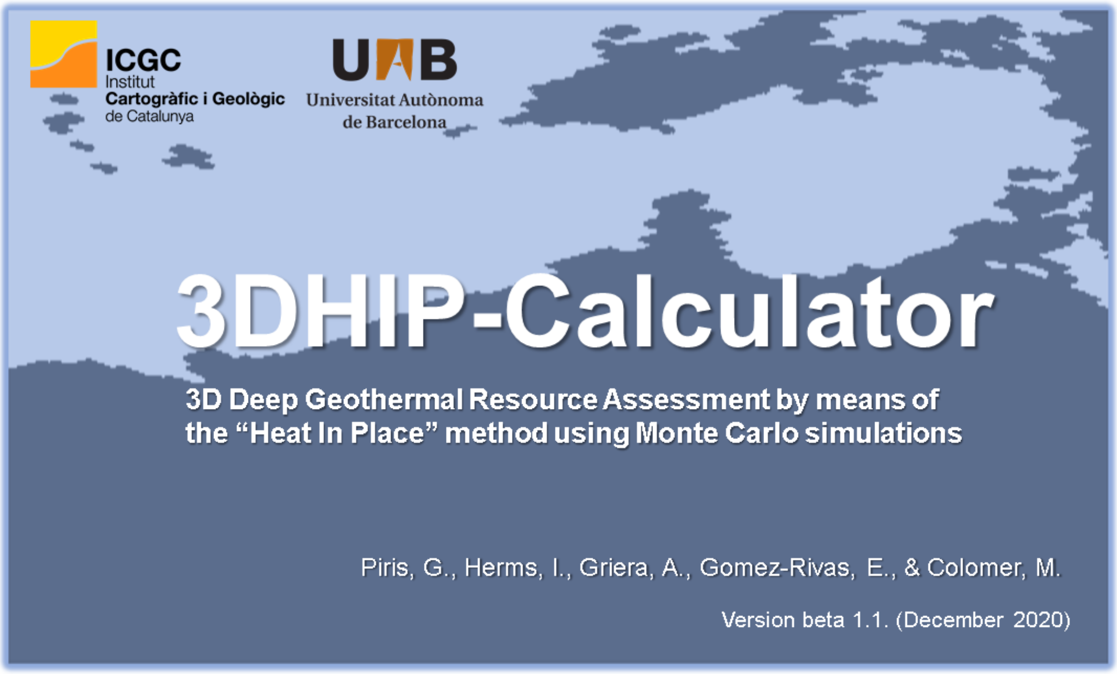

Software User Manual v1.1

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Disclaimer and intellectual property

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Glossary

Parameters	**Description**
HIP	Heat-In-Place [PJ] or [PJ/km^2] according to Muffler and Cataldi (1978)
Hrec	Recoverable heat [kW] or [kW/km^2]
V	Cell or voxel volume [m^3]
ϕ	Porosity [parts per unit]
C	Specific heat capacity [kJ/kg ºC]
T	Temperature [ºC]
Tr	Cell or voxel temperature [ºC]
Ti	Reference or reinjection temperature [ºC]
Tz	Estimated temperature at depth [ºC]
T0	Mean annual surface temperature [ºC]
Dz	Calculated depth [m]
Ce	Conversion efficiency [parts per unit]
R	Recovery factor [parts per unit]
T_{live}	Mean plant lifetime [seconds]
Pf	Plant factor [parts per unit]
gradT	Thermal gradient [ºC/km]
ID	Identifier
PDF	Probability Distribution Function
CRS	Coordinate Reference System

Contents

1 Introduction

1.1 Summary of changes in 3DHIP-Calculator Version beta 1.1

In this version we have added:

- Corrections of internal bugs and typographic mistakes.
- We reconsidered the concept of “rock density” and “rock specific heat capacity” instead “lithology density” and “lithology specific heat capacity” because properly, both lithology and density are rock properties.

We know that these modifications are so light and just look for solve some bugs. However, creating a new version the user knows that these bugs are solved.

1.2 Presentation

3DHIP-Calculator (Fig. 1) is a free software written in MATLAB™ and publicly distributed by the **Institut Cartogràfic and Geològic de Catalunya (ICGC)**. The software uses the stochastic method to estimate the deep geothermal potential of hot sedimentary aquifers (HSA) using the well-known USGS (United States Geological Survey) volumetric Heat-in-Place (HIP) method (Muffler & Cataldi, 1978, Garg & Combs, 2015) based on 3D geological and thermal models. The software utilizes probability distributions function (PDF) to define the input parameters and calculations are performed using the Monte Carlo method (Shah et al., 2018).

The user must provide 3D geological and thermal models (or a temperature gradient to calculate the temperature distribution) in a voxel format (*XYZ* coordinates and geological properties) in which the 3D space is gridded, with each cell or voxel having an attribute to describe the geology and properties within the volume considered. From either kind of input, the code calculates the HIP and Recoverable Heat (Hrec) for the desired lithology/geological formation and depth range. The results are displayed in 2D raster maps and *XY* diagrams (histograms and cumulative frequency plots), which can be saved as image, vector or pdf files. Additionally, the user can save the files containing the input and output data for their post processing, visualization or further evaluations in 2D or 3D with other software packages, and also a short report with the data used in the simulation.

Fig. 1. Logo of the application.

3DHIP-Calculator is provided without support. The code authors/developers would appreciate notification of any errors found in this program by sending an email to: geotermia@icgc.cat,

describing the error details and providing (where possible) a screenshot of the error, the input file used and the MATLAB™ version.

The authors/developers of this tool encourage end-users to obtain quick stochastic HIP and Hrec estimations from their 3D geological models in order to help generate and publish new 2D maps in a GIS environment. The authors/developers also encourage other programmers and scientists to contribute into the project either, by providing feedback of their testing and/or by reporting any bugs they may encounter.

1.3 **Background**

Deep geothermal energy is heat energy originating deep inside the earth. The first step to assess the possibility to take profit of geothermal resources is to quantify the amount of available heat and the part that could be recovered. Muffler & Cataldi (1978) defined the term *geothermal resource base* as "*all the thermal energy beneath a specific area*". The terminology adopted has been highly used at least until now. The geothermal assessment applies for both identified and undiscovered systems and utilizes the definition of *geothermal resource base*. Methodologies used for geothermal resource assessment were reviewed by Muffler & Cataldi (1978) and divided into four main categories, among which the '*volume method'* is the most suitable for many low-temperature reservoirs.

<u>The volumetric method for assessing geothermal resources</u>

The volume method involves the calculation of the thermal energy contained in each volume of rock and water and then the estimation of how much of this energy might be recoverable. The stored heat can be computed by using the equation defined by Muffler and Cataldi (1978) Eq. (1). It can be solved deterministically but also using a probabilistically approach combined with Monte Carlo simulations.

$$HIP = V \cdot [\emptyset \cdot \rho_F \cdot C_F + (1 - \emptyset) \cdot \rho_R \cdot C_R] \cdot (Tr - Ti) \qquad \text{Eq. (1)}$$

As far as the part of energy that could be recovered, as a preliminary assessment, and in case of a direct heat application from a low temperature geothermal reservoir, the accessible resource base ca be converted to recoverable heat by using the following equation Eq. (2) (Arkan & Parlaktuna, 2005; Trumpy et al., 2016; Limberger et al., 2018).

$$Hrec = \frac{HIP \cdot C_e \cdot R}{Tlive \cdot Pf} \qquad \text{Eq. (2)}$$

where:

- V is the cell or voxel volume [m^3]
- $\emptyset$ is the porosity [parts per unit]
- ρ is the density [kg/m^3]
- C is the specific heat capacity [kJ/kg·ºC]
- Tr is the cell or voxel temperature [ºC]

- *Ti* is the reinjection, abandonment temperature [ºC] (as the threshold of economic or technological viability), the ambient temperature, (i.e. the annual mean surface temperature value), or other criteria (e.g. Limberger et al., 2018).
- C_e is the conversion efficiency [parts per unit]. It considers the heat exchange efficiency from the geothermal fluid to a secondary fluid in a thermal plant.
- *R* is the recovery factor [parts per unit]
- T_{live} is the mean plant lifetime or total project live [seconds]
- *Pf* is the plant or load factor [parts per unit]. Most of the direct heat applications (district heating, greenhouse heating, etc.) of geothermal energy are not continuous throughout the year. This factor considers the fraction of the total time in which the heating application is in operation.
- the sub index ‘F’ or ‘R’ indicates fluid and rock, respectively.

<u>The Monte Carlo method</u>

In the first’s phases of geothermal projects, when the resource is preliminary estimated and mapped, the variables of the equation of the volumetric method present uncertainty. To continue with the estimations, the Monte Carlo method can be applied. This method uses stochastic techniques to evaluate the effect of variables uncertainty on the results (Shah et al. 2018). The method uses a repeated process of random sampling of the unknown parameters of the model (the variables) to perform a specific number of simulations to solve the mathematical system (in this case the HIP and Hrec equations).The requirement to use it is that the variables of the equations can be described by probability density functions (PDF's). If this can be assumed, then the first step is to define the uncertainty for the input variables and assign one type of PDF (e.g. normal, triangular etc). Then the Monte Carlo simulation can proceed by random sampling from the different PDFs.

The outcomes will be new PDFs of the HIP and Hrec. If a 3D model is used, at the end each voxel will have a PDF associated with the HIP and Hrec results. Taking these, one can derive the geothermal resource representing different probabilities (e.g. 10% or P10, 50% or P50 and 90% or P90).

2 Software acquisition, use and licence of use

2.1 Acquisition and license of use

The **3DHIP-Calculator** software can be freely downloaded from the ICGC Deep geothermal energy web page to be used without restrictions or limitations. The product is released under the Creative Commons licence Attribution 4.0 International, known as CC BY 4.0.

2.2 Formats and products

3DHIP-Calculator is delivered:

- As a standalone executable MATLAB™-based software compiled for Microsoft Windows™ (**3DHIP_Calculator.exe**). During the installation MATLAB™ libraries will be automatically downloaded and installed to correctly run the app. To install the app just double click on the executable file and follow the installation instructions.

The current version of **3DHIP-Calculator** is beta 1.0. (February 2020). The software has been developed using the MATLAB™ version R2019b and have been tested in Windows 10.

2.3 Software disclaimer

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3 Starting 3DHIP-Calculator

When the user starts the 3DHIP-Calculator software the main window appears (Fig. 2). This contains a brief description of the main characteristics of the software package, information about the authors and their contact details, software version and the institutions involved in the development of this application.

3DHIP-Calculator is divided in different tabs (red rectangle on Fig. 2). The user can go through them either by directly clicking on each label or by using the dark grey buttons (e.g., green rectangle of Fig. 2).

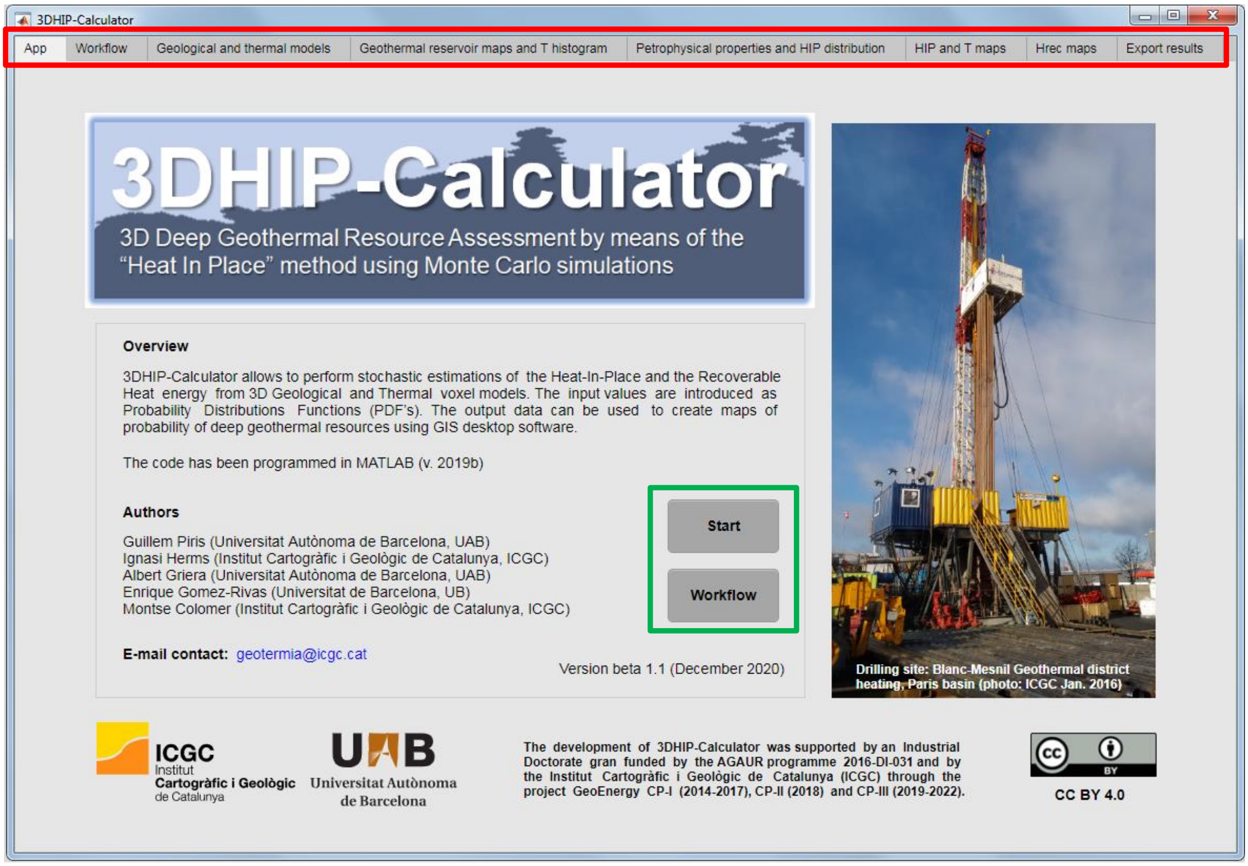


Fig. 2. Screenshot of the main window. The red rectangle indicates the different tabs ('App', 'Workflow', 'Geological and thermal models', 'Geothermal reservoir maps and T histogram', 'Petrophysical properties and HIP distribution', 'HIP and T maps', 'Hrec maps' and 'Export results'). The green rectangle shows the buttons "Start" (takes you to the Geological and thermal models tab) and "Workflow shows a short description of the method.

The application is structured in five blocks, ordered by execution order. Each block contains a light orange "RUN" button that allows running the calculations corresponding to the block and displays the results (Table 1).

Block number	Block Name	Tasks
1	Load data (Geological and thermal models)	Allows loading and defining the geological and thermal data.
2	Heat-In-Place simulation parameters	Allows introducing several fixed parameters for the HIP calculations and select the geothermal target.
RUN 1 & 2 (shows the Temperature-Depth distribution for the selected target)		
3	Depth range selection	Allows selecting the desired depth range where HIP and Hrec calculations will be performed.
RUN 3 (Show the selected depths and some plots of the geothermal target shape)		
4	Petrophysical properties and other parameters	Allows introducing the HIP parameters and selecting the desired PDF type for each parameter.
RUN 4 (Performs the HIP and Hrec calculations and displays the results in plots)		
5	Export files	Allows exporting three files with the HIP results. • File1: Contains the calculated and initial data of the 3D model. • File2: Contains the data to plot 2D maps. • Report: Contains a summary of the values and results of the HIP and Hrec calculations.
RUN 5 (Exports the three files)		

Table 1. Description of each block and run routine of the app.

3.1 **'Workflow'**

The 'Workflow' tab (Fig. 3) provides a brief description of the workflow diagram and the mathematical model applied by the tool, i.e. the HIP and Hrec equations and the description of the main parts (tabs). This tab tries to make the app self-explanatory. The user can find more information by clicking on the "Software user manual" button to open the manual in PDF format.

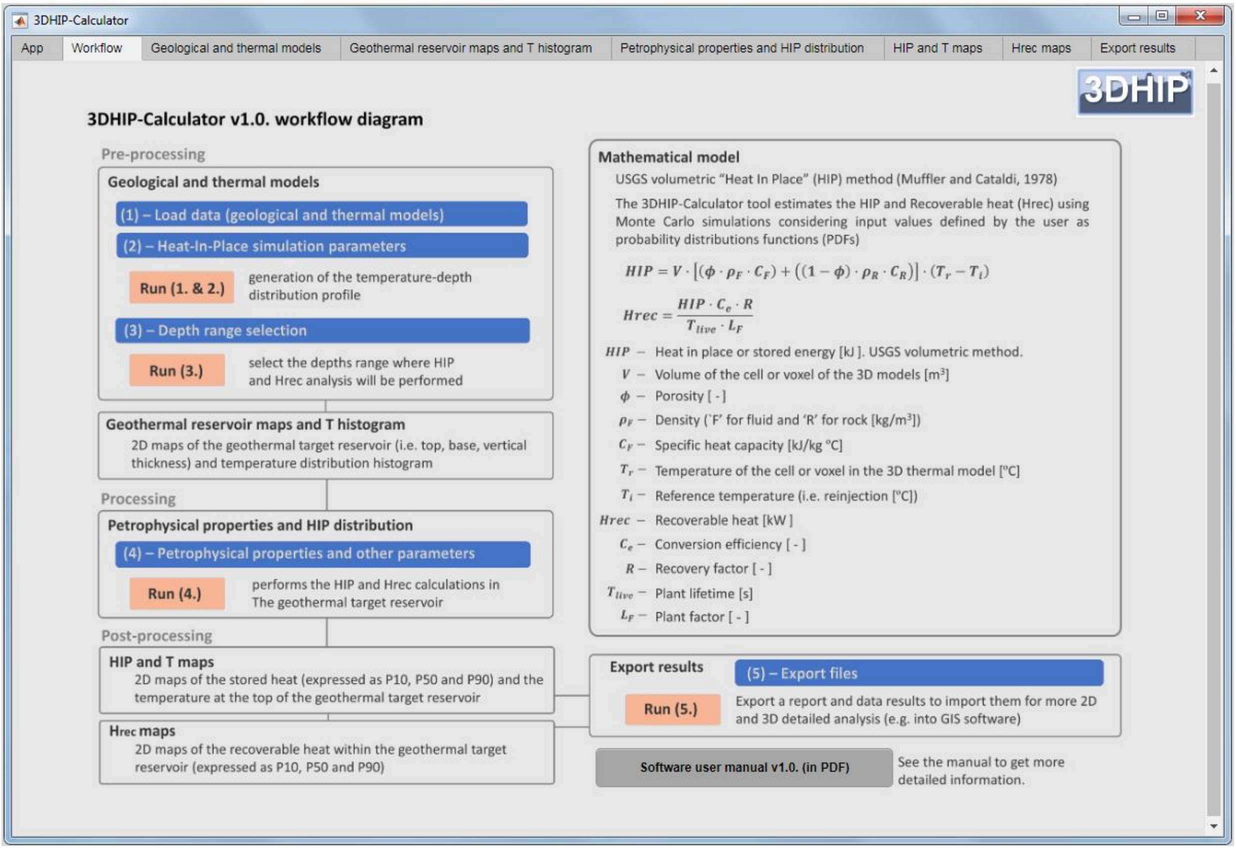


Fig. 3. Screenshot of the 'Workflow' tab. The tab contains a brief description of the application components, the main technical and mathematical concepts, the parameters used, and a brief description of the other tabs of the application.

3.2 **'Geological and thermal models'**

The 'Geological and thermal models' tab offers the user three blocks:

- Load data (Geological and thermal models)
- Heat-In-Place simulation parameters
- Depth range selection

There are two run buttons: RUN (1. & 2.) and RUN (3.) (Fig. 4), which allow saving the data and going forward.

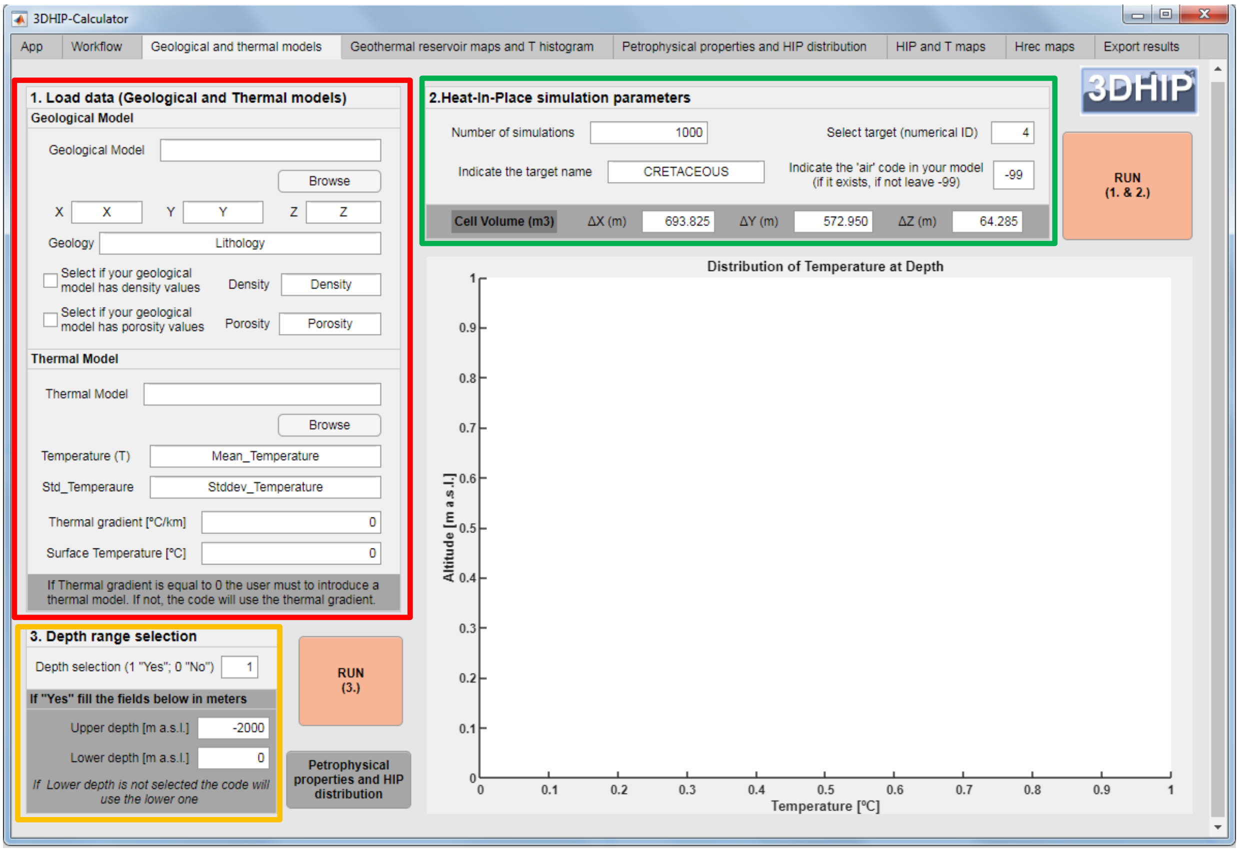


Fig. 4. 'Geological and thermal models' tab view. The area marked by the red rectangle shows the 'Load data (Geological and thermal models)' block 1; the green rectangle shows the 'Heat-In-Place simulation parameters' block 2; and the orange rectangle the 'Depth range selection' block 3.

3.2.1 Block 1: Load data (Geological and thermal models)

In this block the user uploads the geological model, selects the coordinates, geology attributes, and the thermal model. Alternatively, the user can define a thermal gradient to establish a rough generic temperature distribution model according to depth.

Note that in the manual, as well as in the 3DHIP-Calculator, the concept of "target" is used in a general way to refer to the geothermal target. This target could be a certain lithology (e.g. sandstones, limestones, etc.), a geological formation, an aquifer or any other entity. The definition of the target will depend what the user wants to consider in their geological model.

Firstly, the 3D geological model is uploaded using the "Browse" button in the "Geological Model" field. The geological model must follow a voxel format in which each voxel (or cell) is defined by its coordinates and properties. The white rectangles correspond to editable text or numerical fields. The file containing the geological model needs to follow some basic rules:

a) The extension of the file is not important as soon as it corresponds to a text format (i.e. it does not matter if the file extension is *.txt, *.dat, *.vox, etc.).

b) A line with the colheaders needs to appear and be followed by the data. There is no restriction if additional text lines appear before the colheaders.
c) The data can be separated either by space, comma or tabulator.
d) The data file must contain at least the following variables:
   i. *X*, *Y*, and *Z*: coordinates of each voxel, defined in the UTM coordinate system or in geographic decimal degrees.
   ii. Geology (the reservoir/aquifer/target/layer/formation): defined by a numerical identifier (ID).

Once the geological model is introduced, the user must indicate the text identifier for each variable. For example: if the colheader of the "*X*" coordinate is X_cor the field indicated by "X" needs to be filled with "X_cor" and the same for the "*Y*", "*Z*" and "Geology" fields.

Additionally, the geological model can include petrophysical parameters that will be utilized for the HIP analysis (e.g. density, porosity). To do that, just select the box *"Select if your Geological model has density values"* or/and *"Select if your Geological model has porosity values"* and specify the colheaders in the corresponding fields.

If your geological model has more columns, the application will erase them before performing the calculation. The column order is not important as soon as the colheaders are properly identified. Please note that the code will identify the columns by its colheader.

The density value needs to be provided in **g/cm^3** and the porosity in **parts per unit**. An example of the file is displayed in the Fig. 5.

Geological_model.txt

```
X,Y,Z,density,lito,poro
478079.250000,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
478354.494141,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
478629.740234,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
478904.984375,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
479180.230469,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
479455.474609,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
479730.720703,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
480005.964844,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
480281.208984,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
480556.455078,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
480831.699219,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
481106.945313,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
481382.189453,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
481657.435547,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
481932.679688,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
482207.923828,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
482483.169922,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
482758.414063,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
483033.660156,4640278.750000,-6808.750000,2.720000,7.000000,0.15000000
```

Fig. 5. Example file of the Geological model extracted from GOCAD software. The app only will use the columns X, Y, Z, Geology (lito), Density (density) and Porosity (poro) (if the density and porosity boxes are selected).

After that, and following the same procedure as for the geological model, the user can upload the thermal model with the following specifications:

a) The extension of the file is not important as soon as it corresponds to a text format (e.g. *.txt, *.dat, *.vox, etc).
b) A line with the colheaders needs to appear and be followed by the data. There is no restriction if additional text lines appear before the colheaders.
c) The data can be separated either by space, comma or tabulator.
d) The data file must contain at least the following variables:
    i. *X*, *Y*, and *Z*: coordinates of each voxel, defined in the UTM coordinate system or in geographic decimal degrees. The coordinates have to be the same with those of the corresponding geological model in a way that the geological and thermal models are consistent in terms of their dimensions, cell number and cell order.
    ii. Temperature (*T*): defined in Celsius degrees.
    iii. Temperature standard deviation: defined in Celsius degrees (this column can also have 0 values).

The user is required to indicate the colheaders for the temperature and temperature standard deviation. The code only uses the five columns (*X*, *Y*, *Z*, Temperature and Temperature standard deviation). If there are more columns in this file they will not be read and stored.

If a 3D thermal model is not available, the app allows inferring a rough 3D temperature field distribution within the 3D geological model using the ‘temperature gradient approach’ according to the following equation (Eq. 3):

$$Tz = T0 + gradT * Dz, \qquad \text{Eq. (3)}$$

where *Tz* is the estimated temperature at depth, *T0* is the mean annual surface temperature, *gradT* is the measured thermal regional gradient in ºC/km and *Dz* is the depth of the target according to the preliminary 3D model. This calculation considers the surface topography of the model and applies a linear gradient plus the surface temperature and assumes a conductive steady state regime. To calculate the temperature using this approach the user has to fill the fields: “Temperature” and “Std_Temperature” (which will be used as colheaders for the new created columns, in this case the standard deviation temperature will be 0), “Thermal gradient (ºC/km)” and “Surface Temperature (ºC)” and leave empty the field “Thermal model”.

3.2.2 Block 2: Heat-In-Place simulation parameters

Once the geological and thermal models are defined, the user needs to introduce some additional variables for the HIP calculations. Firstly, one has to provide the number of simulations for the Monte Carlo stochastic approach (field “Number of simulations”). A total of 10,000 trials are industry standard although a few thousand might be sufficient (Agemar et al., 2018). Increasing the number of simulations directly affects the computational time required. Secondly, indicate the target (i.e. reservoir, aquifer, geological unit) that is going to be evaluated for the HIP and Hrec calculations. To do this, the user has to provide the corresponding target ID (the numerical identifier defined within the 3D geological model for each layer/lithology/geological formation) in the field “Select target (numerical ID)” and the target name in the field “Indicate the target name” (this name will be used for the titles in the graphs and for the summary report). In the next step the user has to indicate the numerical identifier for the ‘Air’ (the voxels corresponding to the ‘air’ or above the surface level within the 3D geological model). This step is key if you are calculating temperatures from the thermal gradient. To finish block 2, the user has to indicate the cell volume for the HIP calculation (*X*, *Y* and *Z* lengths in meters).

3.2.3 Run (1. & 2.)

After filling the blocks 1 and 2, the user can click on the button “Run (1. & 2.)”. A wait bar will appear to show that the calculation is running. When finished, the Temperature-Altitude distribution that corresponds to the thermal model for the selected target (reservoir/aquifer/layer) will automatically appear in a plot below block 2 (points in blue inside Fig. 6).

3.2.4 Block 3: Depth range selection

In this block the depth range is defined. If the user wants to delimitate a specific depth range, the number ‘1’ must be placed in the field “Depth selection (‘1’ Yes, ‘0’ No)” and then introduce the depth range in the fields below. It is not mandatory to define a lower depth. If no lower depth is introduced the code will automatically use the deepest value.

3.2.5 Run (3.)

After the block 3 is filled, the user must click on the “Run 3.”, and two red lines indicating the selected depth range will be displayed in the diagram (Fig. 6.). Additionally, four plots related to the geothermal shape and temperature distribution will be generated in the ‘*Geothermal reservoir maps and T histogram*’ tab. Once “Run (3.)” is complete, the user can switch to the next tab by clicking on the “Petrophysical properties and HIP distribution” button.

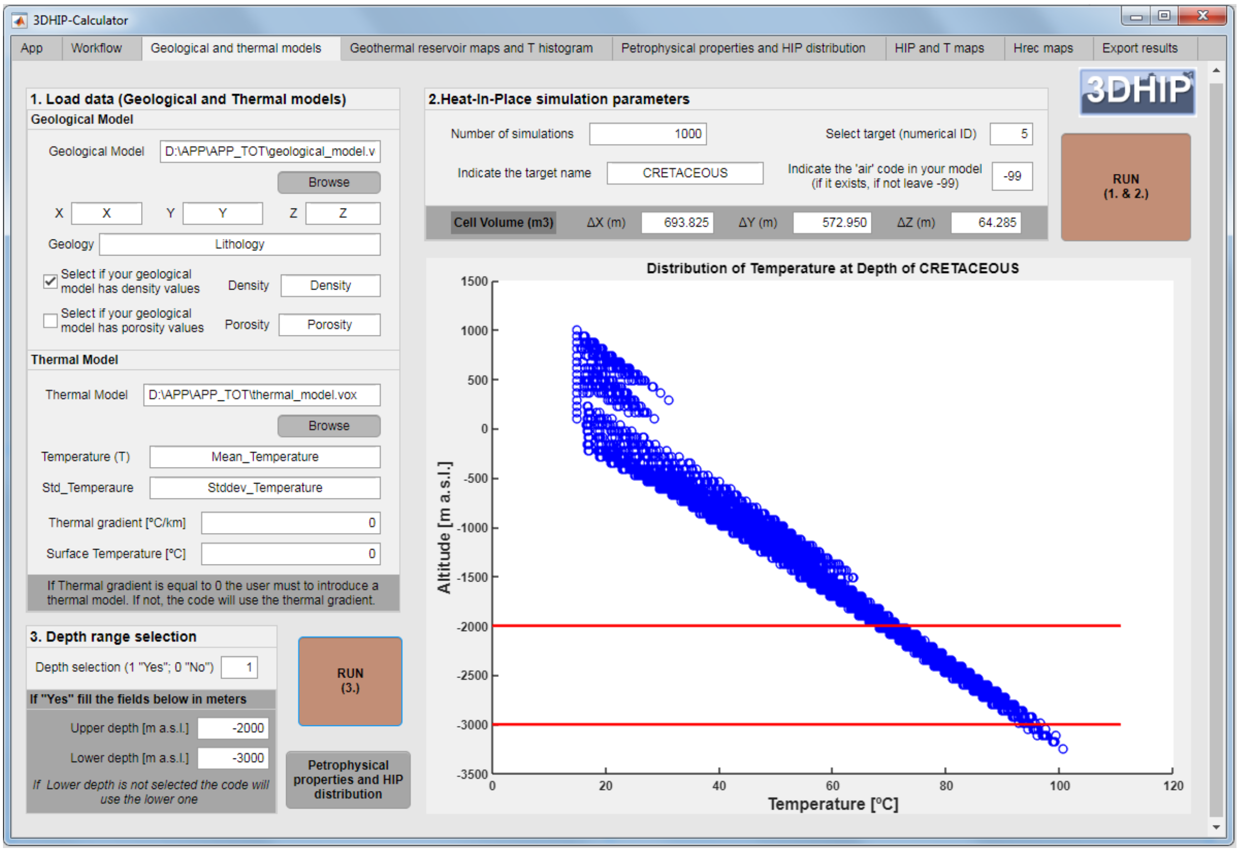


Fig. 6. Screenshot after running the blocks 1, 2 and 3. Each blue circle in the plot represents one cell in the geological and thermal model. The red lines indicate the selected depth range.

3.3 **'Geothermal reservoir maps and T histogram'**

In this tab the user can consult four plots, ordered from left to right and from top to bottom (see Fig. 15 in the section 4): top, base, vertical thickness and temperature histogram of the selected geothermal target and depth ranges.

3.4 **'Petrophysical properties and HIP distribution'**

In this tab the user must introduce all the variables for the HIP and Hrec calculations (Fig. 7):

The HIP and Hrec equations (Eq. (1) and Eq. (2) respectively) are solved for each cell / voxel using as input the random values generated using probability density functions (PDF's) for each parameter. This will be done as many times as to the number of simulations indicated by the user.

3.4.1 Block 4: Petrophysical properties and other parameters

The petrophysical parameters are introduced here (i.e. porosity, fluid density, fluid specific heat capacity, rock density, rock specific heat capacity, recovery factor, reinjection temperature, conversion efficiency, plant factor and mean plant lifetime). The user can indicate the distribution shape (normal or triangular distribution by selecting the corresponding box) and the delimiter fields (mean and standard deviation for normal distribution; lower, maximum and upper values for triangular distribution) (Fig. 7).

If the user has previously indicated that the geological model includes density and/or porosity values, a red label will appear to warn that these values will not stochastically generated (Fig. 7).

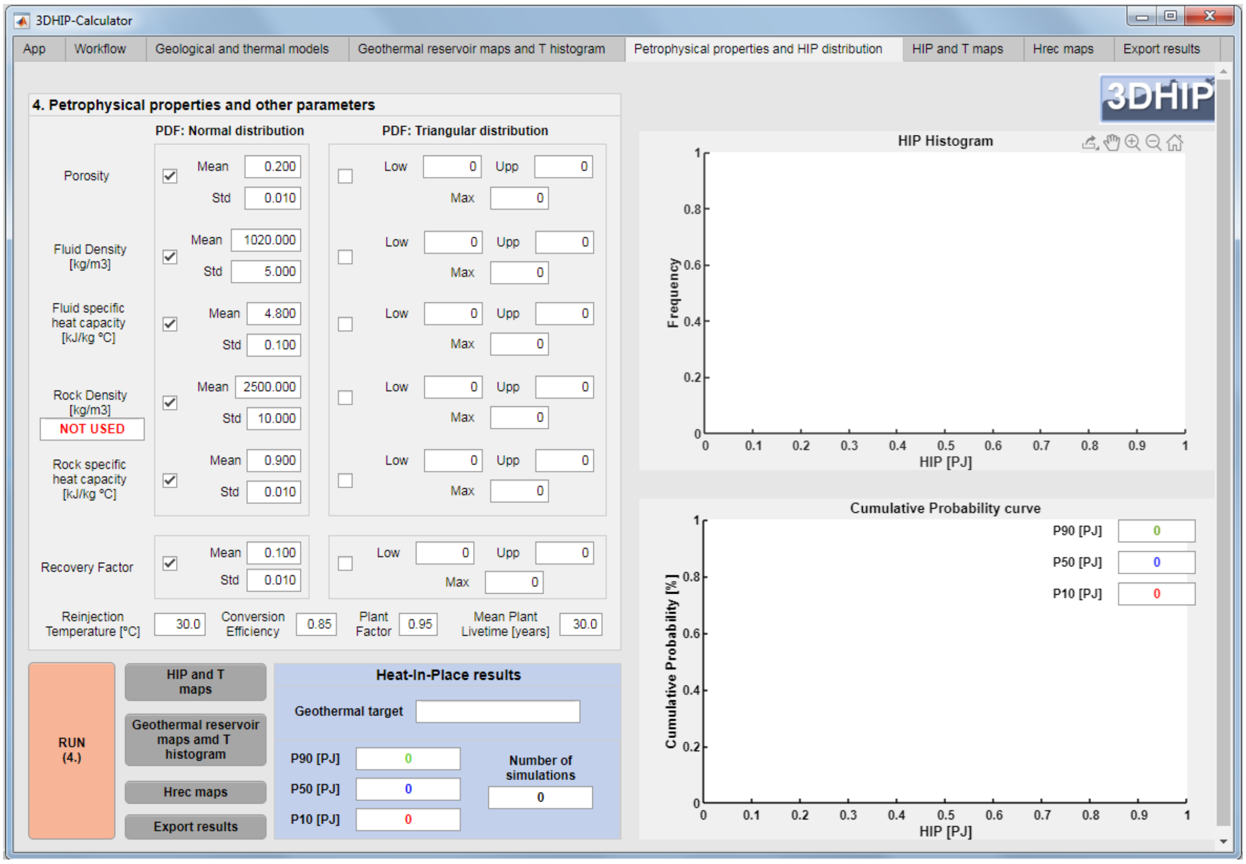


Fig. 7. 'Petrophysical parameters and HIP distribution' tab view.

3.4.2 Run (4.)

Once the parameters in block 4 are already filled, the calculations are done after pressing the button “Run (4.)”. Similarly to previous cases, a wait bar indicates that the application is performing the calculations and preparing the output graphs. It is worth mentioning that the HIP and Hrec parameters are only calculated for cells with a temperature higher than or equal to the re-injection temperature plus five degrees. Otherwise, the assigned HIP and Hrec is directly assigned the value zero.

Once the calculation is complete, graphs are automatically displayed and the main results appear in the blue area of the panel (“Heat-In-Place results”). The right top plot shows a histogram of the HIP values in [PJ], the lower plot the cumulative probability curve of the HIP for the selected target and depth range, highlighting the P10_HIP (probability 10% or very low confidence of the estimation and high values), P50_HIP and P90_HIP (50% and 90% respectively indicating high confidence of the estimation and low values).

All the plots can be saved in image (png, jpg or tif) or vector (pdf) file format. On the right upper part of the graph there is an icon palette to maximize, minimize, rotate, save, restore or pan the image. The user can save the plots by clicking on them (see the icons in the Fig. 17).

Afterwards, the user can go to the following tabs (results) by clicking on the “Geothermal reservoir maps and T histogram”, “HIP and T maps”, “Hrec maps” and “Export results” buttons.

3.5 **‘HIP and T maps’**

Results are displayed in four plots by default, ordered from left to right and from top to bottom (see Fig. 17 in the section “4. Example of application”):

- The P10 HIP distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. HIP units for each cell are PJ/km^2.
- The P50 HIP distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. HIP units for each cell are PJ/km^2.
- The P90 HIP distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. HIP units for each cell are PJ/km^2.
- Distribution of temperatures at the top for the selected geothermal target and depth range.

3.6 **‘Hrec maps’ tab**

Results are displayed in three plots, ordered from left to right and from top to bottom (see Fig. 18 in the section “4. Example of application”):

- The P10 Hrec distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. Hrec units for each cell are PJ/km^2.
- The P50 Hrec distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. Hrec units for each cell are PJ/km^2.
- The P90 Hrec distribution for the selected geothermal target and depth range. The values are calculated as the vertical sum of the grid cells divided by the surface area of the grid cells in km^2. Hrec units for each cell are PJ/km^2.

3.7 **'Export results' tab**

This tab allows exporting the data obtained through the calculations in text format (Fig. 8).

3.7.1 Block 5: Export files

Three types of files are predefined to export data (each one with its own panel):

1. The first file contains the 3D model, i.e. contains all the cells of the selected geothermal target and depth range with the initial data plus the calculated variables (see the list in the Figure 8). The HIP and Hrec results are expressed as they have been calculated, in [PJ] and [kW].

2. The second file contains the 2D data, i.e. contains the vertical sum of the grid cells (for this reason this file only has *X* and *Y* coordinates). The values of HIP and Hrec are not divided by the cell surface and they are expressed as they have been calculated. This is to prevent unit errors if you want to plot these values on a map or sum them by areas or whatever other analysis.

3. Finally, the user can export a brief report with the simulation overview.

To export the files, use the “Browse” button and select the folder and file name. The extension of the file is predefined as .txt. The file name will automatically appear on the file “File name”.

3.7.2 Run (5.)

To export the three files just click on “Run (5.)”. The files will be saved in the folder that the user indicated on block 5. To give an idea of the file’s appearance see Fig. 9 for File 1 (3D Model), Fig. 10 for File 2 (2D Model) and Fig. 11 for the summary Report.

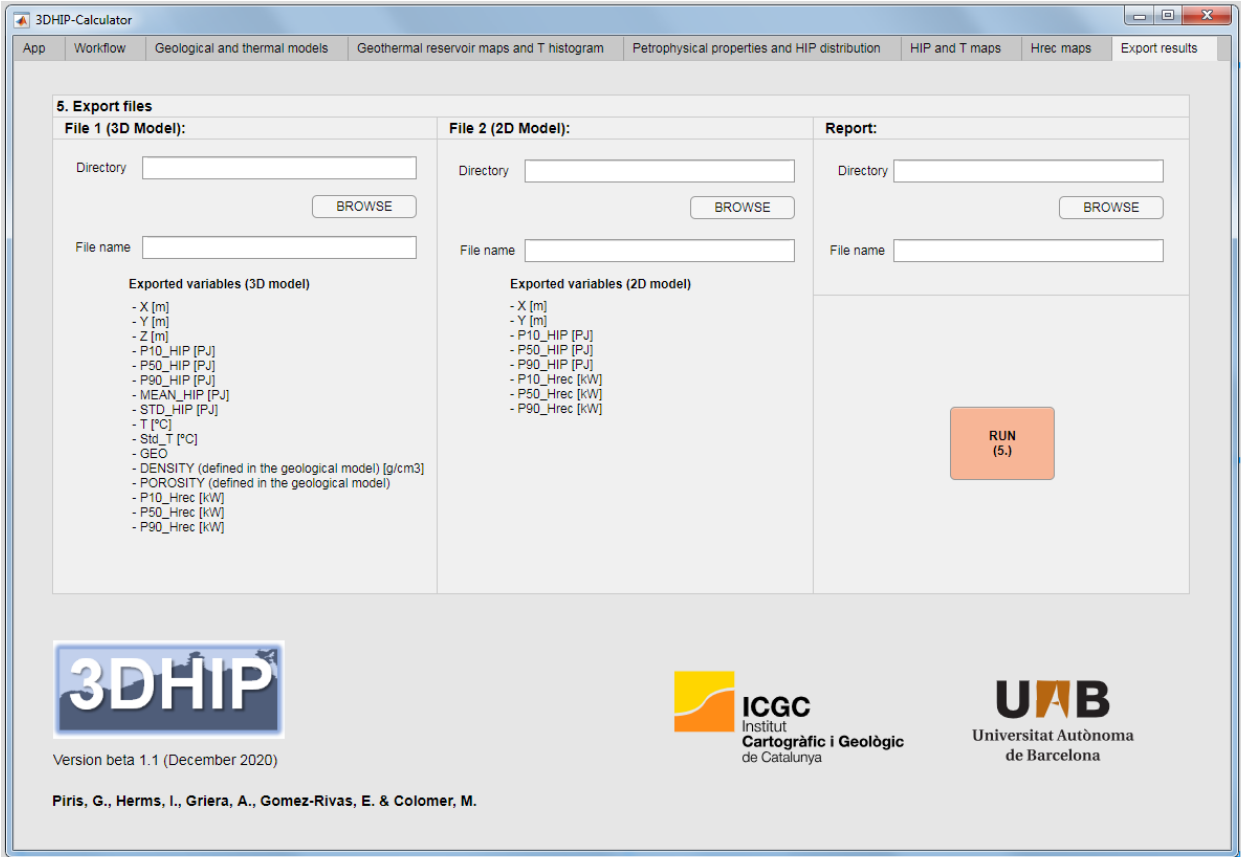
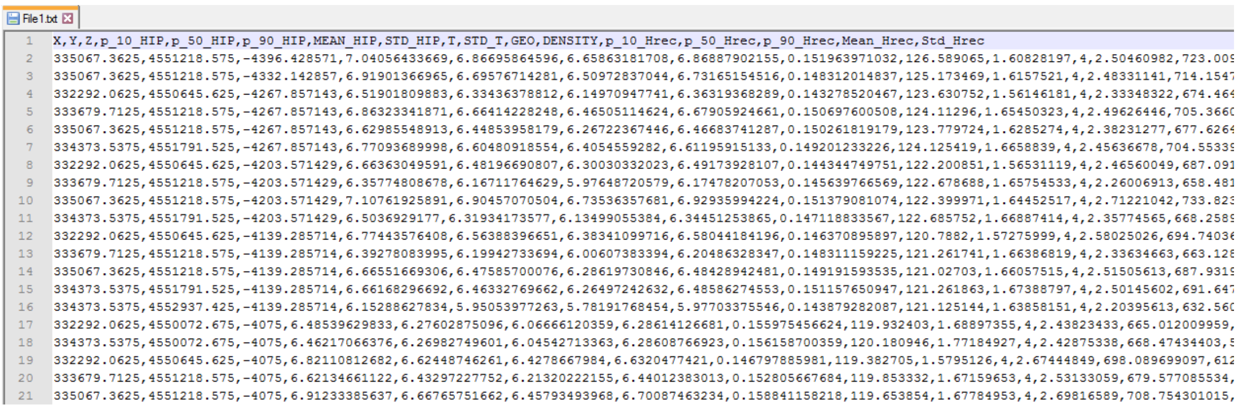


Fig. 8. 'Export results' tab view.




```
X,Y,Z,p_10_HIP,p_50_HIP,p_90_HIP,MEAN_HIP,STD_HIP,T,STD_T,GEO,DENSITY,p_10_Hrec,p_50_Hrec,p_90_Hrec,Mean_Hrec,Std_Hrec
335067.3625,4551218.575,-4396.428571,7.04056433669,6.86695864596,6.65863181708,6.86887902155,0.151963971032,126.589065,1.60828197,4,2.50460982,723.009
335067.3625,4551218.575,-4332.142857,6.91901366965,6.69576714281,6.50972837044,6.73165154516,0.148312014837,125.173469,1.6157521,4,2.48331141,714.1547
332292.0625,4550645.625,-4267.857143,6.51901809883,6.33436378812,6.14970947741,6.36319368289,0.143278520467,123.630752,1.56146181,4,2.33348322,674.464
333679.7125,4551218.575,-4267.857143,6.86323341871,6.66414228248,6.46505114624,6.67905924661,0.150697600508,124.11296,1.65450323,4,2.49626446,705.3660
335067.3625,4551218.575,-4267.857143,6.62985548913,6.44853958179,6.26722367446,6.46683741287,0.150261819179,123.779724,1.6285274,4,2.38231277,677.6264
334373.5375,4551791.525,-4267.857143,6.77093689998,6.60480918554,6.4054559282,6.61195915133,0.149201233226,124.125419,1.6658839,4,2.45636678,704.5533
332292.0625,4550645.625,-4203.571429,6.66363049591,6.48196690807,6.3003033202,6.49173928107,0.14434474975,122.200851,1.56531119,4,2.46560049,687.091
333679.7125,4551218.575,-4203.571429,6.35774808678,6.16711764629,5.97648720579,6.17478207053,0.145639766569,122.678688,1.65754533,4,2.26006913,658.481
335067.3625,4551218.575,-4203.571429,7.10761925891,6.90457070504,6.73536357681,6.92935994224,0.151379081074,122.399971,1.64452517,4,2.71221042,733.823
334373.5375,4551791.525,-4203.571429,6.5036929177,6.31934173577,6.13499055384,6.34451253865,0.147118833567,122.685752,1.66887414,4,2.35774565,668.2589
332292.0625,4550645.625,-4139.285714,6.77443576408,6.56388396651,6.38341099716,6.58044184196,0.146370895897,120.7882,1.57275999,4,2.58025026,694.7403
333679.7125,4551218.575,-4139.285714,6.39278083995,6.19942733694,6.00607383394,6.20486328347,0.148311159225,121.261741,1.66386819,4,2.33634663,663.128
335067.3625,4551218.575,-4139.285714,6.66551669306,6.47585700076,6.28619730846,6.48428942481,0.149191593535,121.02703,1.66057515,4,2.51505613,687.9319
334373.5375,4551791.525,-4139.285714,6.66168296692,6.46332769662,6.2649724263,6.48586274553,0.151157650947,121.261863,1.67388797,4,2.50145602,691.647
334373.5375,4552937.425,-4139.285714,6.15288627834,5.95053977263,5.78191768454,5.97703375546,0.143879282087,121.125144,1.63858151,4,2.20395613,632.560
332292.0625,4550072.675,-4075,6.48539629833,6.27602875096,6.06666120359,6.28614126681,0.155975456624,119.932403,1.68897355,4,2.43823433,665.012009959,
334373.5375,4550072.675,-4075,6.46217066376,6.26982749601,6.04542713363,6.28608766923,0.156158700359,120.180946,1.77184927,4,2.42875338,668.47434403,5
332292.0625,4550645.625,-4075,6.82110812682,6.62448746261,6.4278667984,6.6320477421,0.146797885981,119.382705,1.5795126,4,2.67444849,698.089699097,612
333679.7125,4551218.575,-4075,6.62134661122,6.43297227752,6.21320222155,6.44012383013,0.152805667684,119.853332,1.67159653,4,2.53133059,679.577085534,
335067.3625,4551218.575,-4075,6.91233385637,6.66765751662,6.45793493968,6.70087463234,0.158841158218,119.653854,1.67784953,4,2.69816589,708.754301015,
```

Fig. 9. File 1 (3D Model) views. The first row is the colheaders followed by all the model data. Depending on your initial data some field will be omitted or added (density or porosity) to this example.

File2.txt

```
X,Y,P10_HIP,P50_HIP,P90_HIP,P10_Hrec,P50_Hrec,P90_Hrec
326047.6375,4541478.425,3.92235654724,3.76958524368,3.58625967941,403.205217263,346.710686606,299.631911059
326047.6375,4542624.325,3.77219786427,3.59908408764,3.45482260711,383.944320401,339.714755844,286.639278376
326047.6375,4543770.225,3.81971052049,3.66382676982,3.50794301914,384.32478257,338.145486895,291.96619122
326741.4625,4540905.475,7.95114099271,7.64365391305,7.30646960632,809.197074624,707.758756111,615.400674819
326741.4625,4541478.425,4.1889440175,4.00711804269,3.82529206787,424.908491493,370.811962483,316.715433473
326741.4625,4542051.375,3.89087167387,3.71307110707,3.53527054027,401.012244011,347.442506872,293.872769733
326741.4625,4543770.225,4.04926591555,3.87213522018,3.72452630737,412.158202661,357.90817177,312.699812693
327435.2875,4541478.425,4.07603392697,3.90910078533,3.74216764369,411.269789093,359.375899925,317.86078859
327435.2875,4543197.275,4.22955213645,4.04625807831,3.86296402016,427.477583729,372.332636458,326.378513733
328129.1125,4540905.475,4.38542706139,4.18820298062,4.02384957998,440.313941657,387.929867976,335.545794294
328129.1125,4544916.125,4.14591345623,3.94578565464,3.77901248665,419.375555888,367.810358509,316.245161131
328822.9375,4543770.225,4.18790808833,3.98980742573,3.79170676313,429.415432271,372.069793577,314.724154883
328822.9375,4544916.125,11.7763090159,11.2704497904,10.7350234643,1194.97378195,1051.62050296,908.206874841
328822.9375,4546062.025,13.364955094,12.8488908974,12.3311917148,1363.78003991,1197.74639077,1034.03926965
328822.9375,4547780.875,8.8713713489,8.56981897384,8.2431714871,911.139879422,801.642137325,691.023379382
328822.9375,4548353.825,8.83540541076,8.52379955477,8.21219369879,904.559772393,793.274869194,681.725645416
328822.9375,4548926.775,41.9251668948,40.5376447479,39.259998186,4300.25728404,3771.11331909,3268.68637043
329516.7625,4541478.425,4.75568306752,4.57814054582,4.36508951979,483.344813696,428.189332118,362.002754224
329516.7625,4542624.325,4.45981506821,4.25615960667,4.05250414514,452.890060434,393.941706036,344.818077372
329516.7625,4546634.975,23.1942828454,22.3063681355,21.423750739,2367.44988768,2062.82568034,1780.67845007
```

Fig. 10. File 2 (2D Model) views. The first row is the colheaders followed by all the model data.

```
------------------
SIMULATION REPORT
------------------

3DHIP-CALCULATOR Version 1.1.
Decembrer 2020


1. LOAD DATA (GEOLOGICAL AND THERMAL MODELS)
Input Geological Model: D:\APP\APP_TOT\geological_model.vox
Input Thermal Model: D:\APP\APP_TOT\thermal_model.vox

2.HEAT-IN-PLACE SIMULATION PARAMETERS
Heat-In-Place simulation number: 1000
Target numerical code: 5
Target name: CRETACEOUS
CELL VOLUME [m3]
Delta X [m]: 693.83
Delta Y [m]: 572.95
Delta Z [m]:  64.28

3. DEPTH RANGE SELECTION
Depth range between -2000.00 m and -3000.00 m

4. PETROPHYSICAL PROPERTIES AND OTHER PARAMETERS
HEAT-IN-PLACE VALUES
The Porosity follows a Normal Ditribution
Mean:   0.20
Standard deviation:   0.01
The Rock Density [g/cm3] is already in the geological model
The Fluid Density [kg/m3] follows a Normal Ditribution
Mean: 1020.00
Standard deviation:   5.00
The Fluid Specific Heat Capacity [kJ/kg·°C] follows a Normal Ditribution
Mean:   4.80
Standard deviation:   0.10
The Rock Specific Heat Capacity [kJ/kg·°C] follows a Normal Ditribution
Mean:   0.90
Standard deviation:   0.01
Reinjection Temperature [°C]:  30.00
RECOVERABLE HEAT
The Recovery Factor follows a Normal Ditribution
Mean:   0.10
Standard deviation:   0.01
Plant Factor:   0.95
The Mean Plant Lifetime [Years]:  30.00
Conversion Efficiency:   0.85

HEAT-IN-PLACE RESULTS
The Heat-In-Place results of CRETACEOUS between -2000.00 m and -3000.00 m are:
P90 [PJ]: 9867.88
P50 [PJ]: 10046.07
P10 [PJ]: 10253.97

5. EXPORT FILES
Output File 1: D:\APP\APP_TOT\output files\1.txt
Output File 2: D:\APP\APP_TOT\output files\2.txt
Report File: D:\APP\APP_TOT\output files\re.txt
```

Fig. 11. Reports file views. Depending on your initial data and your preferences during the simulation the report will change.

4 Example of application

The software can be used in different situations and contexts, depending on the data availability. The optimal scenario is when there is a 3D geological model available, including the distribution of petrophysical parameters (e.g. density, porosity, etc) in conjunction with a 3D geothermal model (with the distribution of temperature according to depth). On the contrary, the worst scenario would be when the user only has a 3D geological model and has to infer the rest of the parameters.

This section shows an example of a model based on data from a Neogene basin in the NE of Spain (Herms et al., 2020). According to previous works, the study area has a high potential for deep geothermal project development corresponding to deep hot sedimentary aquifers (Colmenar-Santos et al., 2016). The assessment of deep geothermal resources is achieved by combining 3D geological modelling techniques and stochastic approaches. First, a 3D implicit geological model was built using a litho-constrained stochastic geophysical inversion approach integrated in the software 3DGeoModeller (BRGM, Intrepid-Geophysics). Gravity and magnetic anomalies were used to validate the model. Secondly, a 3D steady state, conductive heat flow was developed to estimate the probable temperature distribution in the whole domain of a fractured deep hot sedimentary aquifer. Heat uncertainties in the basin were modelled using a stochastic approach. Fig. 12 and 13 show the exported 3D geological and thermal voxel-based model data in text format directly obtained from the 3DGeoModeller software. The following variables can be identified in the geological model file:

- ‘X’, ‘Y’ coordinates (in UTM) and ‘Z’ (elevation in meters above sea level [m a. s. l.])
- ‘Lithology’ (characterized by an ID number)
- ‘FixedCell’
- ‘Density’ (in g/cm^3) and magnetic ‘Susceptibility’ (SI units) (*)

(*) The parameters ‘FixedCell’ and ‘Susceptibility’ will not be used for the HIP calculations.

The file can be uploaded successfully to the application as soon as it follows the rules specified in section 4.2.1. (in this case the file extension is *.vox). The first line will not be considered, nor the ‘FixedCell’ and ‘Susceptibility’ columns. The column order does not matter.

geological_model.vox | thermal_model.vox

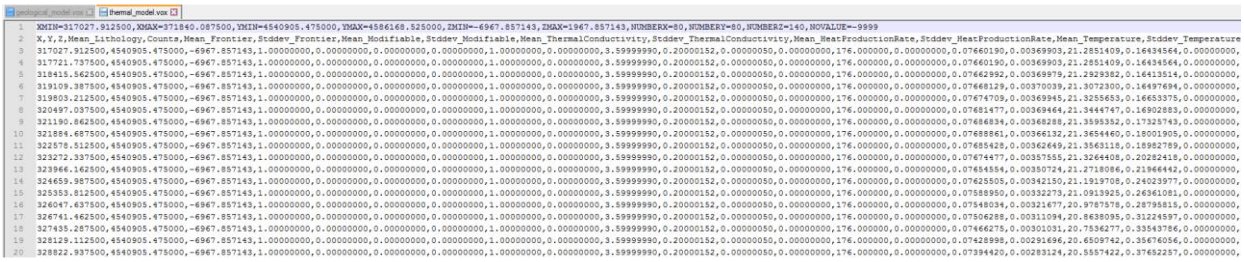
```
XMIN=317027.912500,XMAX=371840.087500,YMIN=4540905.475000,YMAX=4586168.525000,ZMIN=-6967.857143,ZMAX=1967.857143,NUMBERX=80,NUMBERY=80,NUMBERZ=140,NOVALUE=-9999
X,Y,Z,Lithology,FixedCell,Density,Susceptibility
317027.912500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.90372729,0.00028360
317721.737500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.99401951,0.00027906
318415.562500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
319109.387500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.75085640,0.00027336
319803.212500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.97321415,0.00028561
320497.037500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.65498686,0.00028540
321190.862500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
321884.687500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
322578.512500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
323272.337500,4540905.475000,-6967.857143,1.00000000,0.00000000,3.02299905,0.00034152
323966.162500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.62638068,0.00028564
324659.987500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.81234837,0.00027095
325353.812500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.84889984,0.00026874
326047.637500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.70650077,0.00029692
326741.462500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
327435.287500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.92430830,0.00026711
328129.112500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.53909373,0.00024504
328822.937500,4540905.475000,-6967.857143,1.00000000,0.00000000,2.68000007,0.00028000
```

Fig. 12. A 3D voxel-based geological model in text format from the software 3DGeoModeller.

The following variables (among others) can be used for the thermal model file:

- X Y coordinates in UTM and Z (elevation in m a.s.l.)
- Mean_Lithology (characterized by an ID number)
- Mean_Temperature (ºC)
- Stddev_Temperature (standard deviation)

Please note that the column order does not matter. Also note that the spatial position has to be the same between the geological and thermal models (e.g. the coordinates of line 3 are the same for both the geological and thermal models and so on). This is mandatory to correctly run the calculations.




```
XMIN=317027.912500,XMAX=371840.087500,YMIN=4540905.475000,YMAX=4586168.525000,ZMIN=-6967.857143,ZMAX=1967.857143,NUMBERX=80,NUMBERY=80,NUMBERZ=140,NOVALUE=-9999
X,Y,Z,Mean_Lithology,Counts,Mean_Frontier,Stddev_Frontier,Mean_Modifiable,Stddev_Modifiable,Mean_ThermalConductivity,Stddev_ThermalConductivity,Mean_HeatProductionRate,Stddev_HeatProductionRate,Mean_Temperature,Stddev_Temperature
317027.912500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07660190,0.00369903,21.2851409,0.16434564,0.00000000,
317721.737500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07660190,0.00369903,21.2851409,0.16434564,0.00000000,
318415.562500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07662992,0.00369979,21.2929382,0.16413514,0.00000000,
319109.387500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07668129,0.00370039,21.3072300,0.16497694,0.00000000,
319803.212500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07674709,0.00369945,21.3255653,0.16653375,0.00000000,
320497.037500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07681477,0.00369464,21.3444747,0.16902883,0.00000000,
321190.862500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07686834,0.00368288,21.3595352,0.17325743,0.00000000,
321884.687500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07688861,0.00366132,21.3654460,0.18001905,0.00000000,
322578.512500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07685428,0.00362649,21.3563118,0.18982789,0.00000000,
323272.337500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07674477,0.00357555,21.3264408,0.20282418,0.00000000,
323966.162500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07654554,0.00350724,21.2718086,0.21966442,0.00000000,
324659.987500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07625505,0.00342150,21.1919708,0.24023977,0.00000000,
325353.812500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07588950,0.00332273,21.0913925,0.26361081,0.00000000,
326047.637500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07548034,0.00321677,20.9787578,0.28795815,0.00000000,
326741.462500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07506288,0.00311094,20.8638095,0.31224597,0.00000000,
327435.287500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07466275,0.00301031,20.7536277,0.33543786,0.00000000,
328129.112500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07428998,0.00291696,20.6509742,0.35676056,0.00000000,
328822.937500,4540905.475000,-6967.857143,1.00000000,0.00000000,0.00000000,0.00000000,1.00000000,0.00000000,3.59999990,0.20000152,0.00000050,0.00000000,176.000000,0.00000000,0.07394420,0.00283124,20.5557422,0.37652257,0.00000000,
```

Fig. 13. A 3D voxel-based thermal model in text format from the software 3DGeoModeller.

Once the input files have been uploaded just open the application and fill the fields of the ‘Geological and thermal models’ tab. In this case, the headers are:

- ‘X’, ‘Y’ and ‘Z’ for the X and Y coordinates and elevation, respectively.
- ‘Lithology’ for the geology.
- ‘Density’ for the rock density (the box *“Select if your Geological model has density values”* must be selected in this example because the model has density values for each cell).
- ‘Mean_Temperature’ for Temperature.
- ‘Stddev_Temperature’ for Standard deviation of temperature.

In this example, the following options are considered: a total of 10,000 simulations (the default value is 1,000 so you should change it to 10,000 for the current example); the target ID is 4 (corresponding to Triassic); the cell dimensions are 693.825m for X, 572.950m for Y and 64.285m for Z. After filling the values click on “Run (1. & 2.)”.

Afterwards, the selected depth range for calculations must be fixed. In this case the selected values are -1,500m a.s.l (value considered to set the minimum depth to calculate the geothermal potential) and lowest depth (which is -4396.43m, this value will appear in the report file). At the end click on “Run (3.)” (Fig. 14).

Once the lithology and depth range are selected, we can look at the ‘Geothermal reservoir maps and T histogram’ tab (Fig. 15) and continue to the next step, which is the HIP calculation of the tab ‘Petrophysical properties and HIP distribution’.

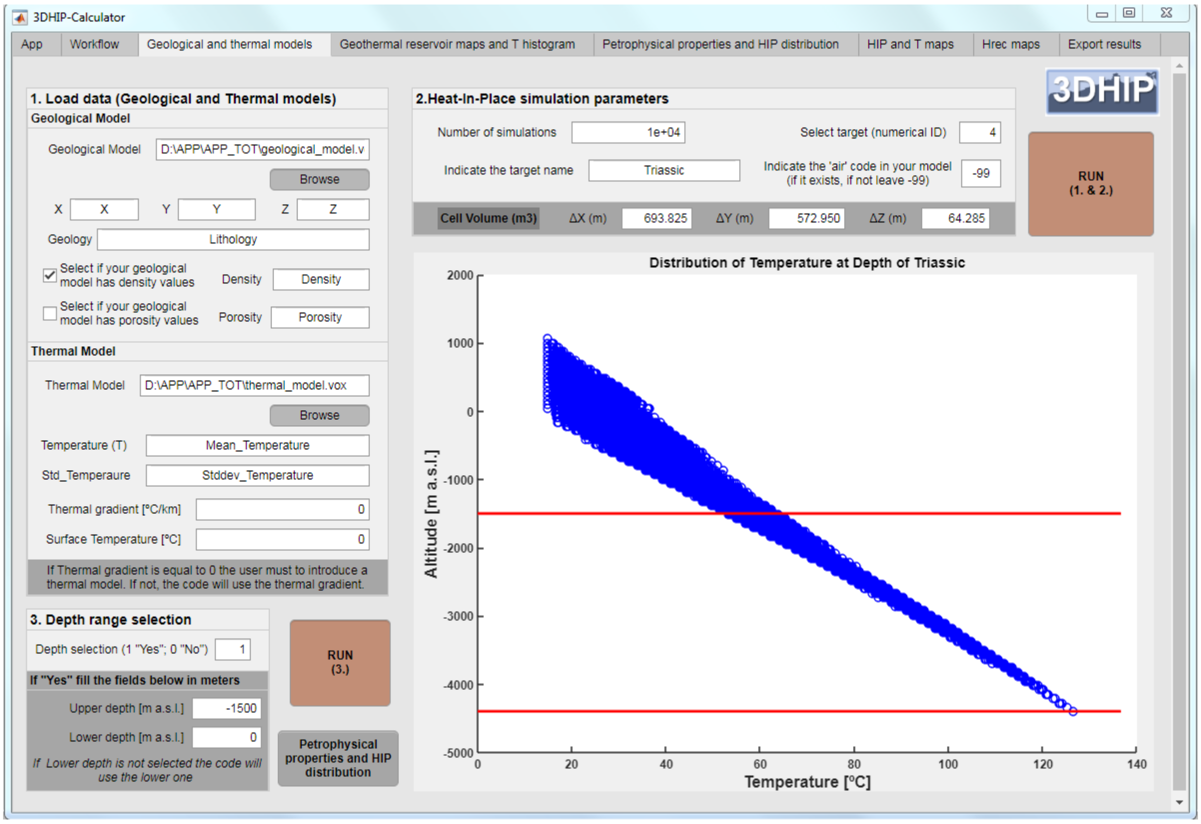


Fig. 14. 'Geological and thermal models' tab for the example.

In the 'Petrophysical properties and HIP distribution' tab, the user must introduce all the variables and select the desired PDF distribution for each one. As this model already has density values, a message will pop up to remind the user that the stochastic values will not be used for this parameter.

By clicking on "Run (4.)" the HIP and Hrec calculations will be performed, showing the cumulated probability curve on this tab (Fig. 16), HIP in the 'HIP and T maps' tab (Fig. 17) and Hrec results in the 'Hrec maps' tab (Fig. 18).

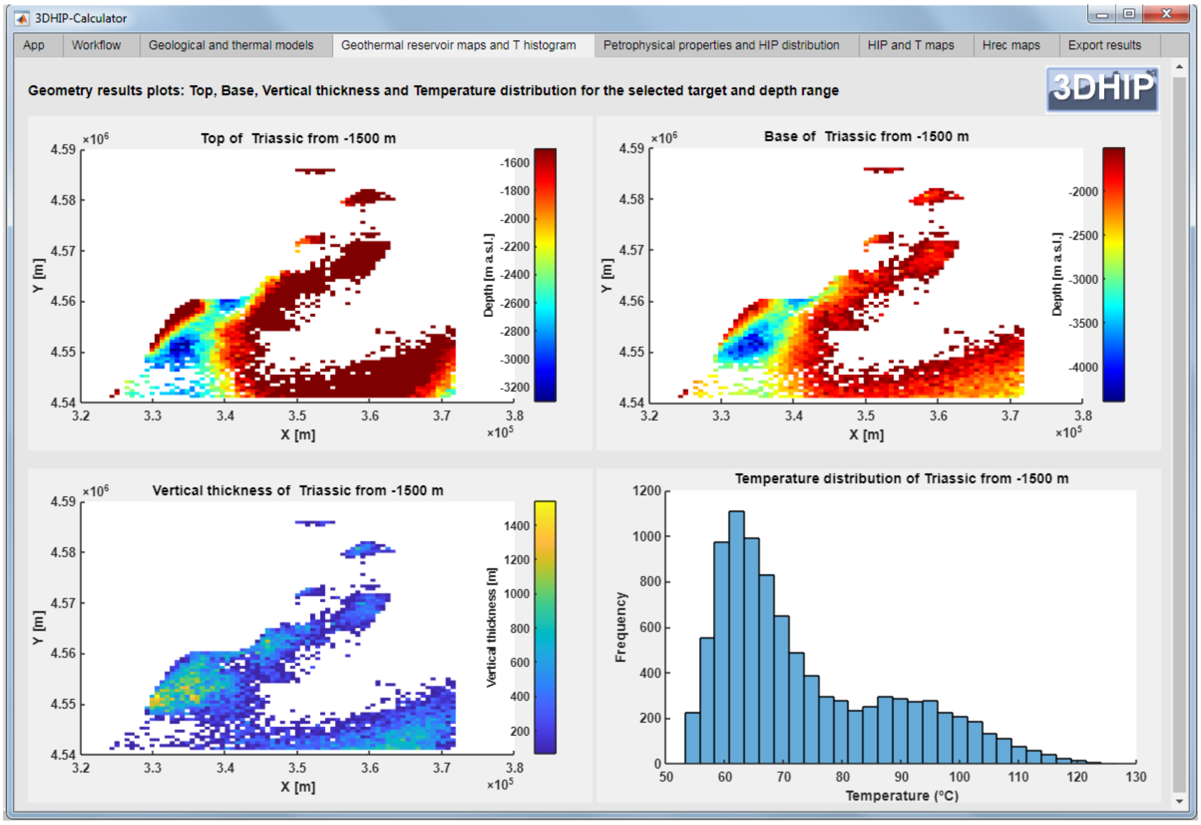


Fig. 15. 'Geothermal reservoir maps and T histogram' tab for the example.

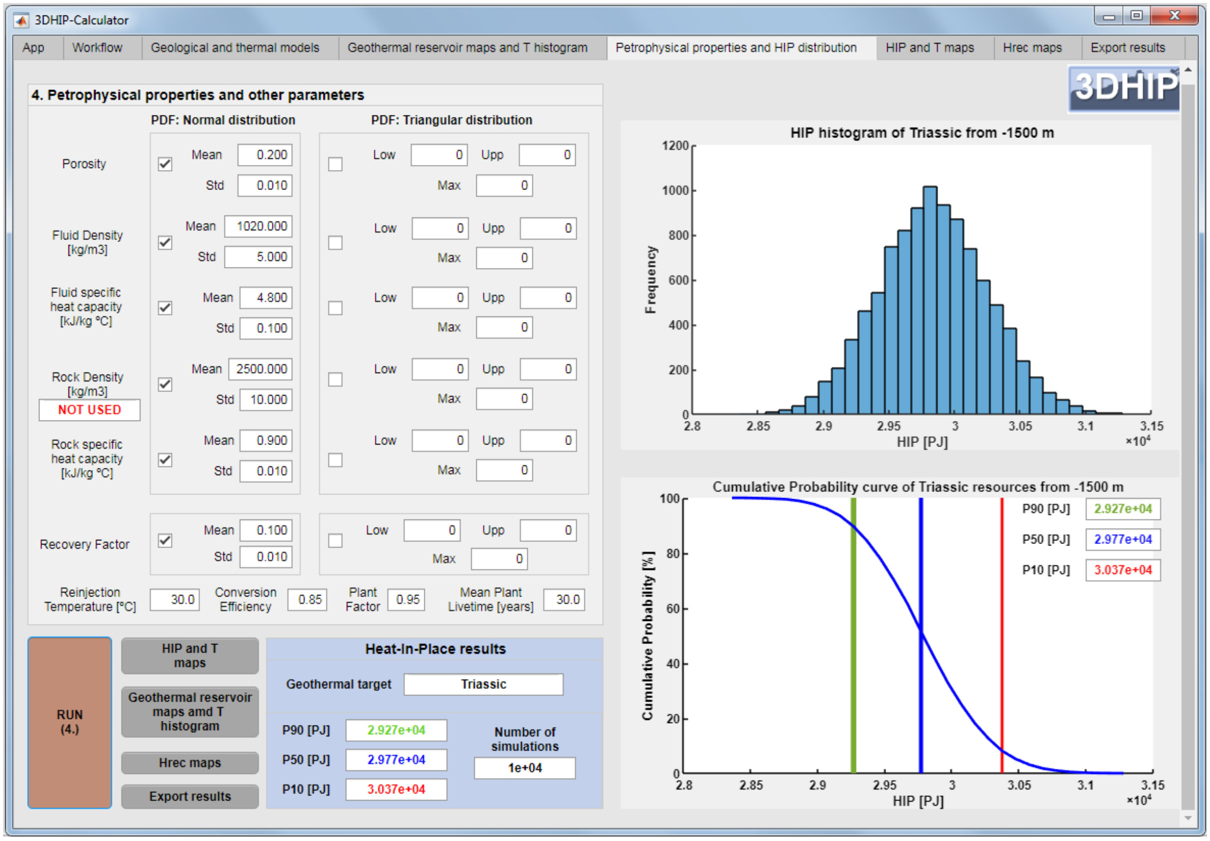


Fig. 16. 'Petrophysical properties and HIP distribution' tab for the example.

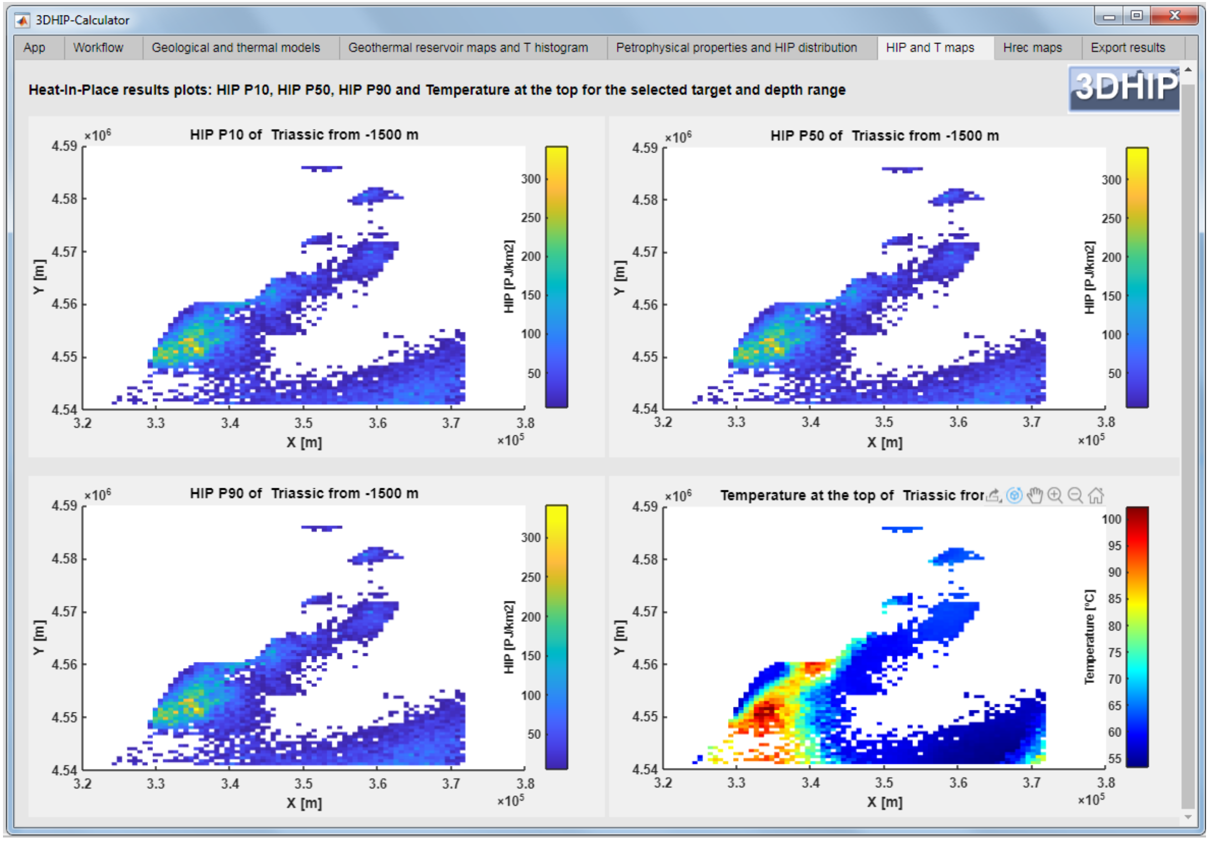


Fig. 17. 'HIP and T maps' tab for the example.

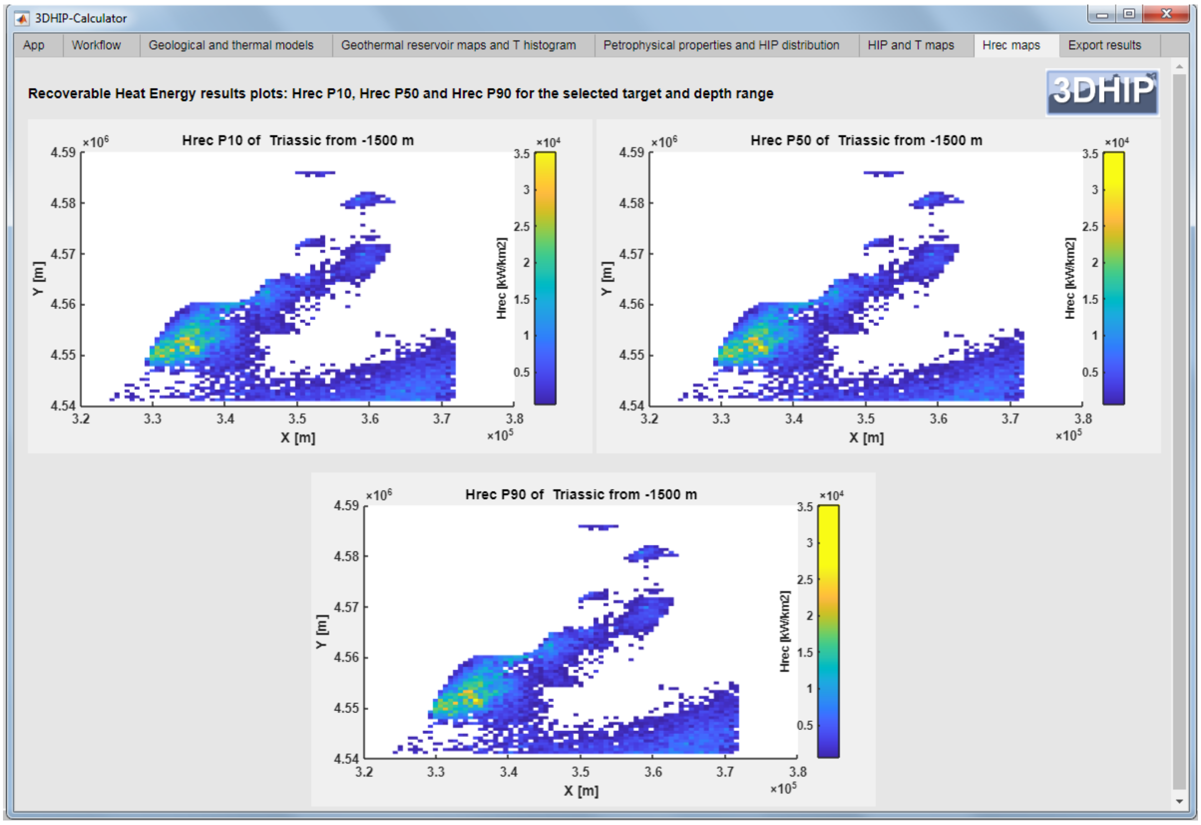


Fig. 18. 'Hrec maps' tab for the example.

After looking at the results, the user can go to the last tab ‘Export results’. Remember that all the plots can be saved or copied directly by the icons which appear when the user passes the mouse on their right top corner. Here we define the names for the export data files (Fig. 19) and click on the “Run (5.)” button. As example, the content of the results summary report file named “Report_Triassic.txt” is shown in the Fig. 20.

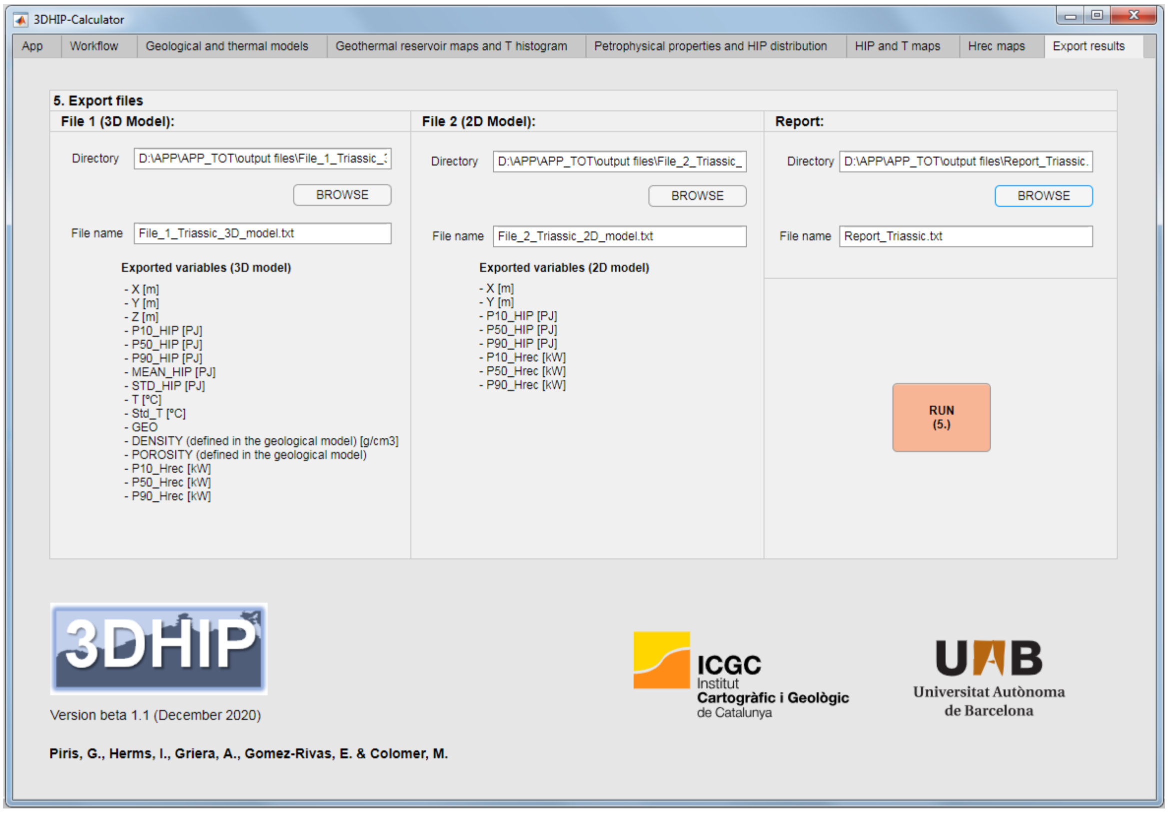


Fig. 19. ‘Export results’ tab for the example.

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SIMULATION REPORT
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3DHIP-CALCULATOR Version 1.1.
December 2020


1. LOAD DATA (GEOLOGICAL AND THERMAL MODELS)
Input Geological Model: D:\APP\APP_TOT\geological_model.vox
Input Thermal Model: D:\APP\APP_TOT\thermal_model.vox

2.HEAT-IN-PLACE SIMULATION PARAMETERS
Heat-In-Place simulation number: 10000
Target numerical code: 4
Target name: Triassic
CELL VOLUME [m3]
Delta X [m]: 693.83
Delta Y [m]: 572.95
Delta Z [m]:  64.28

3. DEPTH RANGE SELECTION
Depth range from -1500.00 m to -4396.43 m

4. PETROPHYSICAL PROPERTIES AND OTHER PARAMETERS
HEAT-IN-PLACE VALUES
The Porosity follows a Normal Ditribution
Mean:   0.20
Standard deviation:   0.01
The Rock Density [g/cm3] is already in the geological model
The Fluid Density [kg/m3] follows a Normal Ditribution
Mean: 1020.00
Standard deviation:   5.00
The Fluid Specific Heat Capacity [kJ/kg·°C] follows a Normal Ditribution
Mean:   4.80
Standard deviation:   0.10
The Rock Specific Heat Capacity [kJ/kg·°C] follows a Normal Ditribution
Mean:   0.90
Standard deviation:   0.01
Reinjection Temperature [°C]:  30.00
RECOVERABLE HEAT
The Recovery Factor follows a Normal Ditribution
Mean:   0.10
Standard deviation:   0.01
Plant Factor:   0.95
The Mean Plant Lifetime [Years]:  30.00
Conversion Efficiency:   0.85

HEAT-IN-PLACE RESULTS
The Heat-In-Place results of Triassic between -1500.00 m and -4396.43 m are:
P90 [PJ]: 29265.69
P50 [PJ]: 29769.21
P10 [PJ]: 30373.42

5. EXPORT FILES
Output File 1: D:\APP\APP_TOT\output files\File_1_Triassic_3D_model.txt
Output File 2: D:\APP\APP_TOT\output files\File_2_Triassic_2D_model.txt
Report File: D:\APP\APP_TOT\output files\Report_Triassic.txt
```

Fig. 20. Report file for the example case.

Exporting the 3D and 2D model results will allow the user to carry out additional post-processing using other software packages or to prepare 2D maps using Geographic Information Systems (GIS) software.

For the extreme case in which the user can only provide the geological model as an input (Fig. 12) (without petrophysical properties or a geothermal model) the calculations can carried out assuming mean values for the area and geological units. For this example, the regional geothermal gradient is about 25ºC/km, the mean annual surface temperature is 10ºC and the Triassic formation density follows a triangular distribution with a lower value of 2400 kg/m^3, a most probable value of 2500kg/m^3 and an upper value of 2560 kg/m^3.

For this case, the geological model is uploaded as in the previous example, but the *"Select if your Geological model has density values"* box must be left unselected. In the thermal model panel, the "Thermal model" field is also left empty. The fields "Temperature (*T*)" and "Std_Temperature" are left as default (*). The geothermal gradient and surface temperature are filled with the 25ºC/km and 10ºC respectively.

Now in the Heat-In-Place parameters in block 2, the simulation number has been changed to 10,000; the target ID is 4 (corresponding to the Triassic, which is introduced in the target name); the cell dimensions are defined as 693.825m for X, 572.950m for Y and 64.285m for Z. Now one has to provide the ID corresponding to the 'air' or above surface formation, which in this case is 0 (this way the application knows the topography and can calculate the depth (*Dz*) for each target cell). After all the fields are filled and clicking on the "Run (1. & 2.)" button the Eq.(3) will be used to estimate the target temperatures according to the Depth range selection of block 3, where the depth range was selected between -1500m a.s.l. and the lower target depth, as in the previous example (Fig. 21).

As in the previous example, after pressing the "Run (3.)" button the red lines indicate the selected depth range and results are displayed at the "Geothermal reservoir maps and T histogram" tab (Fig. 22). Note that *Dz* is only used to estimate the temperature, not to modify the depth coordinates.

In the tab 'Petrophysical properties and HIP distribution', we must introduce all the variables and select the desired PDF distribution for each one, now introducing the density values as a triangular PDF. By clicking on "Run (4.)" the HIP and Hrec calculations are performed, showing the cumulated probability curve on this tab (Fig. 23). From here until the end of the post-processing the steps that the user should follow are similar to those of the previous example. The inputs used in the current simulation (i.e. thermal gradient, surface temperature, used values, results, etc.) are summarised in the exported report.

*Here, the headers corresponding to the Temperature (T) and Std_Temperature fields have not meaning at all. However, they will be used internally to create the temperature values from Eq. (3). When a thermal gradient is used the temperature standard deviation for each cell is 0 and the HIP calculation is performed having the cell temperature as a fixed value.

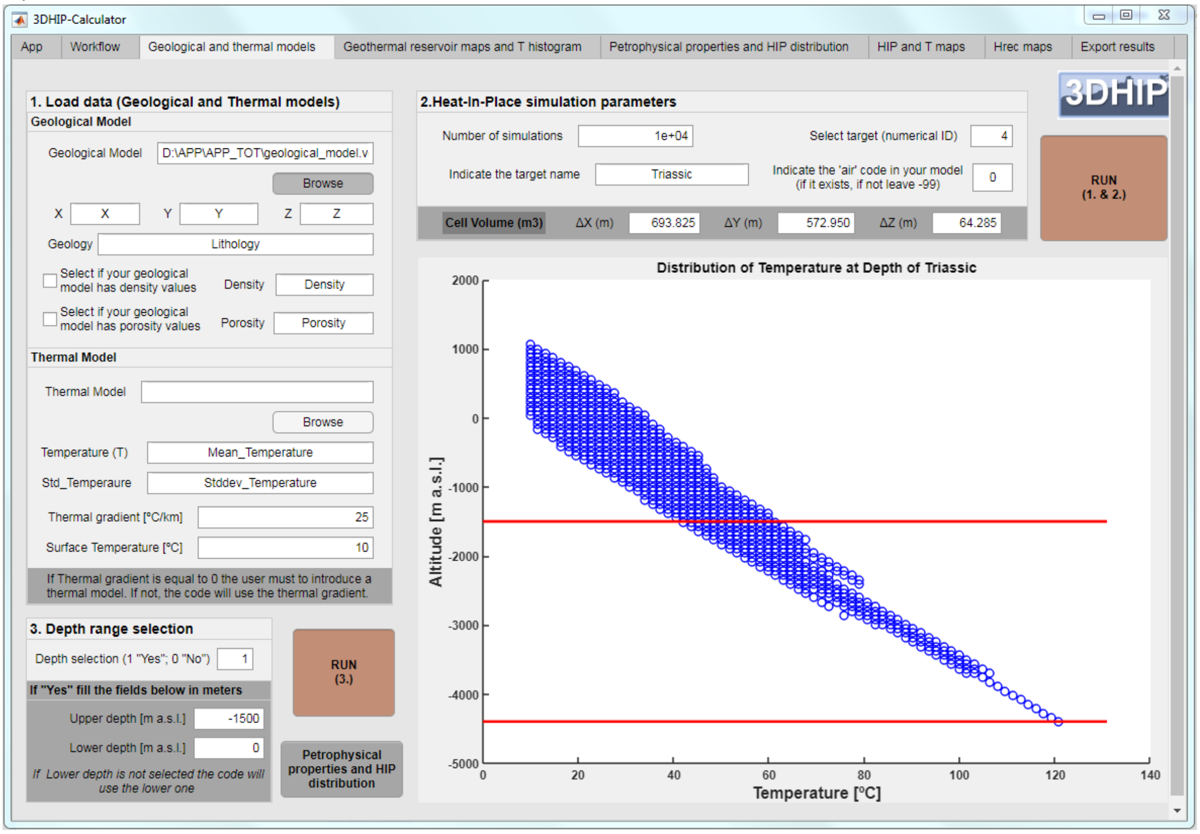

Fig. 21. Geological and thermal models' tab for the example with no thermal model.

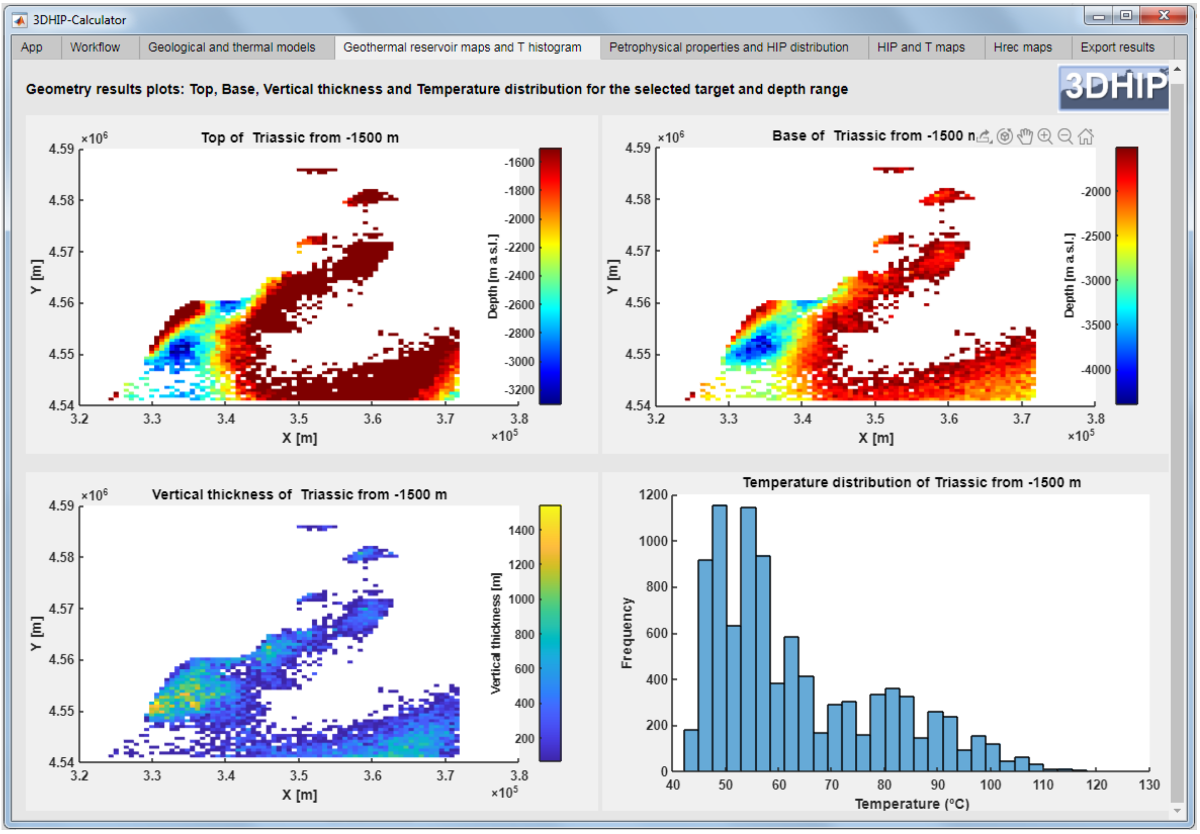

Fig. 22. 'Geothermal reservoir maps and T histogram' tab for the example with no thermal model.

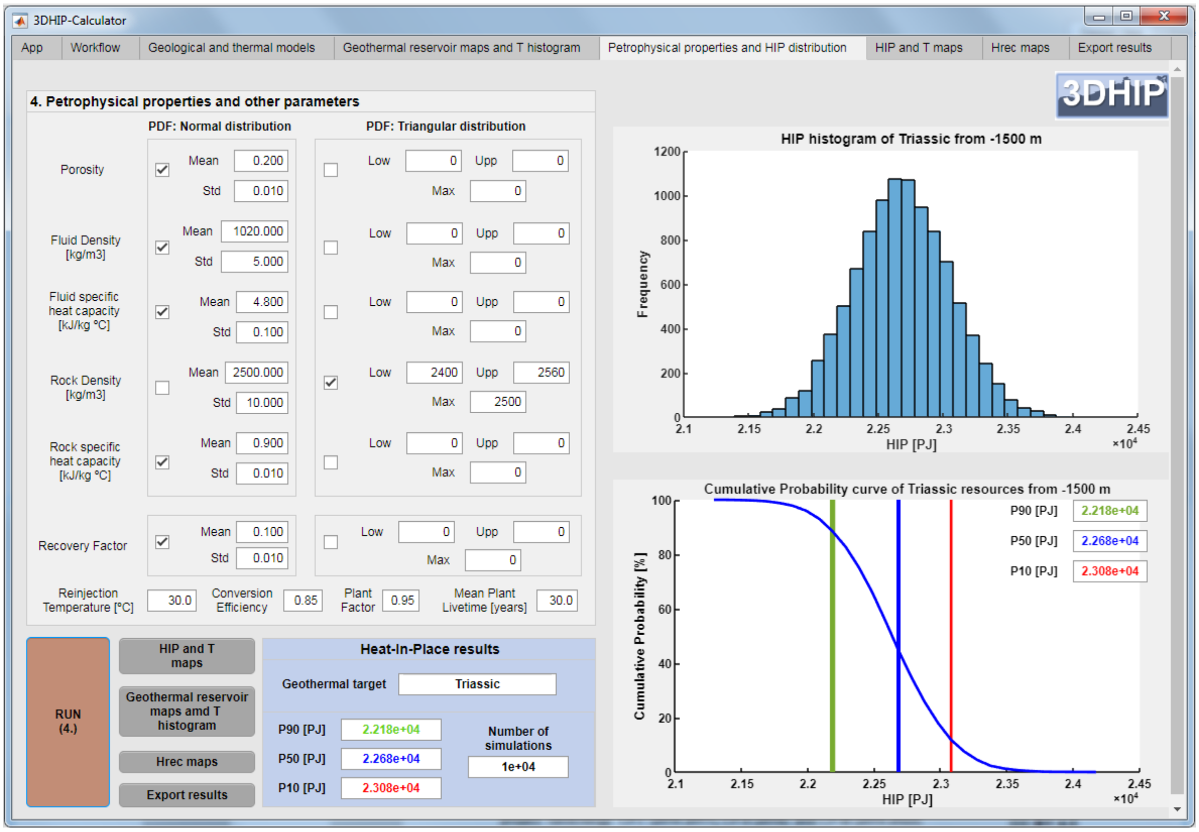

Fig. 23. 'Petrophysical properties and HIP distribution' tab for the example with no thermal model.

5 Preparing 2D maps with desktop GIS software

The **3DHIP-Calculator** was built with the necessary functionalities: 1) to calculate the geothermal potential from 3D geological and thermal models considering the uncertainty of the parameters, and 2) to show the results in different plots (histograms and cumulative probability functions) and 2D maps.

As shown in Figs. 17 and 18, the HIP and Hrec results are expressed in 2D format. These results can be directly exported to GIS software as a dataset of points in order to afterwards create a friendlier or sophisticated 2D raster map representing the HIP or Hrec distribution, combined with topographic or other reference maps.

This step, which is normally straightforward, could slightly change if the distance between X and Y nodes is not the same, i.e. if the resulting raster file does not have square cells.

<u>How to create a non-square raster model from the 3DHIP-Calculator outputs</u>

In order to prepare proper maps, this chapter shows how to create non-square and square cell raster models from the **3DHIP-Calculator** results step-by-step. The example uses the 'File 2' (2D Model) and the open-source software QGIS Desktop 3.4.1. https://www.qgis.org/en/site/).

1) In QGIS import the file 'File2Dmodel.txt' of 2D values provided by 3DHIP-Calculator. Use the option '*Add a delimited text file'* from the '*Layer'* menu (Fig. 24).

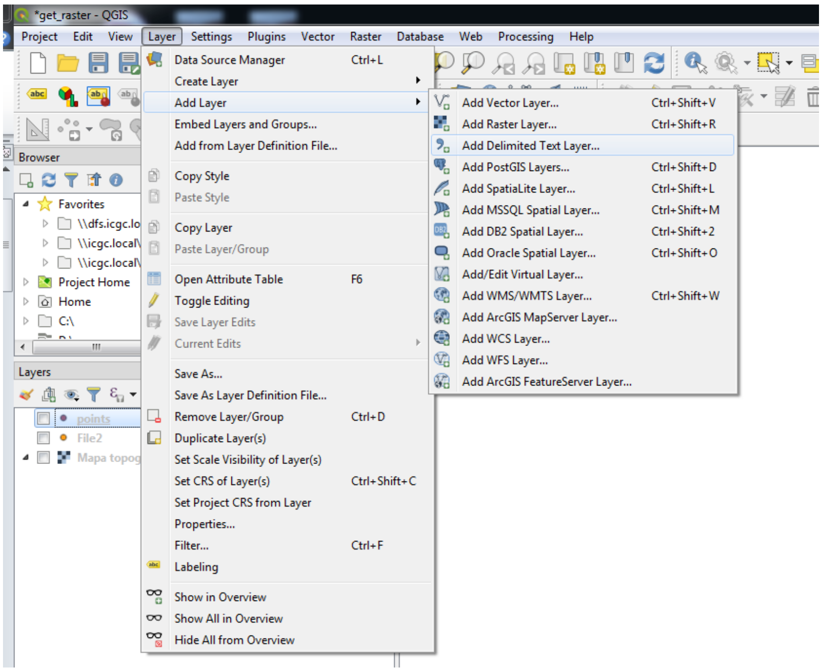

Fig. 24. Import the output data file generated by the 3DHIP-Calculator *using the option 'Add a delimited text file' from the 'Layer' menu.*

2) Fill in all the required parameters. These include the type of format (this case is *.csv), if there is a headline to discard or not, the fields for the X and Y coordinates and the coordinate reference system (CRS) (Fig. 25).

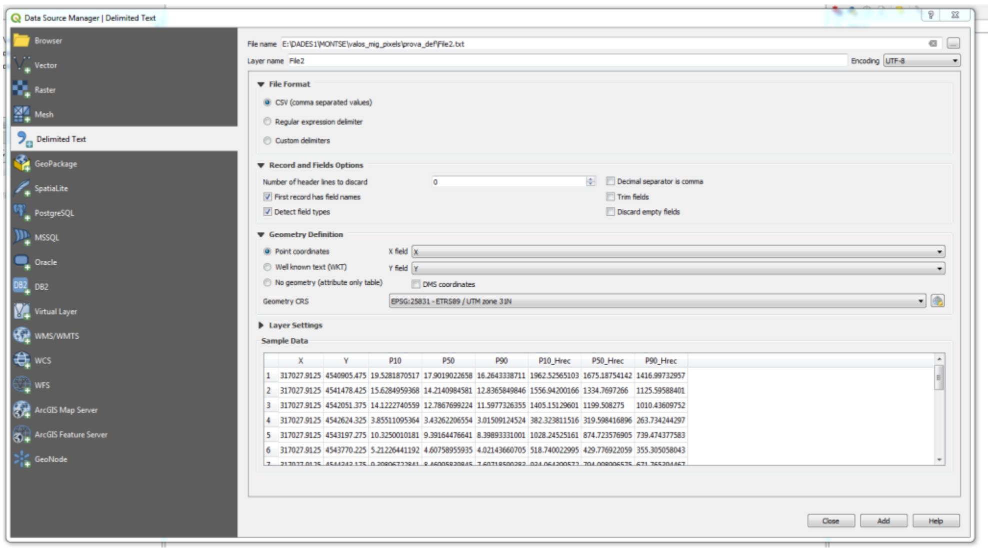

Fig. 25. Pop-up window where the import parameters are defined.

3) At this moment, the user can already see the point layer, but it is still a txt file. The user must convert it to ESRI Shape File format. Click on the right button of the submenu 'Export\ Save Features As…' (Fig. 26).

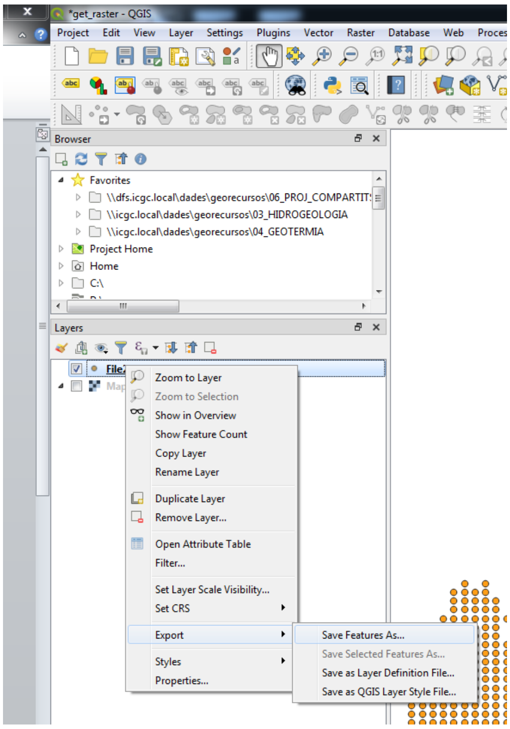

Fig. 26. Access to the pop-up window 'Save Features As…' to convert the format file.

4) Select ‘ESRI shapefile format’ and provide all the parameters of the new layer: CRS, the type of geometry (type point) and the file name (in this case, saved as ‘points.shp’) (Fig. 27). Click on ‘ok’ and a new file named ‘points.shp’ will appear in the Layers window.

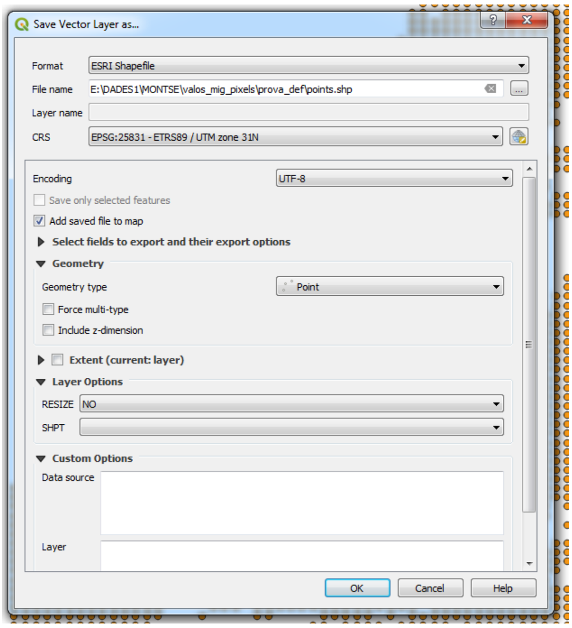

Fig. 27. Pop-up window ‘Save Features As…’.

5) Convert feature file to raster with the ‘Rasterize’ GDAL-tool from vector to raster format. To access to this geoprocessing tool, click on the menu Raster/Conversion (Fig. 28).

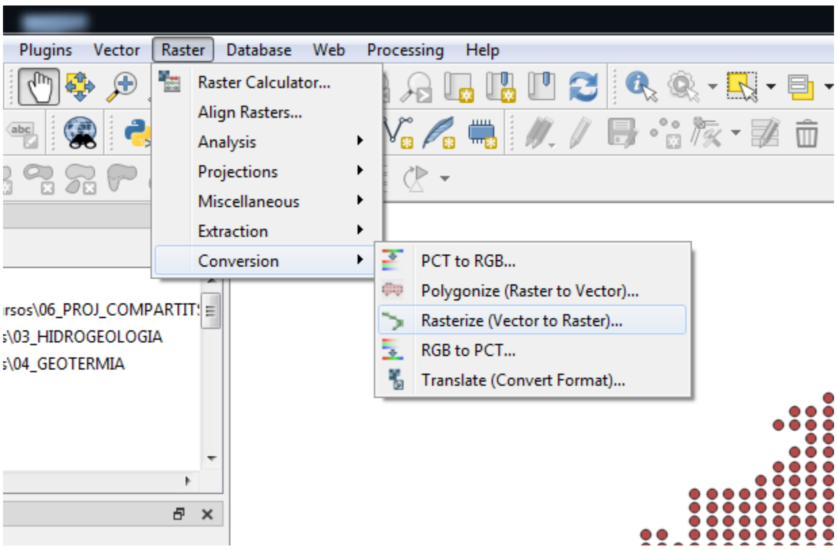

Fig. 28. Access to the geoprocessing tool ‘Rasterize’.

6) In this pop-up window, you will have to select all the following parameters:
   a) Input file: points.shp

b) Select the field to represent: P90_HIP (in this case)
c) Width/Horizontal resolution: the number of pixels in the X-direction (if you choose output raster size units as pixels) or the cell size in the X- direction (if you choose output raster size units as georeferenced units). In this example, georeferenced units and the value of 693.825 meters were taken (this value needs to coincide with the X resolution of the original 3D model).
d) Height/Vertical resolution: number of pixels in the Y-direction (if the users choses output raster size units as pixels) or the cell size in the Y- direction (the user choses output raster size units as georeferenced units). In this example 572.95 meters were used (this value needs to coincide with the X resolution in the original 3D model).
e) Set the georeferenced extent: xmin, xmax, ymin, ymax. Values to input are the coordinates of the model boundaries minus the size of half a cell, in case of the minimum values, and the coordinates of the model boundaries plus the size of half a cell, in case of the maximum ones. The following table shows the final values for this example:

	xmin	**xmax**	**ymin**	**ymax**
Extremities of model	317027.91	371840.09	4540905.48	4586168.53
cell size	693.83		572.95	
Half-cell size	346.91		286.48	
values to input	316681.00	372187.00	4540619.00	4586455.00

Table 2. Coordinates and values taken for this example.

f) Assign a specified nodata value to output bands. The value of '-99' is taken in this example (during the raster creation the user is free to assign the desired value to the nodata cells).

The result is a raster file with values of pixels according to the values of original points (Fig. 29). Remember that the exported HIP and Hrec values are in [PJ] if the user shows a map. If their idea is to represent the HIP or Hrec by surface unit they must divide the value by the cell surface.

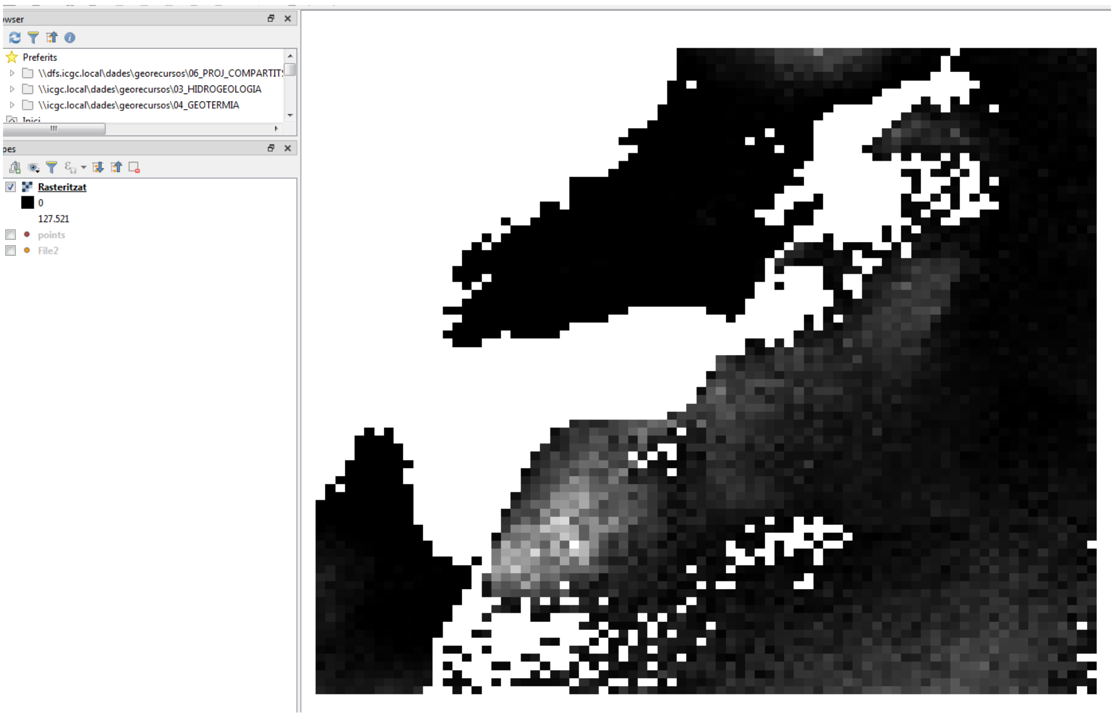

Fig. 29. Raster file obtained

7) Finally, by selecting the appropriate properties and a background map, you will obtain the visual outputs. Just do right-click on ‘Properties’ and select the most suitable representation (colour scale, transparency…) (Fig. 30).

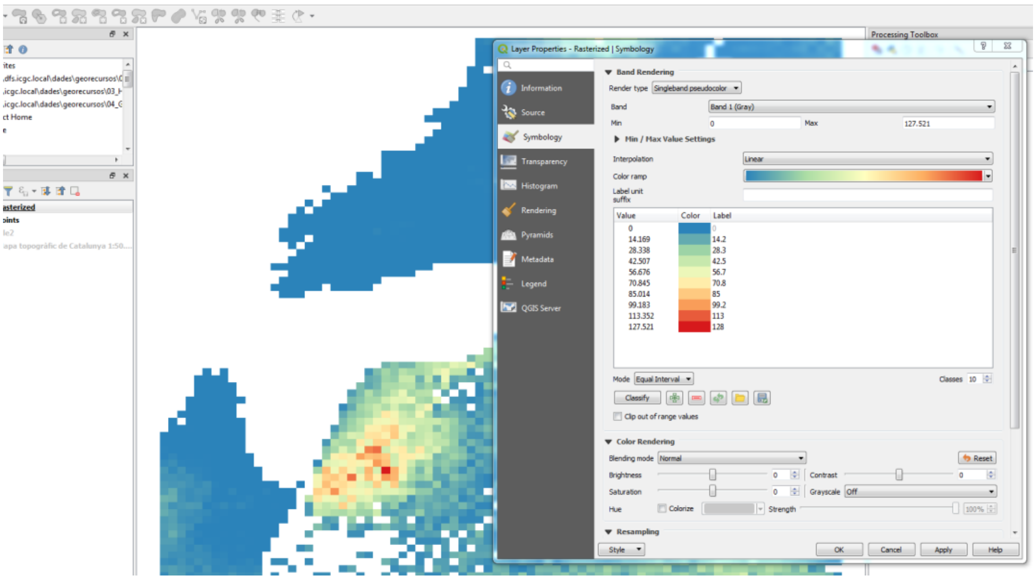

Fig. 30. Properties pop-up window to choose the symbology of the raster file.

8) In order to get a good layout, add a reference background map. For example, choose a WMS map in the option ‘Add a WMS/WMTS file’ of the ‘Layer’ menu and get an available WMS map from a mapping service (Fig. 31).

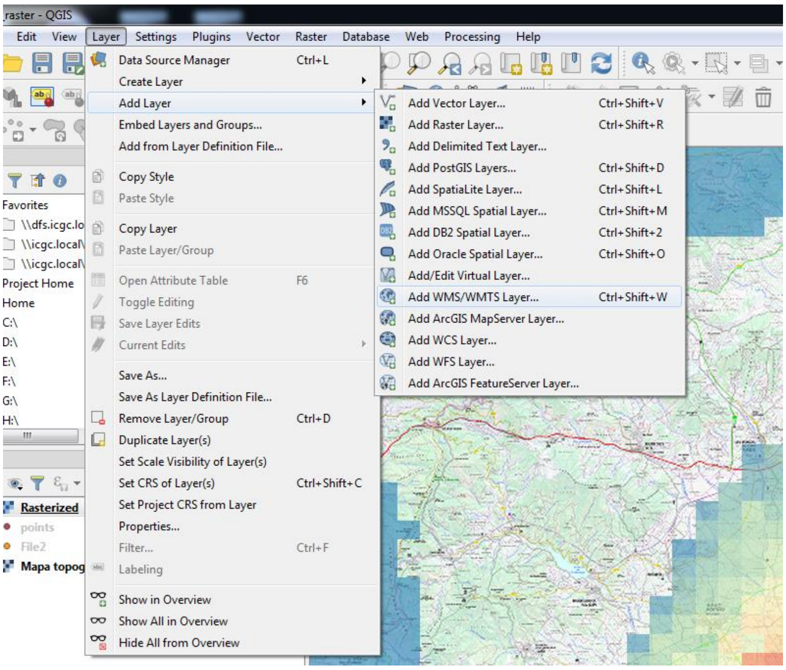

Fig. 31. Import a background map using the submenu 'Add a WMS/WMTS file' from the 'Layer' menu.

9) Moreover, the user can export this raster to different formats by clicking on the right button of the submenu 'Export\ Save As…'. If the user choses 'Raw data' the original data of the raster will be obtained. For an only coloured image, choose 'Rendered image'. The following parameters will allow to choose the format file, extension, and other parameters (Fig. 32).

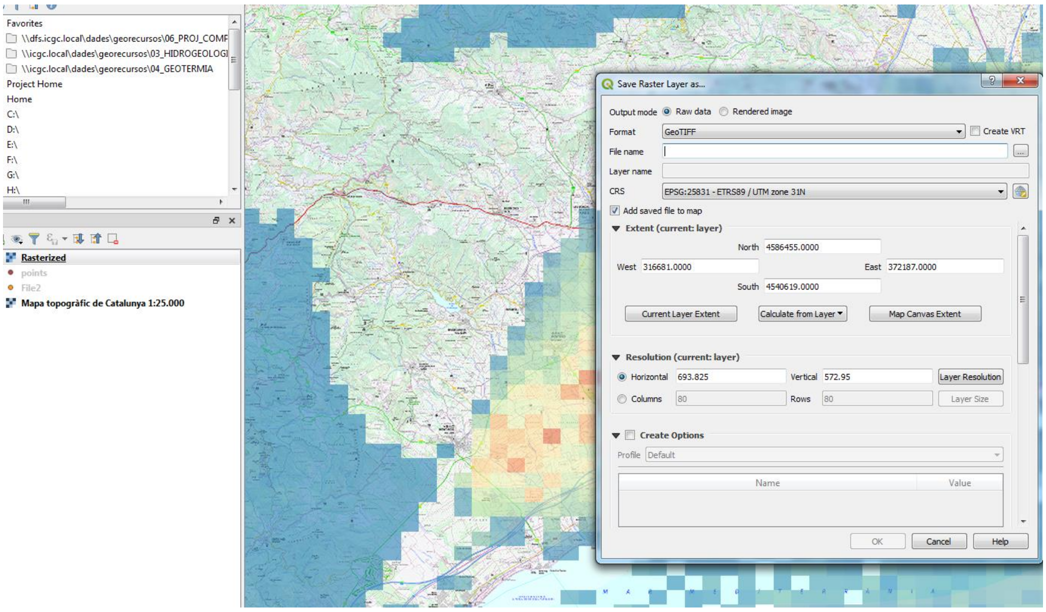

Fig. 32. Pop-up window to export the raster file.

10) In order to generate a final 2D raster map using a GIS software and express the results in PJ/km^2, the value of the cells must be divided by its surface. In this example, the values have been divided by 693.83 m * 572.95 m expressing it in km^2. To present the final map, in this case the cells located over the sea have been masked, as well as the values with HIP equal to zero.

    The following Fig.33 shows the final map of the deep geothermal potential for the target, expressing the results as the probability of 90% stored energy in PJ/km^2.

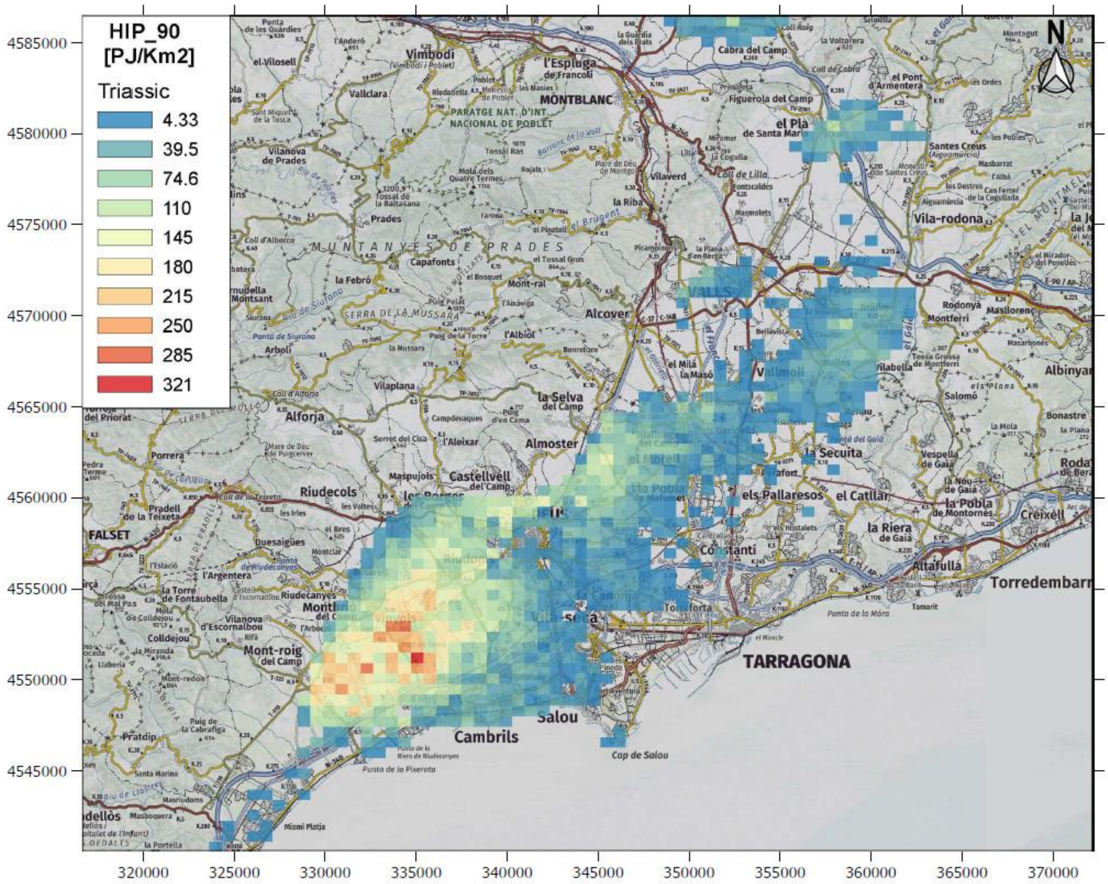

Fig. 33. Deep geothermal potential map of the example. Units: [P90 in PJ/km^2]

6 HIP test

Nowadays some commercial applications allow calculating equations stochastically. For example, Crystal Ball (Oracle) or @Risk (Palisade), are add-in applications inside Microsoft Excel allowing selecting PDF for the input parameter. However, these tools only allow calculating the HIP in 1D, i.e. for an idealized reservoir defined as a unique cell or voxel.

Although 3DHIP-Calculator is defined to obtain the HIP for 3D Geological models divided in multiple cells or voxels, the tool also has the capacity to calculate the HIP for an idealized reservoir defined only by one cell (that the user can create straightforward by himself *), with a constant volume but with parameters defined by PDF.

Thus, we use Oracle Crystal Ball software version 11.1.2 (2016) to test if the HIP calculations are consistent in 3DHIP-Calculator.

We simulate a reservoir with a constant volume of $8 \cdot 10^8$ m^3 (a surface of $4km^2$ by a 200m thickness) and calculate the HIP using both tools, with the same parameters (Table 3) and using 15,000 simulations.

Parameter	PDF	Values
Porosity	Triangular	0.005 / 0.02 / 0.1
Fluid density [kg/m^3]	Triangular	937 / 950 / 970
Fluid specific heat capacity [kJ/kg·ºC]	Triangular	4.17 / 4.2 / 4.22
Rock density [kg/m^3]	Triangular	1900 / 2200 / 2300
Rock specific heat capacity [kJ/kg·ºC]	Triangular	0.78 / 0.83 / 0.85
Reservoir temperature [ºC]	Normal	112 / 4
Reinjection temperature [ºC]	Fixed	30

Table 3. Parameters and values used for the simulation. For triangular distributions the values are ordered by Lower/Most Probable/Upper and for normal distributions by Mean/ Standard Deviation.

The results obtained by 3DHIP-Calculator (Fig. 34) and by Crystal Ball (Fig. 35) are consistent.

*In that case the user just need to create a text file following the rules indicated in the section 3.2.1. Block 1: Load data (Geological and thermal models) i.e. the file needs to contain one line with the headers and one line with the reservoir properties. The minimum number of columns would be *X*, *Y* and *Z* values (that won't be taken into account but must be included), the geology, the temperature and the standard deviation temperature. An example file with these properties is included with the manual: 1D_geological_model. This file must be loaded both for geological and thermal model.

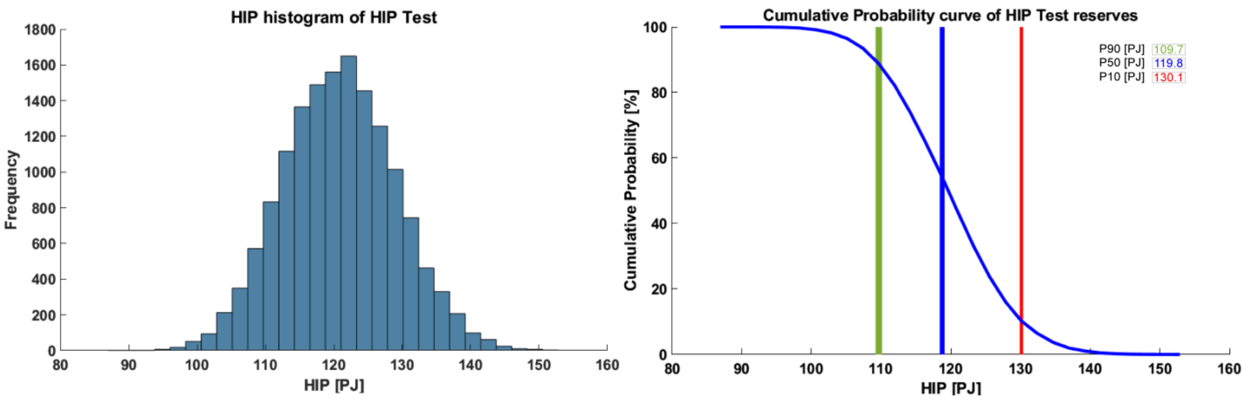

Fig. 34. Results obtained by 3DHIP-Calculator. Left the HIP frequency histogram and right the cumulative probability curve.

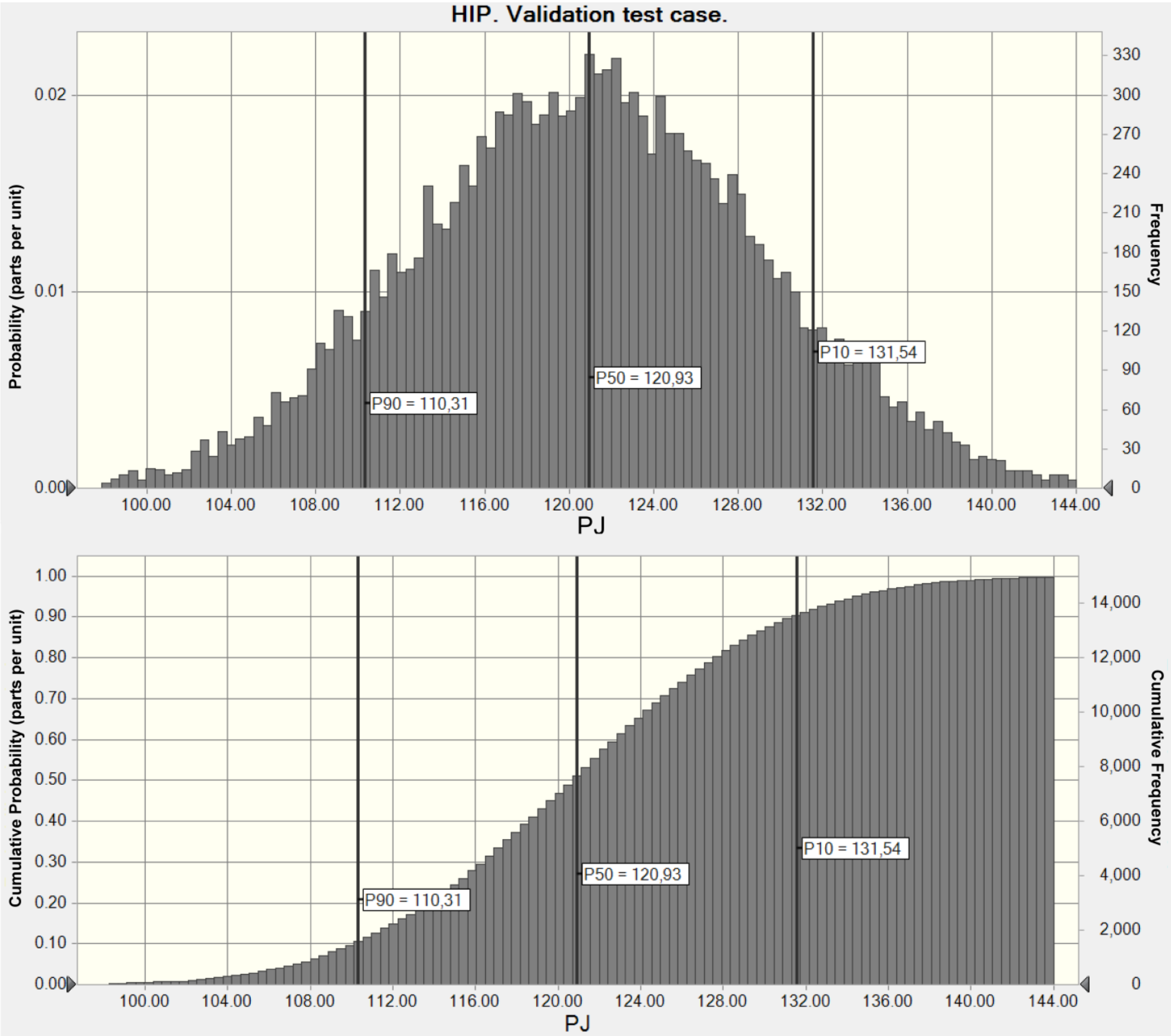

Fig. 35. Results obtained by Crystal Ball (Oracle). Up the Frequency histogram and down the Cumulative Probability-Frequency curve.

If you use 3DHIP-Calculator to calculate the HIP for an idealized reservoir defined just as one cell, the output results will be limited to those obtained and showed on the 'Petrophysical properties and HIP distribution' tab, and it will not produce a 2D raster of the results.

7 Acknowledgements

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