

DosiVox-2D

User Manual

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DosiVox-2D and corresponding documentation are available at <http://www.iram-at-crp2a.cnrs.fr/spip/spip.php?article144>.

Table of Contents

1 – Introduction.....	p.2
2 – Installation	p.5
3 – Create a modelling	p.6
4 – Running a simulation	p.16
5 – Results processing	p.19
6 – References	p.22

Genesis of the software :

Everything in this manual is part of a research initiated a long time ago to which contributed, among others and for different aspects of this research, C. Tribolo (Tribolo et al., 2002; Tribolo, 2003), S. Incerti (Incerti et al. 2009), G. Guérin (Guérin, 2011, Guérin & Mercier, 2012; Guérin et al., 2012), and Alan Guitard (for the Java graphical interface).

-Tribolo C., 2003. Apport des méthodes de la luminescence à la chronologie de techno-faciès du Middle Stone Age associés aux premiers Hommes Modernes du sud de l’Afrique. Thèse de doctorat, Université Bordeaux 1.

-Tribolo C., Mercier N., Valladas H., Selo M., Joron J-L., Reyss J-L., Henshilwood C., Sealy J., Yates R.: Internal dose rate in quartzites: the case of Blombos cave, South Africa. LED 2002 – 10th International conference on Luminescence and Electron Spin Resonance Dating, 24-28 juin 2002, Reno, USA.

-Incerti, S., Seznec, H., Simon, M., Barberet, Ph., Habchi, C., Moretto, Ph. 2009. Monte Carlo dosimetry for targeted irradiation of individual cells using a microbeam facility, Rad. Prot. Dos. 133, 1, 2-11.

-Guérin, G., 2011. Modélisation et simulations numériques des effets dosimétriques dans les sédiments quaternaires: application aux méthodes de datation par luminescence. Thèse de doctorat en Physique des archéomatériaux, Bordeaux, université Michel de Montaigne Bordeaux 3, 242p.

-Guérin, G. , Mercier, N., 2012. Preliminary insight into dose deposition processes in sedimentary media on a scale of single grains: Monte Carlo modelling of the effect of water on the gamma dose rate. Radiation Measurement 47, issue 7, 541-547.

-Guérin, G. , Mercier, N., Nathan, R. , Adamiec, G. and Lefrais, Y., 2012. On the use of the infinite matrix assumption and associated concepts: a critical review. Radiation Measurements 47, 778-785.

1 – Introduction

Principles

DosiVox-2D is a software designed to simulate the beta radioactivity and calculate dose rate in heterogeneous isotropic samples of rocks or sediments (Martin *et al.*, 2018; Fang *et al.*, 2018). It can be freely downloaded with its Java interface and documentation at <http://www.iram-at-crp2a.cnrs.fr/spip/spip.php?article144>. It is derived from DosiVox (Martin *et al.*, 2015a, Martin *et al.*, 2015b, Martin *et al.*, 2015c, <http://www.iram-at-crp2a.cnrs.fr/spip/spip.php?article144>), both created with the Geant4 toolkit (Agostinelli *et al.*, 2003; Allison *et al.*, 2007). DosiVox-2D is based on the concept of 2D-modelling, in which beta particles are simulated in a flat representation of the sample. The software provides at the end of the calculations the distribution of beta dose rates in the different material/mineral modeled phases, as well as average values.

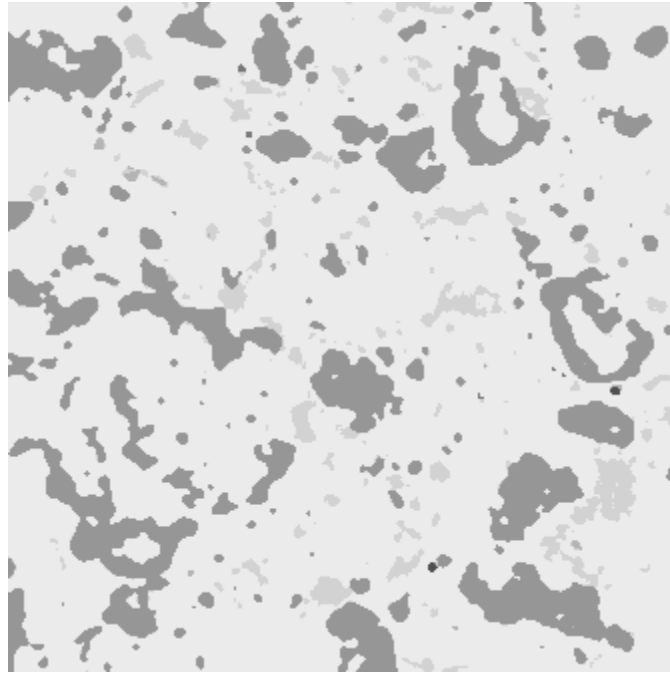
In DosiVox-2D, one constructs the 2D-modelling from a segmented 2D-mapping of a sample, representing the different materials composing this sample. Each pixel of the image becomes a voxel of the modelling, containing the information related to its constituting material (chemical composition, density, moisture, radioactive element contents); the voxel is also able to record doses, what finally allows to calculate dose rates. The software runs the simulation of the beta particle emissions coming from the K or/and U-series or/and Th-series. Alpha et gamma spectra are also available but not tested for 2D-modelling. As explained in Martin (2015), the alpha particle spectra (Ualpha, Thalpha) are constructed from the NIST online database (Kramida *et al.*, 2018). The beta particle spectra (Ubeta, Thbeta, Kbeta) and the gamma particle spectra (Ugamma, Thgamma) are from the work of Nathan (2010) and Guérin (2011) based on the data from the NNDC (Brookhaven National Laboratory, Etats-Unis, <http://www.nndc.bnl.gov/>) online database NuDat (version nov 2009) (Kinsey *et al.*, 1996). The K gamma spectra (Kgamma) is constructed from NNDC online database NuDat (version janv 2013)(Kinsey *et al.*, 1996). It is also possible to use your own energy spectrum for the beta particle emissions, referred as "User-defined" or "Udef". The results are provided as average dose rate in the sample, average dose rate in each material/mineral fraction represented, basic histograms of dose rate distributions for the different elements simulated and for each material, and beta dose rate mappings for the whole sample. The dose rates are calculated using the conversion factors from Guérin *et al.* (2011)The 2D-modelling simulations have been demonstrated to be equivalent to those of standard 3D modellings (Martin *et al.*, 2018) in the limit of representativeness of the modeled slice over the whole sample.

Requirements

The following list contains the basic data and unavoidable considerations to create 2D-modellings with DosiVox-2D. It is important to keep in mind that a modelling is not a perfect representation of the reality, but is circumscribed by the uncertainty on the different parameters and approximations made by the user. Thus, it is possible to construct very accurate and heavy modellings with detailed data, or basic and fast simulations with only the minimum data required. It can be also useful to perform series of simulations with different values for a single parameter (like the moisture), in order to characterize the range of possible dose rates. All these ways to use the 2D-modelling (and any modelling in general) are correct and consistent inside the limits of the accuracy of your parameters and the assumptions made.

- first of all, you need to consider that DosiVox-2D applies only to **isotropic samples**, i.e. a sample where the distribution of the different materials/grains/heterogeneities is similar, in terms of probability, in all directions (Underwood, 1970; Martin *et al.*, 2018). Without this condition, the 2D-mapping of the sample cannot be considered as representative of the whole sample (Fang *et al.*, 2018). The isotropic condition must be considered only at the beta particle scale (millimeter to centimeter), what means that a layer (for instance a sedimentary layer) can be locally isotropic if the different objects and materials composing it are heterogeneous but well mixed together, and even if this layer is actually an anisotropic object by definition. In this case, 2D-modelling can be performed on a sample slice included in the layer under study. The crucial point is to get a sample slice for the 2D-mapping that can be considered as representative of the whole sample, in terms of material proportions and distributions. It is noticeable that 2D-modelling seems to give reliable results as well, even if a slight anisotropy can be observed, like a preferential direction of mineralization (Fang *et al.*, 2018).

Figure 1: Example of a segmented 16 bit image in grey scale (the different grey shades represent the different mineral/material phases).



- The 2D modelling is constructed from a **2D mapping of a slice** of the sample. If the sample is perfectly isotropic, it is possible to cut it in any direction for getting the slice : all possible slices will be equivalent (in the limit of the representativeness of the mapped area). If there is an important (centimeter scale) anisotropy, you should map a sub-sample for which there is no anisotropy (like a layer in a succession of layers). In case of a slight anisotropy (low variation or millimeter scale), the slice should be cut in parallel of the isotropic direction, in order to have the largest representativeness of the sample. The area of a slice should be at least one square centimeter, considering the maximum range of the beta particles in sediments and rocks (3-5mm), and be large enough to be statistically representative of the sample. Notice that it is always possible to test this representativeness by analyzing two slices from the same sample: the different proportions of the area covered by the materials should be similar (at least for the major phases), and the covariograms of the main granulometric fractions should reach a plateau. Different equipments can be used for mapping the different materials constituting a sample : SEM-EDS (Scanning Electronic Microscope – Energy Dispersion Spectrum), μ XRF (micro-Xray Fluorescence), QEM (Quantitative Element Mapping), LA-ICP-MS (Laser Ablation – Inductively Coupled Plasma – Mass Spectrometer), polarising microscope photography, multispectral camera... Some of these techniques can be quantitative and calibrated, but even a qualitative mapping will allow separating the different major material phases. However, the quantitative information are useful to recreate the different materials in DosiVox-2D according to their chemical compositions. Ideally, the resolution of the mapping should be between 50 and 100 μ m. A higher resolution could limit the representativeness of the modelling, and a smaller one would often lead to unnecessarily heavy simulations. The image from a 2D-mapping must be segmented, i.e. each material/mineral phase (you want to consider in the modelling) must be represented by a specific shade of grey in the image (Fig.1). It must be exported as a 8 bit image (in shades of grey, not in color) in TEXT image format (.txt extension), what can be done preferentially in using the ImageJ free software (<https://imagej.nih.gov/ij/> , Rasband, 1997 – 2012) or using a standard spreadsheet software (Microsoft Excel, OpenOffice Calc, LibreOffice Calc, ...). This format corresponds to an ASCII matrix representing the shade of grey of all pixels.
- **The chemical compositions** (at least the major elements) of the major materials present in the sample are required. DosiVox-2D has been made to easily take as inputs the compositions given as percent of oxides, but you can also use the percent of elements, or even give a chemical formula. In addition, the density and moisture of each material

must be given. These data are somewhat difficult to get in case of loose materials, but it is usually possible to estimate these values and test various set of parameters. You might often consider only the major material phases, but other phases could be very important as well (if their radioactivity is significantly higher than the rest of the sample, like K-feldspars or zircons). A quick way to judge if a minor material must be represented or not is to estimate the proportion of beta dose from this material in the sample. Simply multiply the estimated mass proportion of the material by its estimated radioactive content and by the corresponding beta dose conversion factor. If both the resulting dose rate, normalized to the infinite matrix beta dose rate, and the mass proportion of the material are lower than one percent, the material can likely be neglected in the modelling.

- You need to define **the contents of radioactive elements** (K, U-series, Th-series or/and user defined beta spectrum) for each modelled material. It is possible afterwards to adjust manually these values in each voxel. DosiVox-2D provides the beta energy spectrum of the K, the U-series and the Th-series (both at secular equilibrium). A user defined file is available in the software folder (DosiVox-2D/data/spectra/Userdef.txt) for implementing your own energy spectrum (for example a U-series spectrum in disequilibrium), following the defined pattern : the first line contains the conversion factor from element content to dose rate (Gray/ka) followed by a description ; then, a first column lists the energies of the emitted beta particles (in keV) and a second column gives the cumulative probabilities of these energies. The contents of the different radioactive elements can usually be obtained by LA-ICP-MS measurements, or mineral separation followed by ICP-MS or gamma spectrometry measurements. It is also possible to get the K content directly with the slice mapping analysis if a quantitative calibration is set, and possibly the U and Th contents if they are high enough. If the access to these measurement facilities is limited, you might consider the K, U and Th contents from the bulk sample, and test different hypotheses of their distribution in the different materials.
- you need to have the **DosiVox-2D software** installed (This software runs on Linux systems and has been specifically precompiled and tested for the Linux virtual machine available at <ftp://ftp.cenbg.in2p3.fr/info/Vmware/Old-Versions/g4.10.01.p01/> , see part 2), and a Java environment set for running the graphical interface (if you choose to run the software under the proposed virtual machine, the Java environment is already set inside).

→ To sum up, once you have checked that your **sample is isotropic** (or almost) at the scale of the beta dose rate heterogeneity, you need, in order to perform a 2D-modelling with DosiVox-2D, to make a **material mapping** from a slice of the sample, know the **composition of the different major material phases** as well as their contents in radioactive elements, and of course have **DosiVox-2D and its interface installed**.

2 – Installation

The DosiVox-2D software works under Linux. It was developed and tested with Scientific Linux 6.4 (Red Hat™), running on the Geant4 Virtual Machine (freely available at: <ftp://ftp.cenbg.in2p3.fr/info/Vmware/Old-Versions/g4.10.01.p01/>) developed by the Centre d'Etudes Nucléaires de Bordeaux-Gradignan, France (Incerti *et al.*, 2010). This virtual machine itself contains the Geant4 libraries, which are necessary for compiling the source code, if non-compiled or modified DosiVox-2D codes are used.

The provided instructions are given for a PC with the following setup:

Windows 7, 64 bit

Memory: min. 4 GB

1 – Download the virtual machine and unzip it in a folder.

2 – Installing the virtual machine player

DosiVox was tested with VMware™ Workstation 12 Player (free for PC) and VMware Fusion 6™ (available for purchase for Mac).

3 – Opening the virtual machine

Run the virtual machine player and choose to open a Virtual Machine (browse and select the file sl6 x64.vmdk). Play the virtual machine. The Parameters of this machine can be modified by editing virtual machine settings. For further information the user is invited to read the README file on the : <ftp://ftp.cenbg.in2p3.fr/info/Vmware/Old-Versions/g4.10.01.p01/> page.

Note: At the first virtual machine start, VMware Player displays a message asking whether you have moved or copied the virtual machine. You have to answer "I copied it".

Note: The virtual machine works as an independant computer on the user PC or Mac. All the data in the virtual machine are not automaticly saved in the regular computer, for example in the case of the deleting of the virtual machine. To access and save virtual machine data outside of the virtual machine (simulation results for example), use a shared folder between the regular computer and the virtual machine, or copy the data files in the virtual machine and paste them on the regular computer.

4 – Download and unzip the DosiVox-2D folder

The DosiVox-2D folder contains three sub-folders: build, data, results.

The data folder contains the spectra folder where all the spectra used for simulations are stored. All these files are TXT files and therefore can be easily modified. For instance, the file UserDef allows the user to simulate any particle, including ones other than those emitted by the 40K and U- and Th-series. The data folder must also contain the Pilot Text Files (PTF) used by Geant4 to run the simulations (cf. DosiVox manual for further information on the PTFs). The results folder contains the results of the simulation (cf. DosiVox manual for further information).

5 – Copy and paste the DosiVox-2D folder in the virtual machine /local1 folder

If you unzip the DosiVox-2D folder directly under the virtual machine, the access to the file may be restricted by Linux for security. To allow accessing the files and launching the simulations, right-click on the DosiVox-2D folder icon, go in "properties" and select the options « Allow executing file as program » and « Apply permissions to enclosed files » in the "permissions" tabulation.

6 – DosiVox-2D is now ready to work.

Follow the manual in order to build and run a modelling with it.

3 – Create a modelling

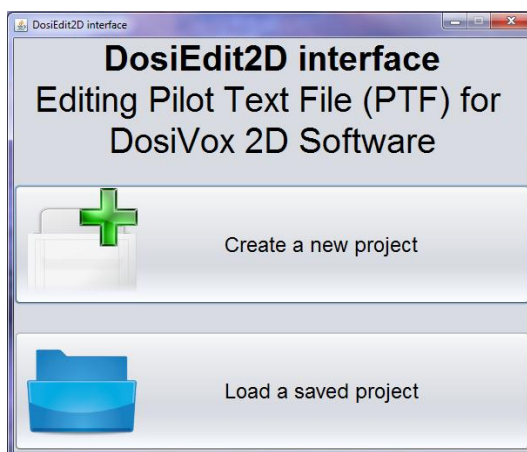
The graphical interface DosiEdit2D

DosiEdit2D is a user-friendly Java Graphical User Interface (GUI) for creating DosiVox-2D simulations. You can not directly run a simulation from it, but it allows creating a Pilot Text File (PTF), as for DosiVox (Martin et al., 2015a). This interface run on any computer with a Java (8 or superior) environment set. To launch it, double-click on the DosiEdit2D.jar file. Notice that a Visual Basic interface is also available at <http://www.iram-at-crp2a.cnrs.fr/spip/spip.php?article144>.

Open/load a new project

At the start of DosiEdit2D, a first window gives you the choice either to create a new project of simulation, or to reload a previous one created on this interface (Fig.2). All the options for creating and setting a simulation will be available whatever the choice.

Figure 2: Interface starting window



Creation of materials

When creating a new project, the first step is to create the different materials that you need for building the geometry of the simulation. These materials correspond to the different phases that you want to represent in your modelling. It could be for instance basic minerals, like quartz, carbonates or feldspars, or mixtures of minerals, like sand or clay, or various materials like air, ashes or bone. In order to create these different materials, you need to know their chemical compositions (at least the major elements), their densities and their moisture content. Each material/mineral phase will be represented as uniform in the modelling, so you only need to know the average values for each one. These data can be obtained from sample analysis (for example, the chemical composition can be provided by an SEM-EDX scan of the slice). The density and moisture can be difficult to determine accurately but standard values for the material type can often be found in the literature. However, as the modelling results accuracy is directly dependent on the input data, we recommend, if accurate analyses are difficult or not possible, to test different hypotheses on the missing data, in order to investigate the possible field of dose rates.

In the DosiEdit2D interface, on the “Forge” tabulation (Fig.3) (1), click on the “Create new material” button (2) in order to add a new material in the material list (3). You can set the name of this material in the box at the top of the tabulation (4), and press “enter” key to validate the name. For setting the chemical composition of the material, choose the components in the “Component list” on the left (5) and press the “Add Component to Material” button (6) to add them one by one to the composition of the material (7). You can then set their mass proportion by selecting one in the composition list, indicating the correct proportion in the “Change mass percentage of the selected component” box (8) and pressing the “enter” key. When setting the mass proportion of all the components of a material, the “total mass %” indicator must be 100% for the material to be validated.

If a material requires a component that is not in the basic component list, you can create it with the “component factory” (Fig.4). Click on the “show/hide component factory” button (9) to display or hide it. Add a new component in the component list with the “create new component” button (10). Select it in the list on the right (11) and choose its name in the box below (12) (do not forget to press the “enter” key to validate the name). You can then set it by constructing its chemical formula by using the periodic table (13) and modifying the number of each element with the “Set the number of atoms for the last selected element” box (14). You can choose the basic density of the new component with the box “Density (g/cm3)” (15). This density is only used for automatically calculating a density value of the materials containing this component. The component factory can also be used for creating a material directly from its chemical formula: create a new component with the chemical formula and density of the material, and then create a new material only constituted of this component.

For setting the density, you can choose the density automatically calculated by the interface, according to the density and proportions of the components, or set manually the density. The calculated density usually corresponds to compact materials or crystals, but it can be necessary to set manually the density for loose materials like sand or clay types. To use the calculated density, tick the “Use Calculated Density” box (16) (Fig.3). To set manually the density, untick the box, set the density value in the “Set manually Density” box (17) and validate with the “enter” key.

The moisture content of a material is expressed in mass percent of water on the dry mass of the material. To set the moisture content of a material, set the value in the “Water fraction in current material” box (18) and validate with the “enter” key.

Repeat the process from the creation of a new material (second paragraph) for each one of the materials that you need for the modelling.

Figure 3: Forge tabulation

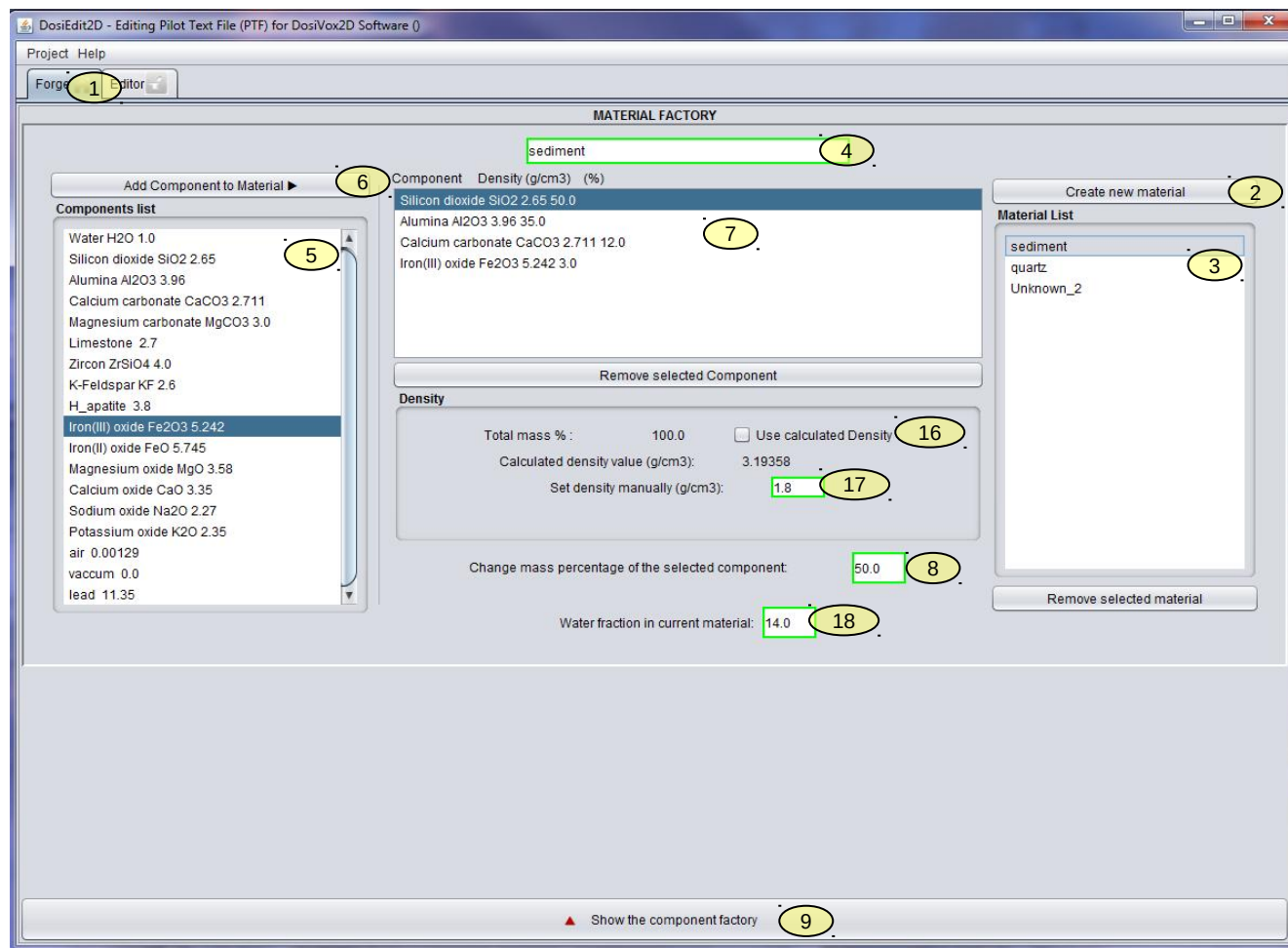
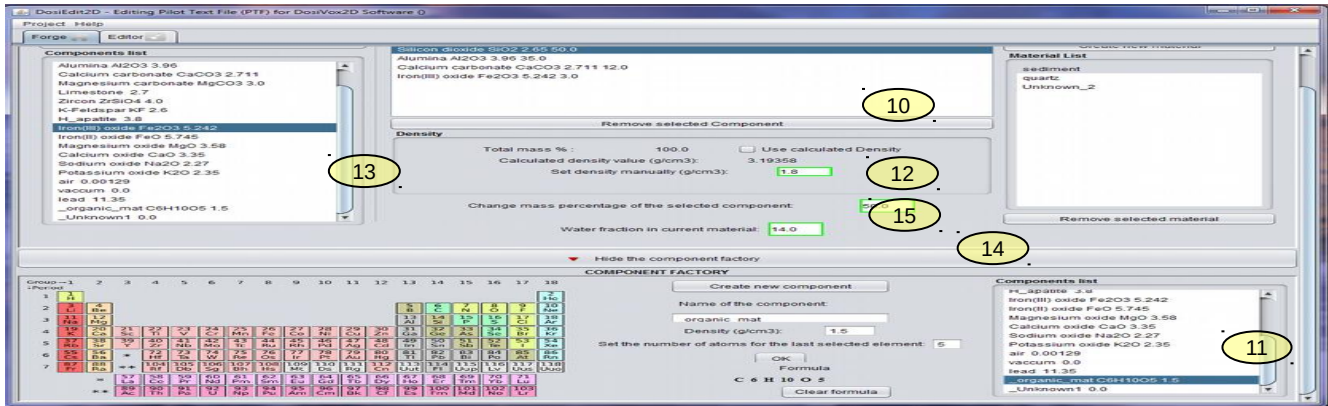


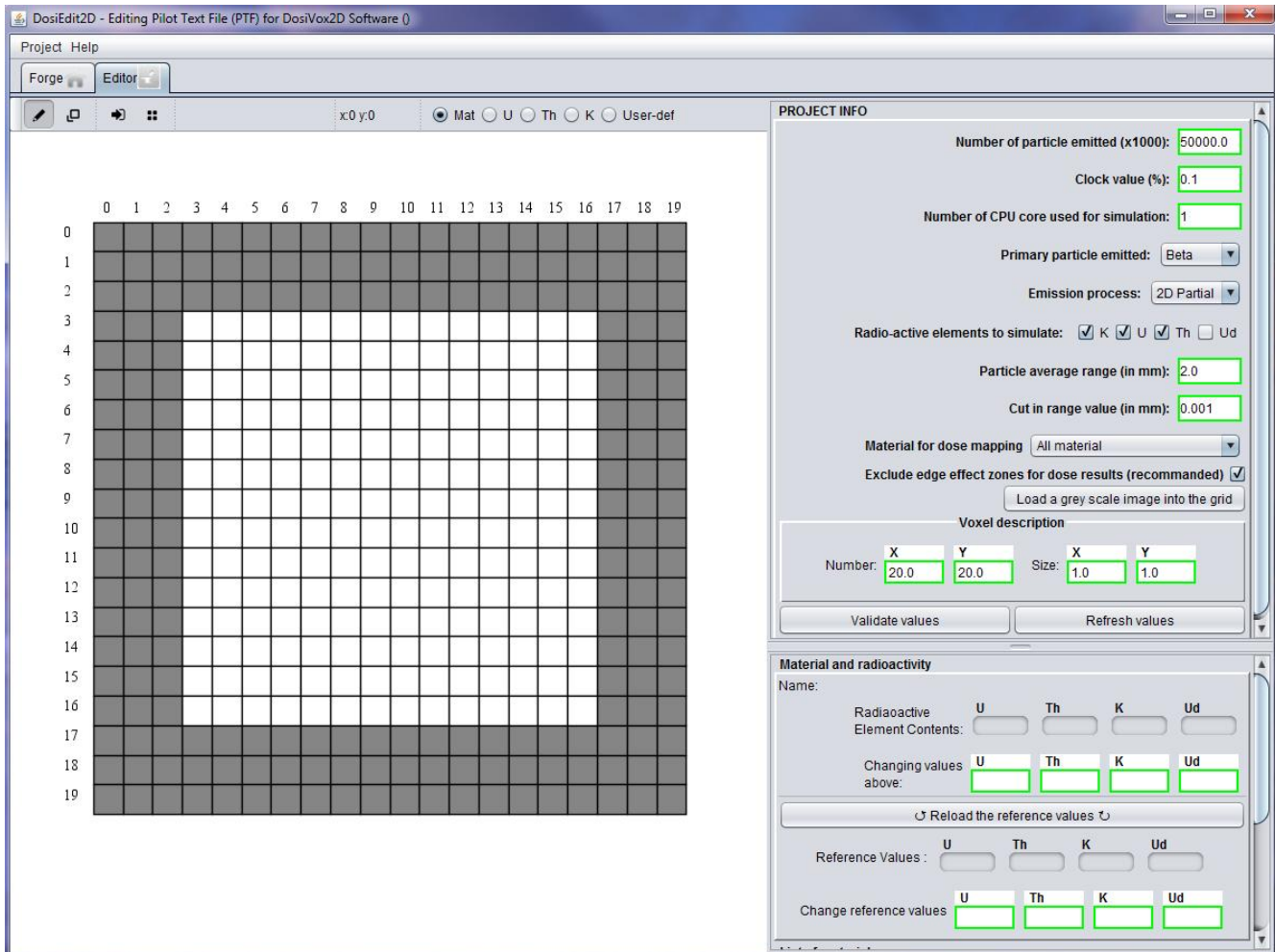
Figure 4: Component factory



Parameters of the simulations

When all the required materials are created, you can go to the “Editor” tabulation (Fig.5). This tabulation allows setting the various parameters of the simulation, and to create and edit the geometry of the modelling.

Figure 5: Editor tabulation



The right-top part of the tabulation allows the settings of parameters and options controlling the simulation:

- Number of particle emitted (x1000) : The quantity of thousand of primary particles (usually beta particles) that is going to be generated during the simulation. The higher this number is, the more accurate will be the simulation but also the longer it will last. For a standard beta dose rate 2D-modelling, 100 000 (x1000) particles give a good accuracy and need about few hours to one day of calculation on current computers (it is common for Monte-Carlo dose rate simulations to last more than few days).

WARNING: The DosiVox-2D_0.9 version can not handle more than 1 000 000 (x1000) particles. The simulation will start, but the results will not be available. This issue will be corrected in the 1.0 version. If you need to simulate more than 1 000 000 (x1000) particles, you can create two simulations of 500 000 (x1000) particles and averaging the results.

- Clock value (%) : The frequency for displaying information about the simulation progression, in percent of particles simulated. The smaller this value, the higher the display frequency of the progression. However, a too high frequency (more than one display by second) can slow down a little bit the simulation speed. If you are not sure about the frequency of display of your simulation, let this value to 1%. The progression of the simulation will be displayed each time 1% of the total number of the particles has been simulated.
- Number of CPU core used for simulation : DosiVox-2D is compatible with multi-threading calculation. You can speed up the simulation by assigning more than one computer core to the calculation. Be careful to not assigning more cores than the number available in the virtual machine where the software runs.
- Primary particle emitted : The type of the primary particles that will be generated during the simulation. DosiVox-2D has been currently tested only for beta particles as primaries, but the user remains free to use other alpha or gamma particles. Other particles may appear from the interactions of the primaries with the matter (X-rays, secondary beta particles, ...), the choice of the primaries doesn't limit it.
- Emission process : Allows the user to choose different emission processes. “2D partial” is the standard process for 2D-modelling: the particles are emitted in the XY plan and reflected at the X, Y and Z edges of the modelling. With the “3D” process, the particles are randomly emitted in the 3 directions and reflected at the edges. It can be used for the modelling of a sample that is invariant (at the particle range scale) in the Z direction. The “2D real” process, still experimental, forces all particles to remain exactly in the XY plan, creating a virtual 2D world. Tests are currently carried on in order to determine its potential.
- Radioactive elements to simulate : Tick the boxes to choose the radioactive elements and series that you want to simulate. DosiVox-2D provides the alpha, beta and gamma spectra of the 40K, the U-series and the Th-series (series at secular equilibrium). The “Ud” boxes corresponds to the user defined spectrum. This file is in the DosiVox-2D/data/spectra folder of DosiVox-2D, you can implement it to create your how spectrum in a similar way than the other available spectra. It can be used for example to simulate a series in disequilibrium.
- Particle average range (in mm) : Indicate the average range of the considered particles in the sample (usually few millimeters for beta particles), in order to determine the area with potential edge effects (edge effect zone, EEZ). This zone is represented in grey tint on the sample map (Fig.5 and Fig.8). If the sample is not symmetrical over the X and Y boundaries, the dose rate in the EEZ may be biased.
- Cut in range value (in mm) : This value represents the distance threshold under which the secondary particles are no more explicitly simulated but replaced by a local deposit of dose (proportionnal to their remaining energy). The smaller the value, the more accurate the simulation. However, decreasing this threshold slows down the simulation (more time is required for secondary particles simulation). It is advisable to keep the cut in range value inferior to the voxel size by one or two orders of magnitude. However, for beta particles, it is not useful to set a cut in range inferior to 0.001 mm.
- Material for dose mapping : This option allows to select just one material for the dose mapping results (see part 5). It simplifies the processing of the dose rate mapping results if you are only interested on the dose rate distribution of this particular material. The average dose rates and basic histograms in all the different materials will still be

provided in the main result file, but the voxels filled by the no-selected materials will get the default value “0” in the dose rate mappings results. If you prefer to get the dose rate mapping in all the materials, just let this option to “All materials”. You will still be able to separate the dose rate mapping of the different materials with a few image processing (see part 5).

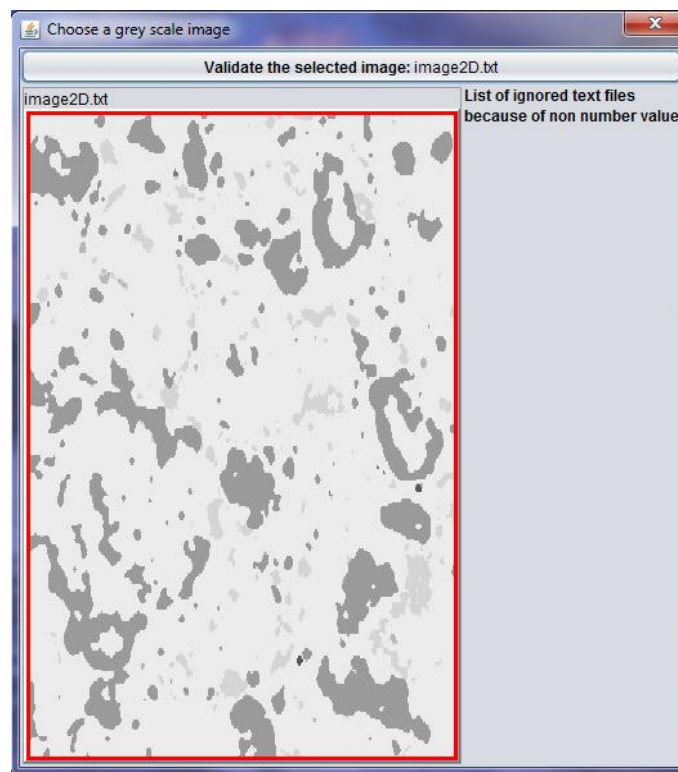
- Exclude edge effect zones for dose results (recommended): this option excludes the voxels in the EEZ for the dose rate calculation and mapping in the result files. It avoids potential bias in the results due to a local break of the isotropy of the modelling at the edges. However, if you want to include these voxels in the results (in the case where you are sure that the statistical isotropy of the modelling is respected), uncheck this box.
- The “Voxel description” box (Fig.5) is used to set the size of the voxel grid. The size of the voxel in the X and Y direction, corresponding to the resolution of the 2D image in these directions, have to be provided here. The number of voxels can be used to modify the voxel grid size when creating manually a 2D geometry, but is useless when loading a 2D image (which is the standard way of using DosiEdit2D).

Do not forget to press the “enter” key to validate any input. You can also use the “Validate values” button to validate all the changes. The “Refresh values” button applies the changes to the voxel mapping when applicable.

We strongly advise you to save the project at this point, before loading a 2D image. Even if a project with an image can be saved, the saved file might be heavy and its reloading might be long and memory consuming. A project saved without an image allows to reload all the created materials and all the set parameters. To save the project, click on the “Project” menu at the top left of the interface, and choose “save” or “save as”.

loading an image

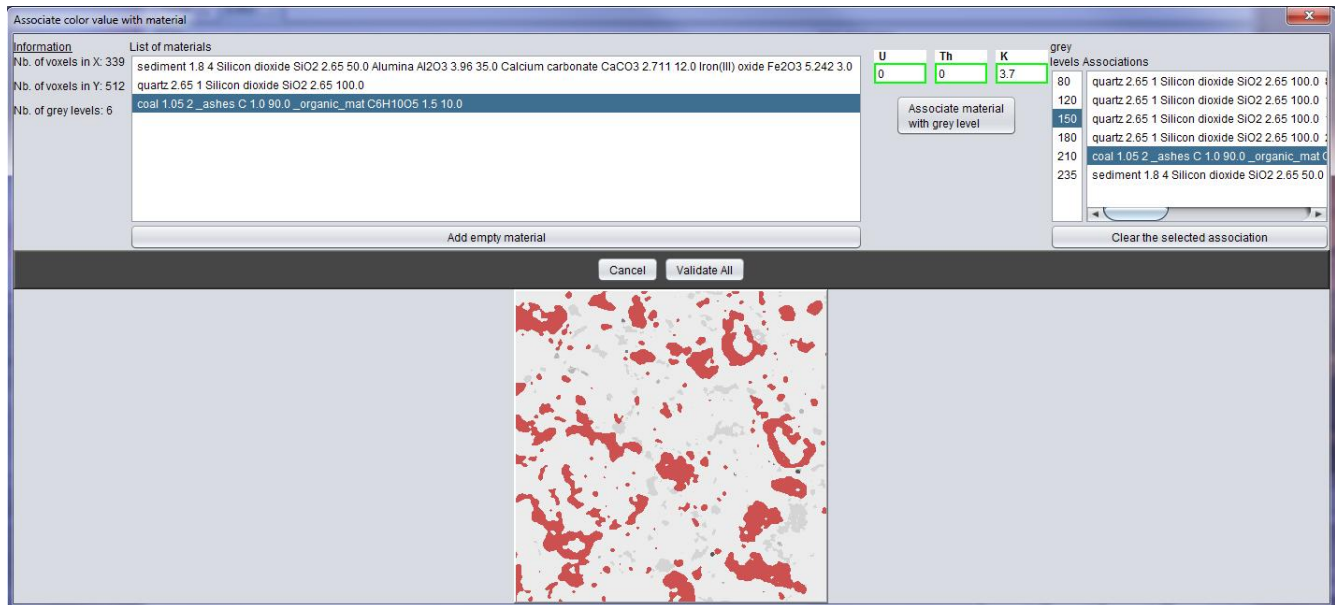
Figure 6: Image selection window



For building the geometry of your sample in the modelling, you have to load a 2D 8bit image in shades of grey. This image has to be segmented, meaning that each material/mineral is represented by one specific grey shade. The image must be in TXT format (available from standard spreadsheet softwares or the free image processing software ImageJ, see Rasband, 1997 – 2012).

For loading an image, click on the “Load a grey scale image into the grid” button, and then select the folder containing the image. A window displaying the different images available in this folder will appear in the interface (Fig.6). From it, you can select the image (Fig.1) by clicking on it and then clicking on the “Validate the select image” button at the top of the window.

Figure 7: Association window

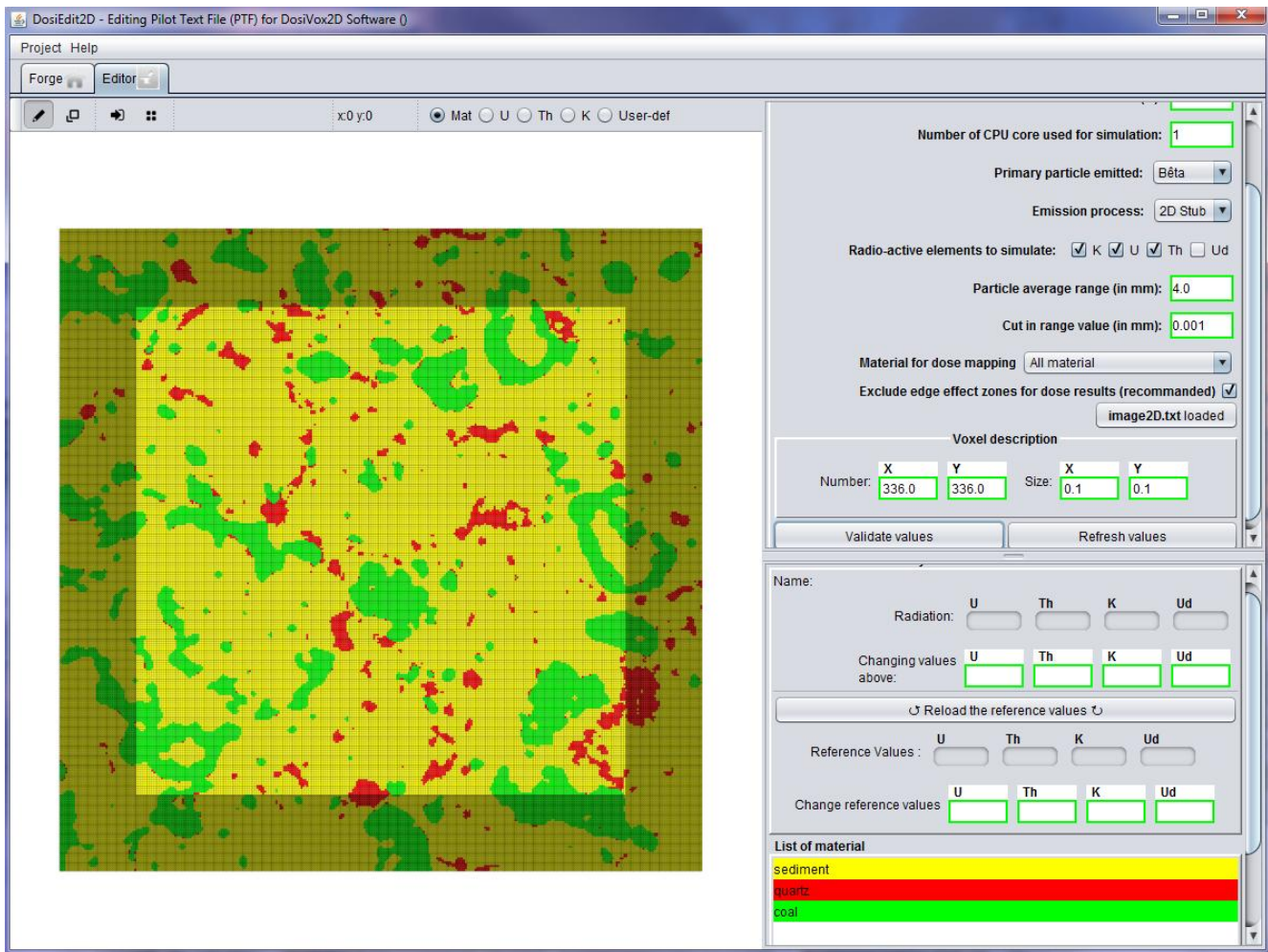


Another window displaying the created materials and the shades of grey of the image will appear. From it, you have to associate each grey value (Fig.7) with a material (select both by clicking on them) and specify the K, U, Th and Ud (representing the element associated with the user defined spectrum) contents. If you do not know the content of one of the radioactive elements or, if you do not want to simulate it, use the “0” value. Once finished, validate the association with the “Associate material with grey level” button. Repeat for each grey shade value of the image. When all shades are associated with materials and radioelement contents, register the associations in the modelling by clicking on the “Validate All” button. This will close the current window and the image, and associations will be displayed in the “Editor” tabulation (Fig.8).

Noticed that if you must associate each shade with a material, you are not obliged to use all the available materials. You can also associate the same material to different shades, but not associate a shade with more than one material. If necessary, you can also create another material in this window, for which you must specify the characteristics afterward in the “Forge” tabulation. You can clear any association of shade/material/radioactive element content by selecting it in the list on the right, and clicking on the “clear the selected association” button.

The interface provides various tools for modifying the material and content of radioactive elements in each voxel after loading the image. To do that, start by selecting a material in the list at the right bottom of the Editor tabulation (Fig.5), and setting the requested contents of radioactive elements in the “changing value above” boxes (validate with the “enter” key). Then, select a tool for filling the voxels (at the left top of the tabulation): the arrows tool allows modifying the content of voxels one by one by clicking on the voxels on the map (you can maintain the click to draw a line on the voxels you want to modify). The selection tool allows to modify all the voxels in a selection square. Be careful: there is no “undo” button.

Figure 8: Displaying of the geometry



It is also possible to modify directly the content of radioactive elements in all voxels containing a particular material. To do that, select a material in the list, then set the requested values of U, Th, K and User defined element in the “Change reference values” boxes (validate with the “enter” key) (Fig.5). You will then modify the contents of these elements in all the voxels filled by the selected material by clicking on the “Reload the reference values” button.

Notice that it is possible to create the whole geometry of the modelling by using the provided tools, instead of loading an image. In order to help the user for this purpose, two additional tools are provided in the left top of the Editor tabulation (Fig.5): "filling all empty voxels with the selected material", and "filling all voxels with the selected material". The contents of radioactive elements/series will be those set in the “Radioactive Element Contents” boxes (Fig.5).

Save a project, create the PTF

If required, you can save at this step the project containing now the image data. To save the project, click on the “Project” menu at the top left of the interface, and choose “save” or “save as”. We remind you that a project saved with an image could be heavy and long to reload in the interface.

The interface and project cannot be directly used to launch the simulation. DosiVox-2D uses a system of pilot text file (PTF) to run the simulation. To create the PTF corresponding to you project, go to the “Project” menu and select “Generate Pilot Text File” (Fig.9). Validate after indicating a file name and a destination folder where the PTF will be created. The generation of the PTF could take some time (few minutes to few hours, depending on the size of the image).

Once it is done, the software will propose you to check the PTF in order to see if the simulation data are correct (Fig.10). You can check this by referring to the PTF layout explained in the next part. If everything is correct, then copy the PTF into the DosiVox-2D/data folder of DosiVox-2D (on the linux virtual machine) : you are then ready to launch the simulation.

Figure 9 Generate the PTF

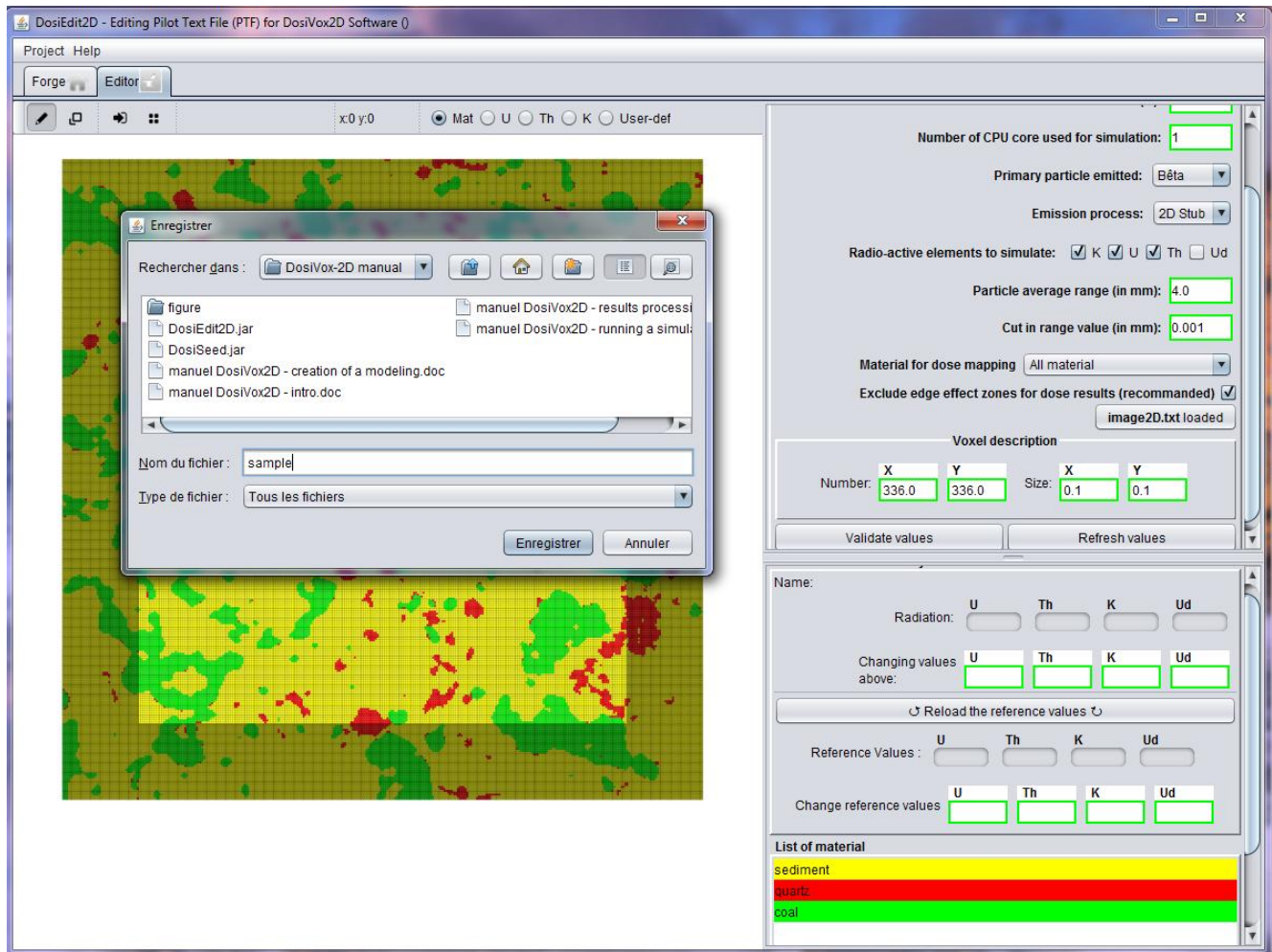
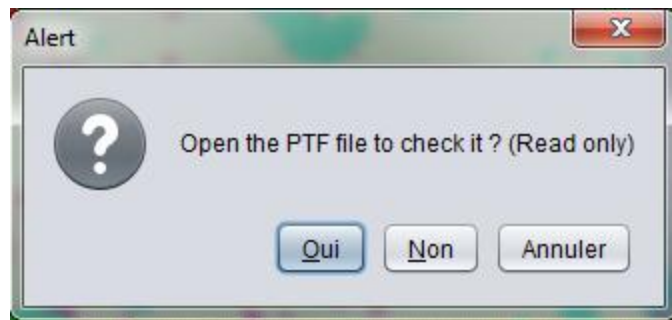


Figure 10 PTF checking



- The first line of the PTF (1) is the name for the results file (or RTF, see part X).
- The first block contains data relative to the general parameters of the simulation (2), like the number and type of the particles to generate, or the radioactive element and/or series to simulate.
- The following series of blocks describes the new components, if any were created by the user (3). Each one is characterized by an index (starting at 18, because indexes 0 to 17 correspond to the basic components available in the interface, see Fig.3-(5)), its name, its density (only used in the interface for calculating the default density of the materials containing it), and the number of elements it contains, followed by the list of symbols and numbers of atoms of each element composing it.
- The second series of blocks describes the different materials filling the voxels (4). Each one is characterized by an index, allowing to represent it in the material mapping: its name, its density, its moisture content, and the number, indexes and proportions of its components.
- After the material description, a data block defines the voxel grid where the sample is represented (voxel sizes and numbers in the X and Y direction) (5).
- The first matrix below is the material mapping (6). It is a matrix representing the material filling each voxel of the grid. This matrix has the size of the grid (the lines and columns represent respectively the X and Y axis, each value represents a voxel) and each material is represented by its index issued from the data blocks of material description.
- The four following matrices, sharing the same layout than the material mapping matrix, represent the mapping of the radioactive contents. The order of the matrices is ⁴⁰K, U-series, Th-series and User Defined element.

It is possible to edit (or create, for experimented users) a PTF with a text editor software. Please find below some rules and advices:

- You must respect the layout and the order of the data blocks presented above.
- The data blocks, the components and the materials must be separated by one and only one empty line
- The data in a line must be separated by at least one space. Avoid using tabulation.
- The decimal separator is the point. Do not use comma.
- Do not use complex notation for numbers (with power of ten for example).
- The indexes of the new components starts at “18”, those of the material at “0”.
- The unit of the U, Th and Udef mapping is ppm. The unit of the K mapping is %.

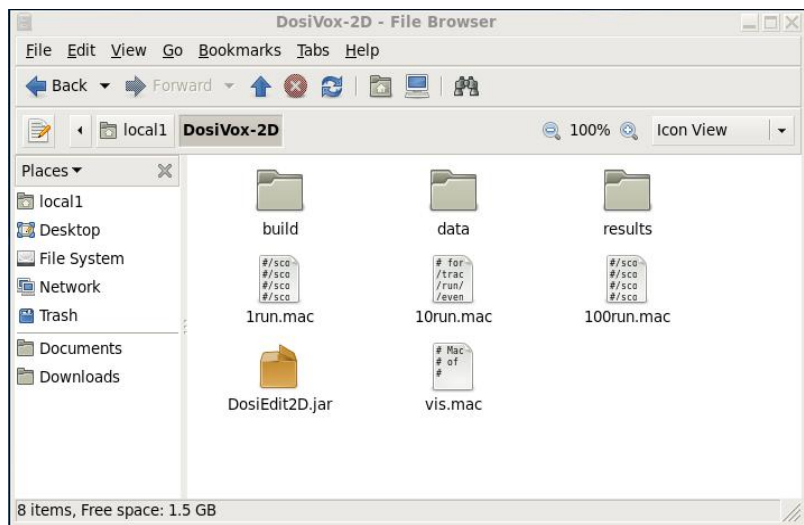
4 – Running a simulation

Launching a simulation

The simulation of a modelling is launched from a Linux terminal, using a command line and the name of the corresponding PTF. The PTF must be stored in the “DosiVox-2D/data/” folder. To **open a terminal**, go to the DosiVox-2D/ folder (Fig.12), right-click in the folder and select “Open in Terminal” (Fig.13). You can open as many terminals as you need, in order to launch several simulations in parallel for example. If a terminal is open but indicates a different address than the DosiVox-2D/ folder, you can navigate in the folder using the commands “cd + name of the folder” to enter a folder, “cd ..” to move back in the folder hierarchy, “cd” to return at the user home folder, and “ls” to list the available files and folders in the current folder. For more information and more command lines, see the Linux documentation.

WARNING: The DosiVox-2D_0.9 version can not handle more than 1 000 000 (x1000) particles. The simulation will start, but the results will not be available. This issue will be corrected in the 1.0 version. If you need to simulate more than 1 000 000 (x1000) particles, you can create two simulations of 500 000 (x1000) particles and averaging the results.

Figure 12: The DosiVox2D folder



Once the terminal is located in the DosiVox-2D folder, you can launch a simulation by using inside the command line “**build/DosiVox-2D**” followed by a space and the name of the PTF that you want to use (Fig.14), and then validate the command with the “enter” key. For example, with the previous PTF, the command to launch the simulation would be “build/DosiVox-2D Sample2D.txt”. The simulation will start and display various data about the modelling and the Geant4 processes.

If the terminal indicates that the PTF name given in the command line does not correspond to any PTF in the DosiVox2D/data/ folder, the name might contain a mistake, or the PTF could be not in the data folder. If the terminal indicates that the command line is unknown, the terminal might be not open in the DosiVox-2D folder, or the user access rights for the folder can limited the launching of the software (see the installation manual or the Linux documentation). In the last case, you can allow the launching by right-clicking on the DosiVox2D folder icon, and going in the "properties" options. Then go to the "permissions" tabulation, and tick the option "Allow executing file as program". Close the “Properties” window to validate.

Figure 13: Open a terminal in the DosiVox-2D folder

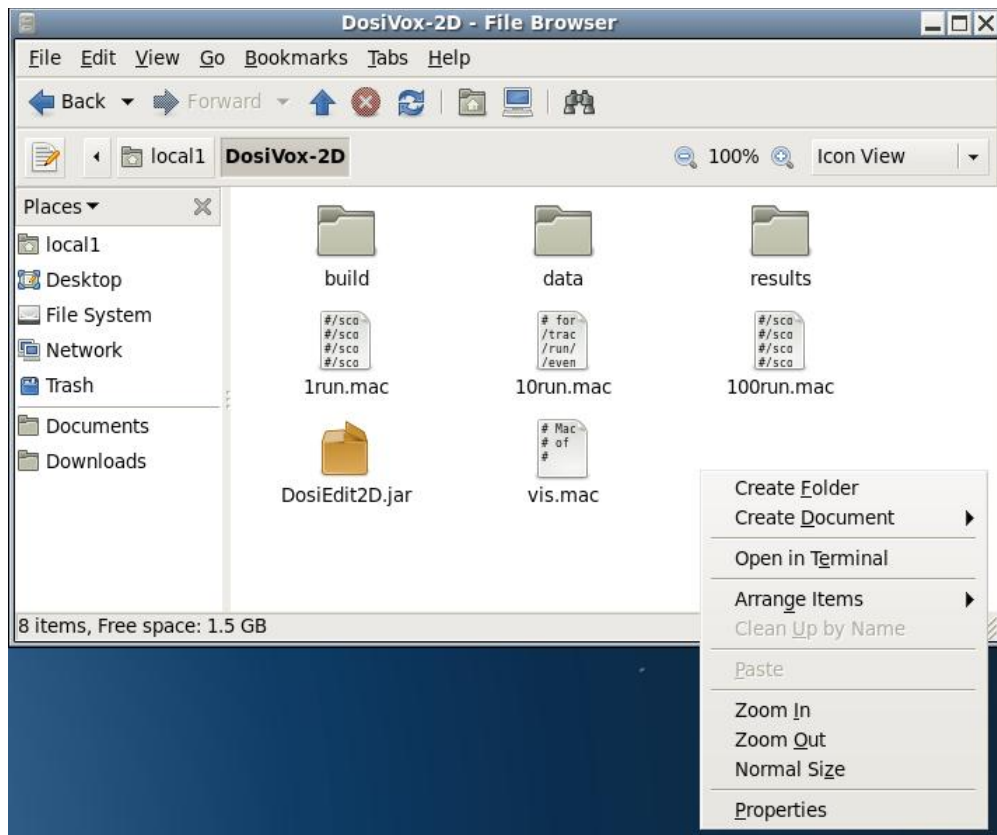
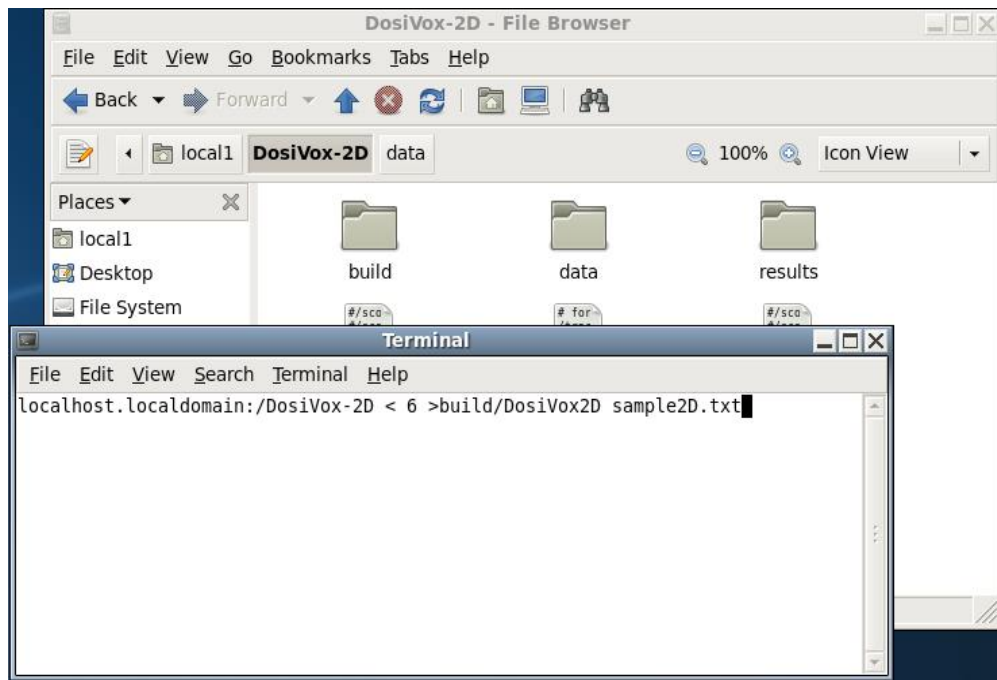


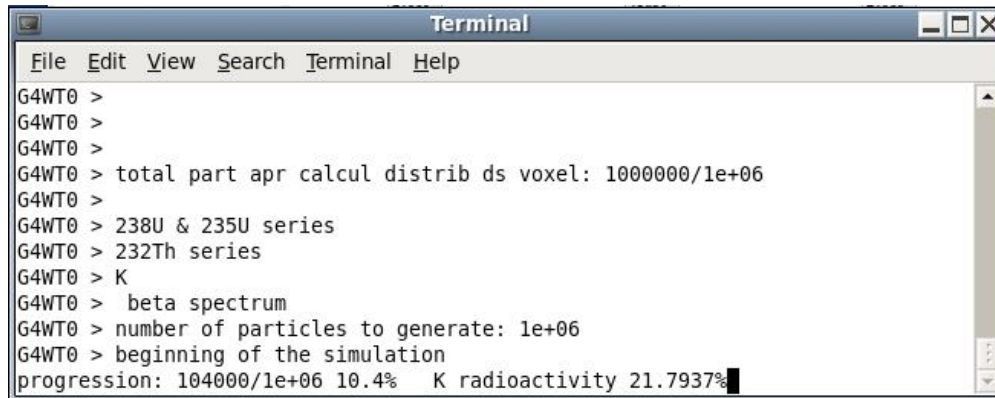
Figure 14: Command line for launching a simulation



You can cancel a simulation launched by using in the corresponding terminal the “control + C” keys. To launch a simulation in the background of the terminal and get back the console line, add the symbol “&” at the end of the command

line for launching the simulation (for example “**build/DosiVox-2D Example.txt &**”). You will be able to enter other command lines in the same terminal (for example to launch several simulations in a same terminal), but you will not be able to cancel a simulation with the “**control + C**” keys (it is still possible to cancel a simulation with the command “kill” followed by the process number of the simulation, see Linux documentation for more information)

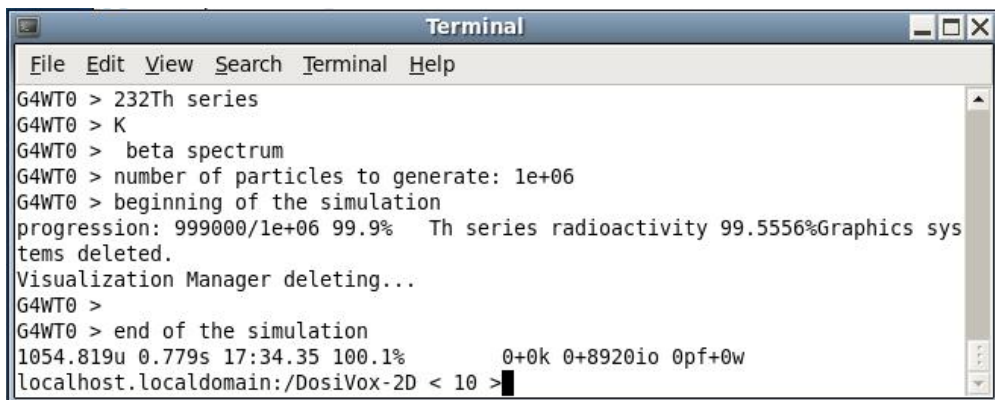
Figure 15: Progression of the simulation

A terminal window titled "Terminal" with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal shows a series of commands and their outputs. The commands are: G4WT0 >, G4WT0 >, G4WT0 >, G4WT0 > total part apr calcul distrib ds voxel: 1000000/1e+06, G4WT0 >, G4WT0 > 238U & 235U series, G4WT0 > 232Th series, G4WT0 > K, G4WT0 > beta spectrum, G4WT0 > number of particles to generate: 1e+06, G4WT0 > beginning of the simulation, and progression: 104000/1e+06 10.4% K radioactivity 21.7937%.

```
G4WT0 >
G4WT0 >
G4WT0 >
G4WT0 > total part apr calcul distrib ds voxel: 1000000/1e+06
G4WT0 >
G4WT0 > 238U & 235U series
G4WT0 > 232Th series
G4WT0 > K
G4WT0 > beta spectrum
G4WT0 > number of particles to generate: 1e+06
G4WT0 > beginning of the simulation
progression: 104000/1e+06 10.4% K radioactivity 21.7937%
```

The progression of the simulation is displayed in the terminal, at a frequency (in percent of the total number of particles to emit) depending of the PTF parameter “clock value” (Fig.15). However, this progression is not exactly proportional to the duration of the simulation, because all the particles do not require the same time to be simulated (depending on their energy, on the cut in range asked, on the materials crossed, on the proximity of the edges of the modelling, ...). The simulation ends when the number of particles requested in the PTF has been simulated. The message “end of the simulation” is displayed in the terminal (Fig.16).

Figure 16: End of the simulation

A terminal window titled "Terminal" with a menu bar (File, Edit, View, Search, Terminal, Help). The terminal shows the continuation of the simulation. The commands and outputs are: G4WT0 > 232Th series, G4WT0 > K, G4WT0 > beta spectrum, G4WT0 > number of particles to generate: 1e+06, G4WT0 > beginning of the simulation, progression: 999000/1e+06 99.9% Th series radioactivity 99.5556%, Graphics systems deleted., Visualization Manager deleting..., G4WT0 >, G4WT0 > end of the simulation, 1054.819u 0.779s 17:34.35 100.1% 0+0k 0+8920io 0pf+0w, and localhost.localdomain:/DosiVox-2D < 10 >.

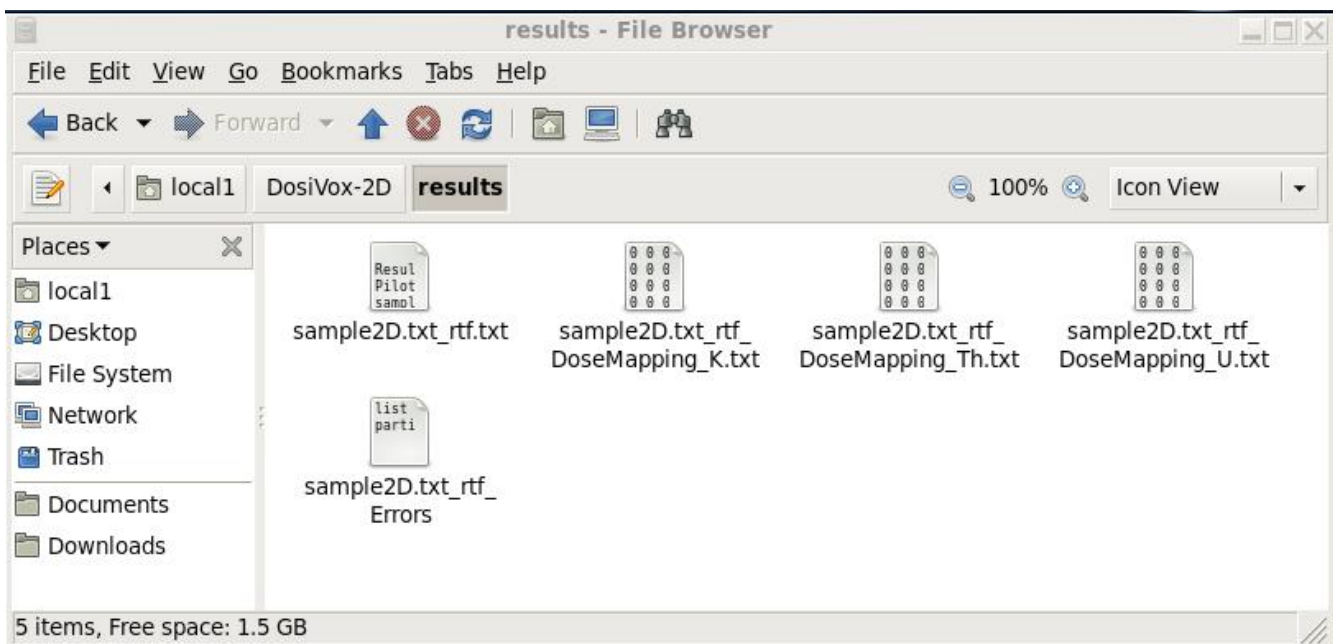
```
G4WT0 > 232Th series
G4WT0 > K
G4WT0 > beta spectrum
G4WT0 > number of particles to generate: 1e+06
G4WT0 > beginning of the simulation
progression: 999000/1e+06 99.9% Th series radioactivity 99.5556%
Graphics systems deleted.
Visualization Manager deleting...
G4WT0 >
G4WT0 > end of the simulation
1054.819u 0.779s 17:34.35 100.1% 0+0k 0+8920io 0pf+0w
localhost.localdomain:/DosiVox-2D < 10 >
```

5 – Result processing

The Result Text Files (RTF)

At the end of each simulation, DosiVox-2D provides 3 types of Results Text Files (RTF), created in the DosiVox-2D/results folder (Fig.17): the first one, with the same name indicated in the first line of the corresponding PTF, is the main RTF, and contains data about EmMass, doses simulated and corresponding dose rates for the bulk sample and for each material. The second type of RTF is the dose rate mapping, that can be recognized by the RTF name followed by the “DoseMapping” and the letter of one of the simulated beta spectra (K for the potassium 40, U for the U-series, Th for the Th-series and Udef for the user defined spectrum). These are the dose rate mapping RTF (one by element simulated). The last RTF is the error file, named by the RTF name followed by “Errors”. It contains a list of particles suppressed during the simulation. Actually, it can happen that particles enter into an infinite loop calculation: a security inside the software stops the simulation of these particles in order to avoid blocking the whole calculation. The total kinetic energy loss because of this process is indicated and compared to the total kinetic energy simulated. Usually, the energy loss is null or negligible in regard to the total energy. If it is not the case, the simulation could be biased, please report it to the support of DosiVox-2D.

Figure 17: the Result Text Files



The main RTF

This file can be opened in any standard text editor or spreadsheet software (import as a non-formatted text file, select “space” as separator and detection of special number), however it is usually easier to read it and process the results using a spreadsheet. It contains a series of data blocks with the dose rate results and the data useful for processing (Fig.18).

(1) The first data block contains information about the whole modelling composition (average content of radioactive element/series, average content of water, average density, ...) and dosimetric results (average dose rates of the bulk). It is preceded by a description line detailing each value or information.

(2) The second data block retakes the same layout, but gives the data for each material. It allows to get the effective beta dose rate in the different material/mineral phases of the sample.

(3) The third data block presents basic histograms (25 channels) of dose rates for each radioactive element/series and for each material. The channels are ranking from the minimum dose rate to the maximum dose rate of voxel for each radioactive element or series simulated. The purpose of these histograms is to give the user a quick view of the dose rate

distributions in the different material/mineral phases. If required, more detailed histograms can be obtained from image processing of the dose rate mappings.

(4) The next data block contains data relative to the size of the modelling: voxel sizes and numbers in the X, Y and Z axis (the Z axis is only mentioned as an additional information).

Figure 18: The main Result Test File (open in a spreadsheet)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1																	
2	Results of the whole sample																
3	Pilote_File	Number_of	Number_of	Average_dens	Average_w	K_AverageC	Series_Ave	Thseries_Av	UserDefined	K_AverageE	Series_Ave	Thseries_Av	UserDefined	K_AverageD	Series_Ave	Thseries_Av	UserDefined
4	sample2D.txt	3	64516	1.71321	12.3881	0.947004	1.61448	4.84345	1.61448	2.44E-006	7.63E-007	4.36E-007	0	2.46E-006	7.61E-007	4.36E-007	0
5																	
6	Results by materials																
7	Material_Nar	material_num	Number_of	density	water_conten	K_AverageC	Series_Ave	Thseries_Av	UserDefined	K_EmMass	Series_Em	Thseries_Em	UserDefined	K_Dose(Gr	Series_Dos	Thseries_Do	UserDefined
8	sediment	0	49569	1.8	14	0.5	2	6	2	1.29E-006	9.45E-007	5.41E-007	0	2.06E-006	8.35E-007	4.83E-007	0
9	quartz	1	3507	2.65	0	0	0	0	0	0	0	0	0	1.19E-006	4.32E-007	2.29E-007	0
10	coal	2	11440	1.05	10	5	0	0	0	1.29E-005	0	0	0	6.41E-006	4.66E-007	2.45E-007	0
11																	
12																	
13	Dose_rate_histogrammes																
14	DoseRate(G	0	0.157712	0.315425	0.473137	0.630849	0.788562	0.946274	1.10399	1.2617	1.41941	1.57712	1.73484	1.89255	2.05026	2.20797	2.36569
15	sediment_K	0.264278	10.2322	30.4626	23.4078	12.1649	7.33119	4.85182	3.60306	2.58831	1.95889	1.30122	0.788799	0.512417	0.266295	0.127096	0.0685913
16	sediment_U	10.6175	66.1764	21.9048	1.28911	0.0121043	0	0	0	0	0	0	0	0	0	0	0
17	sediment_Th	60.0052	38.7682	1.22254	0.00403478	0	0	0	0	0	0	0	0	0	0	0	0
18	quartz_K_dose	16.0821	40.7471	21.8991	9.06758	4.30567	2.90847	1.25463	0.940975	0.912461	0.741374	0.427716	0.342173	0.199601	0.171086	0	0
19	quartz_User	68.5486	30.6815	0.769889	0	0	0	0	0	0	0	0	0	0	0	0	0
20	quartz_Thseries	96.5498	3.45024	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	coal_K_dose	0	0	0.13986	0.664336	1.5472	2.7535	3.72378	4.10839	5.20105	6.26748	7.9021	9.07343	10.7867	10.4545	10.0524	9.09965
22	coal_User	63.2692	34.4668	2.2028	0.0611888	0	0	0	0	0	0	0	0	0	0	0	0
23	coal_Thseries	93.2955	6.61713	0.0874126	0	0	0	0	0	0	0	0	0	0	0	0	0
24																	
25	Dose_rate_mapping_data																
26	Scale	Xaxis	Yaxis	Zaxis													
27	VoxelSize(m	0.1	0.1	8													
28	Number_of	336	336	1													
29																	
30	Dose_rate	MapValue	K(Gray/ka)	Series(Gray	Thseries(Gr	UserDefined(Gray/ka)											
31	Minimum_va	1	0.00339553	0	0	Non-simulated											
32	Maximum_va	65535	3.94281	0.735905	0.522926	Non-simulated											
33																	

(5) The last data block is the calibration values (minimum and maximum dose rates for each of the element/radioactive series simulated) for the dose mapping results. The minimum dose rate and maximum dose rate of the voxels are associated with their corresponding values in the dose mapping matrices, for a linear calibration in Gy/ka.

The dose rates for each radioactive element/series presented in the result files are calculated according to the following formula:

$$Dr_x = Dose_x / EmMass_{bulk} \cdot Content_{bulk} \cdot F_c$$

Where Dr_x (Gy/ka) is the dose rate of the material x, $Dose_x$ (Gy) is the dose recorded during the simulation by the voxel containing the material x, $EmMass_{bulk}$ (Gy) and $Content_{bulk}$ (in ppm or percent) are respectively the quantity of kinetic energy by unit of mass simulated and the average content of the corresponding radioactive element/series over the whole modelling. F_c (Gy/ka/ppm or Gy/ka/percent) represents the conversion factor for content of radioactive element (according to the particle type and to the element/series considered) to dose rate. The conversion factor, given at the first line of each spectrum text file (in the folder DosiVox-2D/data/spectra), is by default from (Guérin *et al.*, 2011), but the user is free to replace it with the factor he prefers.

If the objects of interest are grains inside one of the material/mineral phases of the modelling, the dose rate calculated for this phase can be considered as the dose rate coming from the environment containing the grains. Therefore, it is possible to calculate the dose rate in grains just by applying an attenuation factor for moisture (Zimmerman, 1971, Nathan and Mauz, 2008) and grain size (Aitken, 1985, Guérin *et al.*, 2012). However, users have to consider that these tabulated factors were calculated for environments with poor and scattered grains fraction, surrounded by a homogeneous fine matrix. Published data show that they may not be suitable for materials presenting a significant coarse fraction of grains (Guérin and Mercier, 2012) or if the material contains radioactive hotspots that are not represented in the modelling (Guérin *et al.*, 2012). However two particular cases can be highlighted: if the grain size is very small compared to the particle range (as it is for fine grains under 10µm and beta particles) or if the grain fraction totally fills the material (for example if the material is composed of an agglomerate of grains of the same mineral), then there is no need to apply attenuation factor for grain size as the dose rate received by the grains will be the same than in the material/mineral phase. However it is still necessary to remove the part of the dose rate absorbed by the moisture.

The dose rate mappings

The dose mapping results are text matrix with the same layout than the 2D image used for the model creation. Each value of the matrix represents the dose rate recorded by the voxel at this location. There is one mapping file by element simulated, plus a total dose rate mapping file. These files can be opened into a spreadsheet, or read as a 16 bit text image (with ImageJ for instance). The dose rate of each file is distributed from the values 1 (corresponding to the minimum dose rate of a voxel) to 65535 (maximum value of a 16bit image, corresponding here to the maximum dose rate of a voxel). The value “0” corresponds to the EEZ (Edge Effect Zone) when it is excluded from the results or to the materials not represented if you chose the dose mapping option for one material only (see part 3). To calibrate the dose mapping files in Gy/ka (linear calibration), use the values of the last data block of the main result file.

In addition to the visualization of the dose rates, the dose mapping files, once calibrated, allow to use image processing for investigating dose rates distribution. It is therefore possible to obtain histograms of dose rates distribution for different areas of the modelling. You can also isolate the dose rates in a material/mineral phase using the original segmented image of the sample slice by creating ROI (Region of Interest) or a binary mask of the material/mineral phase, and applying it to the dose mapping (<https://imagej.nih.gov/ij/>). It is also possible (by using for example the mathematical process of ImageJ or a simple spreadsheet) to apply attenuation factors for moisture and grain size (when required) to the dose mapping or to a ROI, and also to add/average different dose mappings together (once the attenuation factor are applied for example, or if several simulations were carried on with the same modelling). Notice that if you use the ImageJ software, it is recommended, once the dose mappings have been calibrated as 16bit images, to convert them in 32bit images. More process options will be available, and the results of the mathematical processes will be more accurate.

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DosiVox-2D and corresponding documentation are available at <http://www.iram-at-crp2a.cnrs.fr/spip/spip.php?article144>.