete graphical interface. It is used in THYRSIS to generate large and accurate unstructured grids of triangles (Fig. 3(a)). cfMesh is an opensource library for automatic mesh generation implemented within the OpenFOAM framework. It is used in THYRSIS to generate large unstructured grids of quadrangles (Fig. 3(b)).

The domain to be modelled as well as optional sub-domains, lines and fixed points are first defined interactively as vector layers with the QGIS tools. In each case, the required mesh size is specified. Boundary conditions are set in the same time as (i) fixed hydraulic head along rivers or outcrops (Dirichlet condition), (ii) zero flux along other boundaries (Neuman condition).

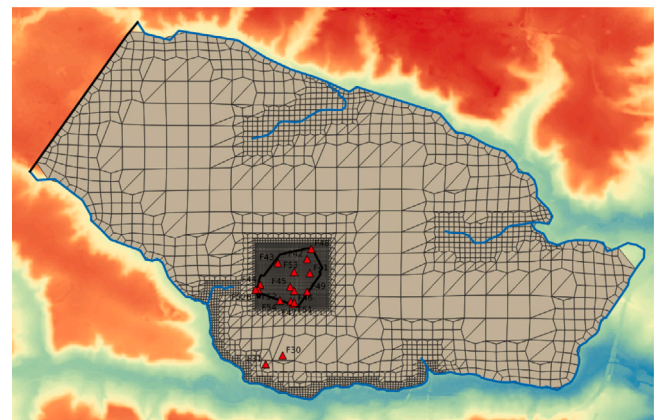
The elevation of the top and bottom of the aquifer are defined using two raster layers.

THYRSIS then builds the required files as input of the selected mesh builder and runs it as external software. The result files are finally interpreted to build the mesh layers with meshes and nodes and display in QGIS.

Model parameters. After building of the mesh, a permeability field is defined which makes it possible to determine a steady-state groundwater flow model that is stored in a SpatialLite database and then used in simulations of transient flow or solute transport. The permeability field can be defined in three ways: (i) specifying a uniform permeability value over the entire domain, (ii) importing a permeability field as a raster file, (iii) using an inversion procedure inspired by the pilot point method (Renard and Jeannée, 2008; Renard and Tognelli, 2016).



(a) GMSH



(b) cfMesh

Fig. 3. QGIS interface displaying the results of GMSH and cfMesh meshing, with the digital terrain model in the background. The blue lines represent rivers, with fixed hydraulic heads. The black contour inside the modelled domain outlines the experimental site. The black line at top left represents a zero flux boundary. Red triangles represent boreholes used as fixed points.

Table 1
Main subsurface characteristic parameters.

Name	Description	Unit
VGA	Van Genuchten α	m^{-1}
VGN	Van Genuchten n	–
VGR	Residual saturation	–
VGS	Maximal saturation	–
VGE	Air-entry value of the pressure head	m
WC	Effective porosity	–
WT	Total porosity	–
VM	Volumic mass	kg/m^3

Once the permeability field is defined, a steady-state flow simulation is used to generate all the fields describing the model (hydraulic head, piezometric level, Darcy velocity, unsaturated zone thickness, topographic and bedrock elevation), which then are stored in a SpatialLite database. The porousMultiphaseFoam solver used for this stage is *steadyGroundwater2DFoam*.

Scalar model parameters such as the van Genuchten parameters (α , n , θ_r and θ_s), the effective and total porosity or dispersivities, are also stored in the SpatialLite database (Table 1).

All the representative fields of the steady-state groundwater flow model can be represented and analysed in QGIS using THYRSIS.

2.4.2. Flow and transport in unsaturated zone

The unsaturated zone is modelled by 1D vertical columns, each column describing an input zone and its thicknesses calculated by

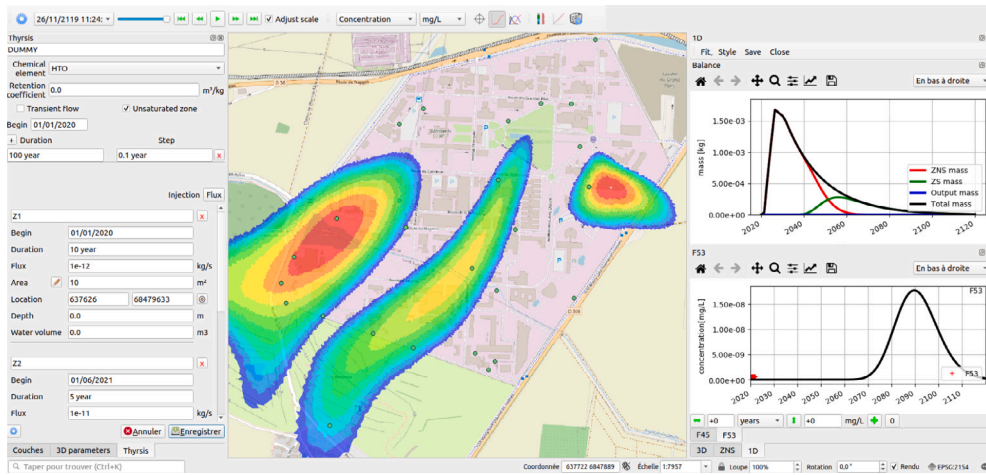


Fig. 4. Example of THYRSIS interface, with panel for the definition of injections (left), the main 2D map displaying the simulation results (centre), the mass balance graph and the time-concentration graph (right).

subtracting the steady-state piezometric level from the topographic elevation.

Flow is calculated by solving the Richardson-Richards' equation (Richardson, 1922; Richards, 1931), using the van Genuchten closed-form laws (Van Genuchten, 1980), modified by Ippisch et al. (2006):

$$S_e = \begin{cases} \frac{1}{S_c} [1 + (\alpha h)^n]^{-m} & h > h_e \\ 1 & h \leq h_e \end{cases}$$

$$K = \begin{cases} K_s \sqrt{S_e} \left[\frac{1 - (S_e S_c)^{1/m}}{1 - (S_c)^{1/m}} \right]^2 & S_e < 1 \\ K_s & S_e \geq 1 \end{cases}$$

where K is the hydraulic conductivity (LT^{-1}), K_s the saturated hydraulic conductivity (LT^{-1}), h the pressure head (L), h_e the air-entry value of the pressure head (L), θ the volumetric water content, θ_r the residual water content, θ_s the saturated water content, $S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$ the effective saturation, $S_c = [1 + (\alpha h_e)^n]^{-m}$ the effective saturation at the cut-off point h_e , n and α (L^{-1}) the fitting parameters with $m = 1 - \frac{1}{n}$.

When $h_e = 0$, then $S_c = 1$ and the equation regresses to the original van Genuchten formula. The highly non-linear conservation equation is solved using an iterative algorithm (Picard or Newton's method) with user-defined tolerances.

The columns are automatically discretized into cm-sized elements to ensure good numerical stability even for low dispersivities and a conservative mass balance.

In addition, the mesh thicknesses are constrained to remain less than $\frac{0.1}{\alpha}$ to ensure good numerical stability at high values of α .

The unsaturated zone simulations are broken down into a steady-state flow simulation (*steadyGroundwaterFoam* solver of the porousMultiphaseFoam toolbox) to obtain initial conditions followed by a transient flow and transport simulation (*porousScalarTransportFoam* or *groundwaterTransportFoam* solvers of the porousMultiphaseFoam toolbox).

Unsaturated column simulations are independent and can be automatically run in parallel on multiple machines using an MPI implementation (Clarke et al., 1994; MPICH, 2024; OpenMPI, 2024).

2.4.3. Flow and transport in saturated zone

Groundwater flow modelling of the saturated zone is simplified to a two-dimensional problem by considering the Dupuit-Forchheimer assumption. Transport is modelled by a general convection-dispersion equation including an optional decay rate for radionuclide modelling and a retardation factor R describing the effect of a partitioning coefficient K_d by $R = 1 + \frac{(1-\omega)}{\omega_c} \rho_s K_d$ where ω is the total porosity, ω_c the cinematic porosity and ρ_s the solid matrix density.

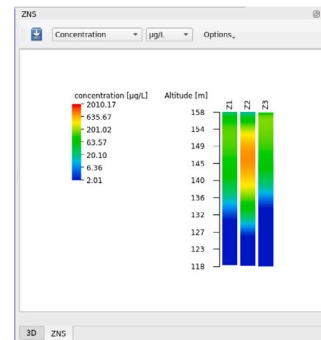


Fig. 5. Example of simulation results in an unsaturated zone.

The porousMultiphaseFoam toolbox has three solvers to handle the different configurations: *groundwater2DFoam* for transient flow without transport, *porousScalarTransport2DFoam* for passive transport in a pre-computed flow field, and *groundwaterTransport2DFoam* for flow modelling coupled with transport.

1D+2D coupling is achieved simply by considering the water and solute outflows at the bottom of the unsaturated columns as boundary conditions of the saturated 2D model.

2.4.4. Input characteristics

Multiple water or solute inflows can be defined through the interface (Fig. 4), specifying their properties: coordinates of the centre of the input zone, depth, area, value of the water or solute inflow and duration. The solute inflow can be calculated from a mass input, taking into account the solubility limit. Coordinates and surfaces can be defined interactively through the QGIS interface.

THYRSIS can also handle diffuse water or solute inflow over the whole modelled domain, either by simulating the same number of unsaturated vertical columns as there are mesh nodes, or by simulating groups of columns (composed of similar thickness and permeability) to reduce the number of simulations.

2.4.5. Uncertainty management

Uncertainty calculations can be performed with the Latin Hypercube method (McKay et al., 1979; McKay, 1992), by defining a number of simulations as well as ranges of variation and probability laws for the main parameters. The calculations can be automatically run in parallel on several computers using an MPI implementation. THYRSIS aggregates the results in order to calculate the mean and standard deviation

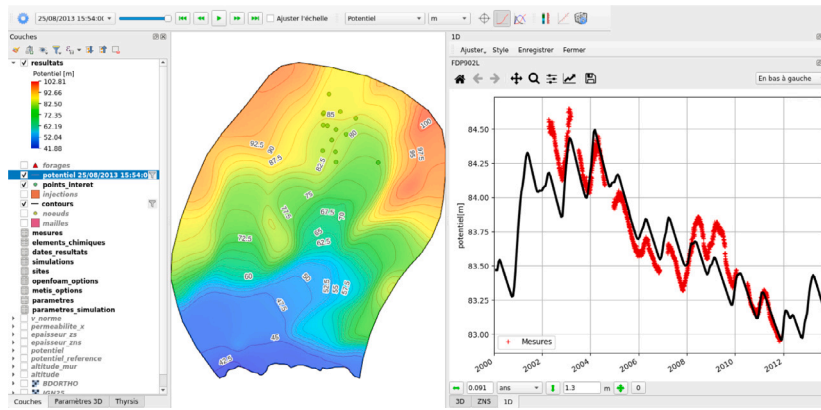


Fig. 6. Example of time-potential graph with measurements (right) and isovalues on a 2D map (centre).

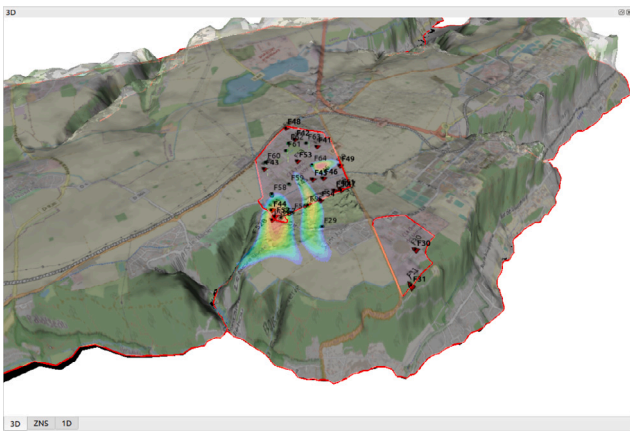


Fig. 7. Example of 3D display.

OGC_FID	groupe	nom	longueur_element	potentiel_impose	epaisseur
1	site	centre	50	0	5
2	contour	sw	500	1	50
3	contour	sud	100	1	10
4	contour	se	500	1	50
5	contour	nord	500	1	50
6	contour	ouest	500	0	50
7	contour	canal	100	1	10
8	contour	corbeville	250	1	25
9	contour	vauhallan	250	1	25
10	contour	montbron	250	1	25

Fig. 9. Contour layer attributes: “longueur-element” defines the mesh size (m), “potentiel_impose” defines the contour elements with fixed hydraulic head and “epaisseur” is used by cfMesh to define the range (m) of the corresponding mesh size.

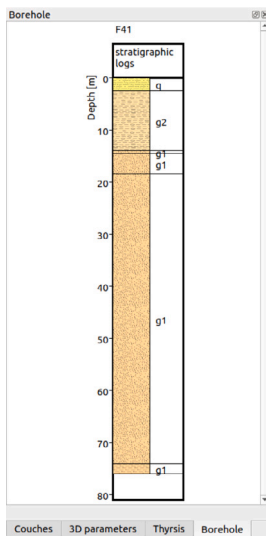


Fig. 8. Example of borehole display, using (i) geological time scale codification from BRGM (2006), (ii) RGB colorimetric codification from the Commission for the Geological Map of the World (CGMW) (Gradstein et al., 2020), and (iii) lithology pattern chart from USGS (2006).

for each simulated variable. Graphs are used to display confidence intervals or probability maps.

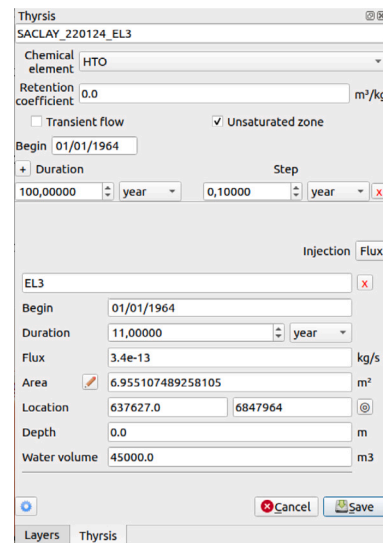


Fig. 10. THYRSIS interface used here to define tritium injection conditions.

2.5. Interface

THYRSIS is fully integrated in QGIS with (i) a drop-down menu for selecting the main actions of the plugin, such as the choice of solver and mesh generator, the choice of model or study, the creation of isolines, the running of uncertainty calculations by Latin Hypercube, etc. (ii) a dockable window for defining injections (Fig. 4), (iii) a menu bar for managing the display of results (Fig. 4), (iv) a dockable window for the display of unsaturated columns (Fig. 5), (v) a dockable window for the display of results and mass balances as a function of time (Figs. 4 and 6), (vi) a dockable window giving a 3D representation of the modelled

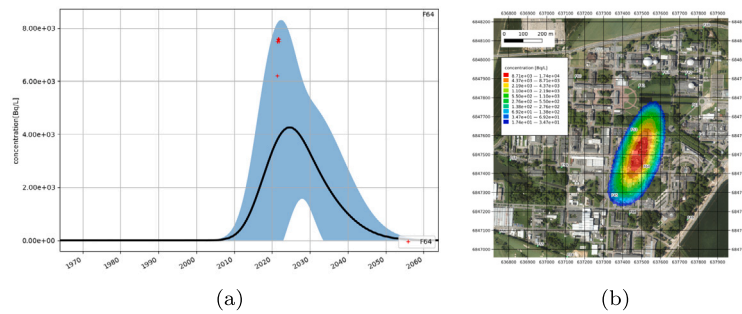


Fig. 11. (a) Mean concentration and 95% confidence interval estimated at piezometer F64. The red crosses indicate measurements. (b) Mean concentration map for January 2022.

domain (Fig. 7), (vii) a dockable window for displaying stratigraphic logs (Fig. 8).

2.6. Software packaging

THYRSIS is distributed via the QGIS plugin repository and can be run on Linux/Ubuntu or Windows.

Some Python libraries needed by THYRSIS are not available in QGIS Windows; to avoid manual installation by users, GitLab Continuous Integration (CI) is used to install the missing libraries and store them in the plugin archive.

OpenFOAM and porousMultiphaseFoam are mainly supported on Linux operating systems; to enable Windows support, a pre-compiled version of OpenFOAM is available from <https://www.openfoam.com/>. Opensuse (OpenSUSE, 2024) and mingw (MinGW, 2024) are used to create a docker image for porousMultiphaseFoam. This image contains an OpenFOAM built from sources with the mingw compiler. A GitHub action is then used to compile porousMultiphaseFoam and generate an archive that contains porousMultiphaseFoam solvers.

GitLab Continuous Integration includes numerous tests to ensure non-regression of code during development.

Documentation is available online in French or English, along with a tutorial and a user’s manual.

3. THYRSIS application

THYRSIS is used here to illustrate the hydrogeological modelling of the Plateau de Saclay, a large area located about 20 km south-west from Paris (France) and covering about 80 km². A complete hydrogeological description can be found in Renard and Tognelli (2016).

After a description of the model building process, two examples of application are developed: the first one describes a classical use of THYRSIS, with the simulation of a tritium release from a potential source, and the second one illustrates the capacity of THYRSIS to simulate rainfall infiltration over the whole modelled domain and including the vadose zone.

3.1. Model building

The hydrogeological model is built using two topological datasets: (1) a raster file defining the topographic elevation with a resolution of 5 m, and (2) a raster file defining the bedrock elevation with a resolution of 50 m. A contour vector layer is then constructed to define the domain boundaries, the mesh size and the fixed hydraulic head boundaries (Fig. 9). The mesh is automatically generated after selecting the mesh builder – GMSH or cfMesh – from the THYRSIS options (Fig. 3). A permeability field is obtained by the inversion method used by THYRSIS based on steady-state simulations to minimize the differences between simulated and measured hydraulic heads. The effective porosity is then estimated by using transient flow simulations and adjusting the range of the variations in simulated hydraulic head with

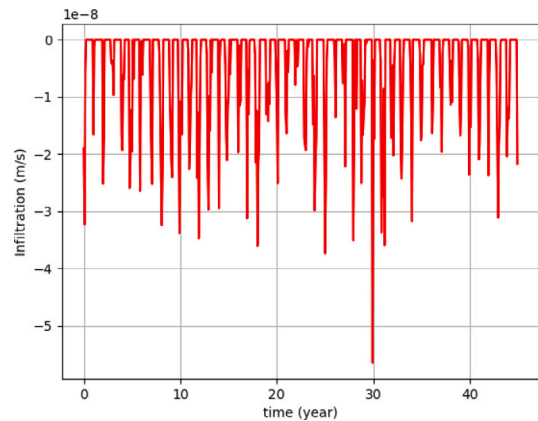


Fig. 12. Transient rainwater infiltration.

Table 2

Mean values of soil water characteristic parameters in the vadose zone.

θ_r (-)	θ_s (-)	α (m ⁻¹)	n (-)	m (-)
0.03	0.49	13	1.43	0.30

respect to the measurements (see 3.2.2). Finally, the van Genuchten parameters of the unsaturated zone are set in the parameters table (Table 2) and the whole model is stored in a sqlite database which can be used later for different case studies.

3.2. Case studies

3.2.1. Simulation of tritium infiltration

The first case deals with the modelling of tritium transport, motivated by the detection of an abnormal amount of tritium in a new borehole. A potential source of tritium leakage between 1964 and 1974 was identified from hydrological modelling and the analysis of flow directions and velocities, as well as from evidence of an excess of deuterium compared to the levels measured in remote boreholes.

Based on estimates of the amounts of tritium released, simulations of tritium transport can be performed using the THYRSIS interface (Fig. 10), while considering the variability of the parameters to estimate confidence intervals (Fig. 11).

3.2.2. Simulation of transient rainwater infiltration

The second case illustrates the ability of THYRSIS to simulate transient rainwater infiltration flows over the entire modelled domain, whether considering or not the unsaturated zone. With the 1D+2D modelling approach of THYRSIS, it is possible to avoid carrying out 3D simulations, which are much more cpu-expensive and barely converge at times. Convergence issues arise especially in the case of a thick

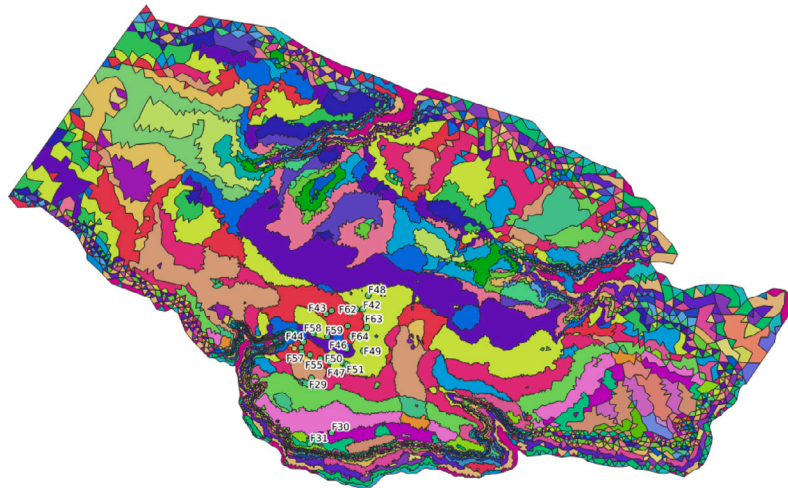


Fig. 13. Display of 56 injection zones created by THYRSIS to sample the unsaturated zone in columns of similar thickness and permeability. Note that the injection zones are not necessarily contiguous.

vadose zone with a low van Genuchten alpha coefficient as is the case with the modelled domain.

The average monthly infiltration is estimated over the period 1970–2014 and using a Thornthwaite water balance model (Renard and Tognelli, 2016). The results are stored in an ASCII file providing the infiltration for each month and shown in Fig. 12.

When modelling the unsaturated zone, the checkbox “Unsaturated zone” is selected and the parameters “thickness_sampling_step” and “permeability_ratio” must be defined by the user. The thickness sampling step defines the maximum variation in thickness of unsaturated columns within a group. For example, if the step is defined as 5 m (default value), groups of columns considered as identical will be defined as [0, 5 m], [5 m, 10 m], [10 m, 15 m], etc. Decreasing the sampling step increases the number of 1D simulations required but also improves the resolution of the injection in the saturated zone. The second parameter is the maximal ratio of permeability tolerated in a given group of columns, by default equal to 10. In the considered case with default parameters, THYRSIS creates 56 unsaturated columns, to be compared to the 60 000 nodes of the mesh (Fig. 13). Note that the injection zones are not necessarily contiguous.

Simulation can be automatically performed using MPI parallelization on a personal multi-core computer.

Fig. 14 highlights the influence of the unsaturated zone when simulating the transient flow of rainwater infiltration: the unsaturated zone induces a delay of about 2 years and produces a much smoother signal.

3.3. Validation

Two kinds of validation of THYRSIS calculations are presented: (i) a comparison of THYRSIS results with measurements and (ii) a comparison of THYRSIS results obtained with METIS and PMF.

3.3.1. Comparison of 1D+2D calculation with measurements

On the same domain as that used in Latour et al. (2023), THYRSIS 1D+2D transient flow simulations were carried out over a 14-year period, where detailed measurements are available. The resulting simulated hydraulic heads are in very good agreement with the measurements, as shown in Fig. 15, demonstrating the relevance of the 1D+2D approach.

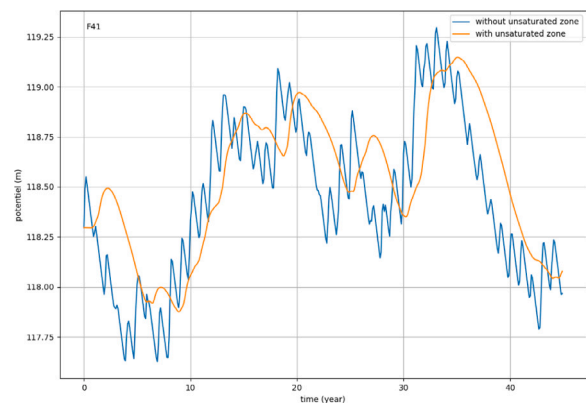


Fig. 14. Simulated hydraulic head with or without unsaturated zone.

3.3.2. Comparison of THYRSIS calculations with METIS and PMF

Comparing THYRSIS results obtained with METIS and PMF calculations is relevant because of the very different conceptual approaches of the two software packages. In particular, METIS is a finite element code where hydraulic heads and concentrations are calculated at mesh nodes, whereas PMF is a finite volume code whose variables are calculated at mesh centres. These differences require distinct processing and interpolation procedures to restore the results at the mesh nodes and meshes and display them in the QGIS mesh layers.

Concerning the Plateau de Saclay’s model and the flow simulation based on transient infiltration (Section 3.2.2), we compare below the water flows leaving two 1D columns, with thicknesses of about thirty metres (Fig. 16(a)) and sixty metres (Fig. 16(b)) respectively, then the total flow entering the saturated zone and calculated from all the 1D columns (Fig. 16(c)). The unsaturated water outflows are very similar and the total saturated inflow shows local differences up to ten per cent, which may explain the small deviation observed on the hydraulic levels shown in Figs. 17(a) and 17(b).

4. Conclusion

THYRSIS is a new opensource QGIS plugin dedicated to hydrogeological modelling. It allows us to build simple hydrogeological models

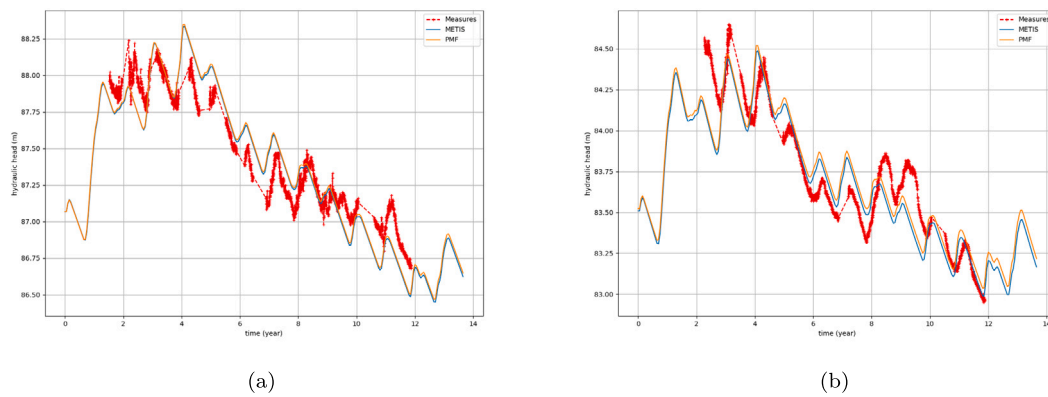


Fig. 15. Examples of 1D+2D THYRSIS transient flow simulations at two locations, with comparison between METIS and PMF results, and measurements.

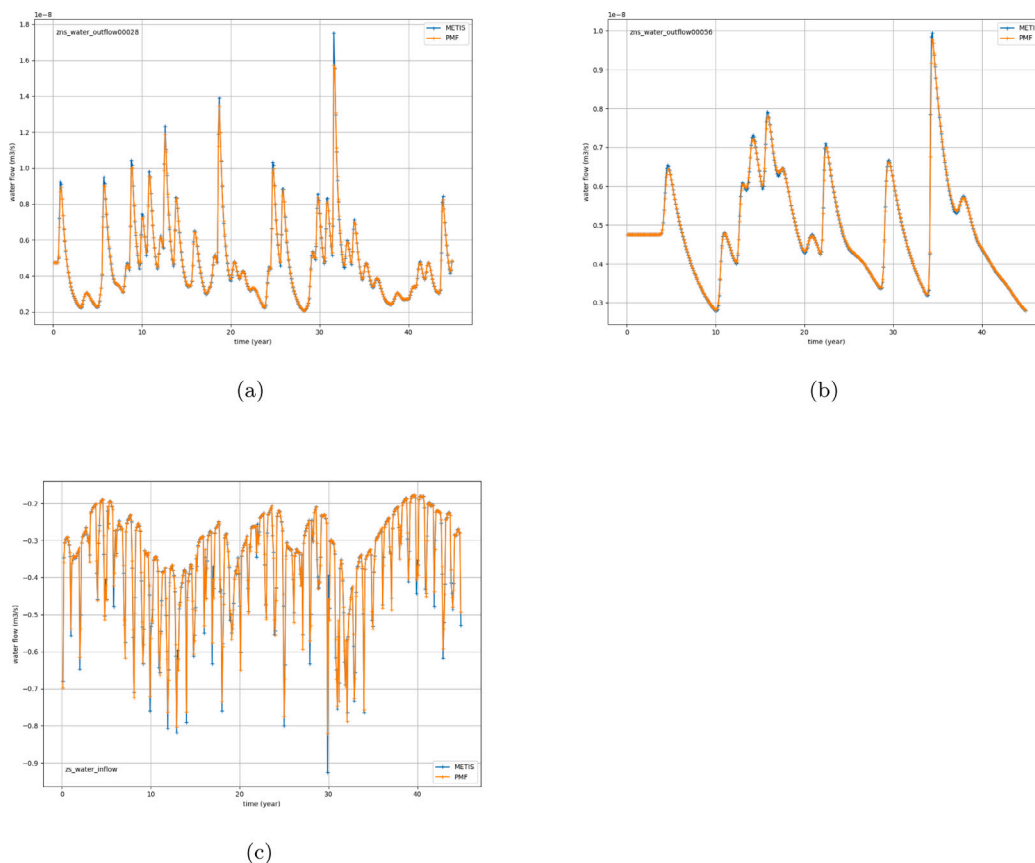


Fig. 16. Comparison of METIS and PMF (a) water outflow from column 28 with thickness 30 m, (b) water outflow from column 56 with thickness 60 m and (c) total water inflow in saturated zone.

at multiple scales, from local to regional, and to run flow and transport simulations by coupling 1D unsaturated column modelling with a 2D model of the saturated zone. The design is based on a new meshlayer module which implements data providers for steady-state data and time-dependent NumPy result files, ensuring very good performances and smooth display for meshes comprising several million elements. Steady-state groundwater flow models can be built via the QGIS interface and stored in SpatiaLite databases, to instantly serve as initial state for transient flow and transport simulations. With a very simple interface, THYRSIS can be used easily to simulate several flow and transport situations and is particularly well suited to provide a rapid response in accidental situations. For example, THYRSIS can simulate the effect of heterogeneous and transient infiltration to reproduce variations in piezometric levels and adjust the effective porosity, or the

transport of solute in the subsurface, from the ground to groundwater outlets, in order to estimate groundwater concentrations. THYRSIS is a simple and effective alternative to 3D models that are often rather complex to implement and converge.

In addition to its modelling and simulation capabilities, the full integration of THYRSIS into QGIS makes it easy to build models and use the results, with all the geospatial functions of QGIS available, and the addition of specific functions such as uncertainty and mass balance calculation, or graphical representation of potential and concentration as a function of time.

Several developments are being studied, such as (i) implementing geostatistical techniques to interpolate piezometric measurements, which would be useful for preparing the inversion of the permeability field, (ii) interfacing with public libraries to generalize inversion

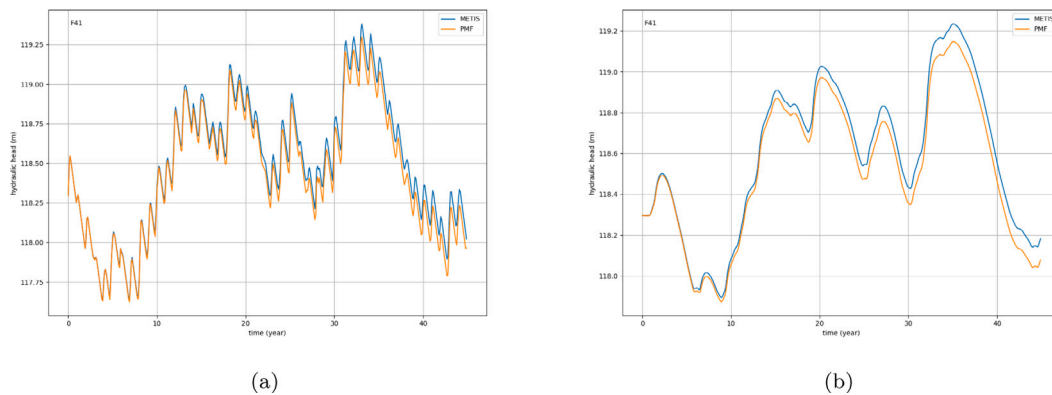


Fig. 17. Comparison of METIS and PMF simulated hydraulic heads (a) without or (b) with unsaturated zone.

techniques, (iii) implementing a dual-medium approach, using recent developments in porousMultiphaseFoam solvers or (iv) using THYRSIS to generate full 3D hydrogeological models, which could be used to treat configurations with high vertical heterogeneity, that are more difficult to model using a 1D+2D approach.

Software availability

Software name: THYRSIS

Developers: François Renard, Vincent Mora, Jean-Marie Kerloch

Year first available: 2022

Operating System Required: Linux, Windows 10

Software required: QGIS 3.22 or later

Licence: GPL2 and CeCILL 2.1

Availability: <https://gitlab.com/Oslandia/qgis/thyrsis> or <https://plugins.qgis.org/plugins/thyrsis>

Cost: free

Program language: Python 3

CRediT authorship contribution statement

F. Renard: Conceptualization, Data curation, Methodology, Project administration, Software, Supervision, Validation, Writing – original draft, Writing – review & editing. **V. Mora:** Conceptualization, Methodology, Software, Writing – review & editing. **P. Horgue:** Validation, Writing – review & editing. **J.M. Kerloch:** Software, Validation, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

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