DosiVox-2D
User Manual

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1 – Introduction

Principles

DosiVox-2D is a software designed to simulate the beta radioactivity and calculate the dose rate in heterogeneous isotropic samples (e.g., rock and sediment; Martin et al., 2017). It is derived from DosiVox (Martin et al., 2015a, Martin et al., 2015b, Martin et al., 2015c), and created with Geant4 toolkit (Allison et al., 2007). DosiVox-2D is based on the concept of 2D-modelling, in which beta particles are simulated in a representative surface of the sample. For simulation,

2D geometry can be manually built or uploaded from a mapping image. Each voxel contains the information of constituting material (chemical composition, density, moisture, radioactive element contents) and records the doses generated by K, U-series, Th-series or any user-defined spectrum. The results are given as an average dose rate of the bulk sample, an average dose rate and dose distribution histogram of each material and a dose rate distribution map of the sample.

Requirements

The input data required and unavoidable considerations are listed below for creating a model with DosiVox-2D. One should keep in mind that a modelling reflects the input parameters and the user-defined approximations, which may not perfectly represent the reality.

**DosiVox-2D applies to isotropic samples** (i.e. the distribution of different materials/grains/heterogeneities is similar, in terms of probability, in all directions; Martin et al., 2017; Underwood, 1970). The isotropic condition is required at the beta particle scale (millimeter to centimeter), which means a layer (e.g., a sedimentary layer) can be locally isotropic if its constituting materials are well mixed, even if this layer is actually an anisotropic object in a larger scale. In such case, 2D-modelling can be performed on a sample slice from this layer. The crucial point is to get a sample slice for the 2D-mapping representative to the whole sample, in terms of material proportions and distributions. It is noticeable that 2D-modelling seems to give reliable results in case of slight anisotropy, like a a partial or small ranged layering (Fang et al., 2017).

If the sample is perfectly isotopic, a slice can be cut from any direction: every possible slice is 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 co variograms of the main granulometric fractions should reach a plateau.

**2D mapping of a representative slice is prerequisite to construct a model.** 2D image processing techniques are used depending on the sample size and the chosen magnification: SEM-EDS (Scanning Electronic Microscope – Energy Dispersion Spectrum), µXRF (micro-Xray Fluorescence), QEM (Quantitative Element Mapping), LA-ICP-MS (Laser Ablation – Inductively Coupled Plasma – Mass Spectrometer), polarising microscope photography, multispectral camera, etc. Some techniques can acquire quantitative information of the material, which is 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 µm. A higher resolution could limit the representativeness of the modelling, and a smaller one would often lead to unnecessarily heavy simulations. However, in the case of the presence of small grains of interest (grains for dating, or higly radioactive grains like zircon), it can be necessary to choose a resolution for which they will be accurately represented (in term of proportion mainly, as the shape of small grains will have low effect on the beta dose rate). The image from a 2D-mapping must be segmented, i.e. each material/mineral phase must be represented by a specific shade of grey in the image (Fig.1). It must be exported as an 8 bit image (in shades of grey, not in color) in TEXT image format (.txt extension), what can be done preferentially in using the free software ImageJ (https://imagej.nih.gov/ij/, Rasband, 1997-2012) or using standard spreadsheet software (Microsoft Excel).
Excel, OpenOffice Calc, LibreOffice Calc, etc.). This format corresponds to an ASCII matrix representing the shade of grey of all pixels.

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

The chemical composition (at least the major elements) of the each material presents in the sample is required. The chemical compositions can be defined in several ways: by percent of oxides, 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 the 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 (when 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 concentrations and by the corresponding beta dose conversion factor. If 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.

The concentrations of radioactive elements (K, U-series, Th-series or/and user defined beta spectrum) must be defined for each modelled material. These values are possible to be adjusted manually for each voxel. DosiVox-2D provides the beta energy spectrum of the K, the U-series and the Th-series (both at secular equilibrium). Besides, 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, the first column lists the energies of the emitted beta particles (in keV) and the second column gives the cumulative probabilities of these energies. The concentrations of radioactive elements can 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 from the quantitative mineral mapping, but the U and Th concentrations are usually under the detection limit.
2 – Installation

The DosiVox-2D software works under Linux environment. It was developed with Scientific Linux 6.4 (Red HatTM), running on the Geant4 Virtual Machine developed by the Centre d'Etudes Nucléaires de Bordeaux-Gradignan, France (Incerti et al., 2010). This virtual machine contains the Geant4 libraries, which are necessary for running DosiVox-2D, or for compiling the source code, if non-compilated or modified codes are used.

The provided instructions are given for a PC with the following setup:
# Windows 7, 64 bit  
# Memory: min. 4 GB

**Download virtual machine and DosiVox-2D.**


**Installing the virtual machine player**

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

Run the virtual machine player and choose to open a Virtual Machine (browse and select the file sl6 x64: vmdk). The properties of the machine can be modified in editing virtual machine settings. For further information, please read the README file at [ftp://ftp.cenbg.in2p3.fr/info/Vmware/Old-Versions/g4.10.01.p01/](ftp://ftp.cenbg.in2p3.fr/info/Vmware/Old-Versions/g4.10.01.p01/).

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".

The virtual machine works as an independent computer on the user PC or Mac. All the data in the virtual machine are not automatically 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.

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

The DosiVox-2D folder contains three sub-folders: build, data, and 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 contain the Pilot Text Files (PTF) for running simulations. The results folder contains all simulation results.

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

The graphical interface DosiEdit2D

DosiEdit2D is a user-friendly Java Graphical User Interface (GUI) for creating Pilot Text Files (PTF) for DosiVox-2D simulations. You cannot directly run a simulation in DosiEdit2D. This interface runs on any computer with a Java (8 or superior) environment. To launch it, double-click on the DosiEdit2D.jar file.

Create/load a project

At the start of DosiEdit2D, one can choose either to create a new project, or editing a previous project (Fig.2).

Figure 2: Interface starting window

Creation of materials

When creating a new project, the first step is to create all materials (i.e., different phases in the modeling) for building the geometry of simulation. These materials could be basic minerals (e.g., quartz, carbonates or feldspars), or mixtures of minerals (e.g., sand, clay), or others (e.g., air, ashes or bone). For material creation, you need to know its chemical composition (at least the major elements), density and moisture content. In the modeling, we assume all above properties are uniform in a material/mineral phase, which can be obtained from sample analysis (e.g., the chemical composition can be provided by an SEM-EDX scan of the slice) or literatures (the density and moisture can be difficult to determine accurately but standard values can be found in literatures). The accuracy of modelling results directly depends on the input data, and thus we recommend testing different hypotheses on the missing data to investigate its influence on the dose rate if accurate analyses are not available.

In the DosiEdit2D interface, on the “Forge” tabulation (Fig.3) (1), click on the “Create new material” button (2) to add a new material in the material list (3). You can edit the name of material in the box at the top of the tabulation (4), and press “enter” key to validate the name. For setting the chemical composition, 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 (7). You can then set their mass proportion by selecting one component in the composition list, making the correct proportion in the “Change mass percentage of the selected component” box (8) and pressing the “enter” key. The “total mass %” of all components must add to be 100% for validating the material.

If a material requires a component not in the component list, you can create it with the “component factory” (Fig.4). Click “show/hide component factory” button (9) to display or hide. 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)
The component can be set by constructing its chemical formula using 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 define the density in the box “Density (g/cm3)” (15). 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 in the Forge, that only contains this component.

Setting the density for a material, you can use the density automatically calculated from its components, or manually with a theoretical/experimental value. 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. It can be set in “Water fraction in current material” box (18) and validate with the “enter” key.

Repeat the process of new material creation until all materials required are ready for modelling.

Figure 3: Forge tabulation
Parameters of the simulation

When all the required materials are created, you can go to the “Editor” tabulation (Fig.5). This tabulation allows setting the various parameters, create and edit the geometry of the modelling.
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 primary particles (usually beta particles) that is going to be generated during simulation. The accuracy of the simulation will be increased by using a larger number, but the simulation time will last longer. For a standard modelling, 100 000 (x1000) particles can provide good accuracy and need about few hours to one day of calculation on common computers (it is common for Monte-Carlo dose rate simulations to last more than few days).

**WARNING:** The DosiVox-2D 0.9 version cannot 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 of displaying simulation progression, in percent of particles simulated. The smaller this value, the higher the display frequency of the progression. However, a high frequency (more than one display per second) may slow down the simulation speed. The default value is 1%, indicating every 1% change in the total number of emitted particles will be displayed.

- **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 for calculation. Be careful to not assigning more than the number of cores available in the virtual machine where the software runs.

- **Primary particle emitted:** The type of primary particles generate during simulation. Only beta particles have been tested in DosiVox-2D at the moment, but the user remains free to use alpha or gamma particles. Other particles may appear from the interactions of the primaries with the matter (X-rays, secondary beta particles, etc.), and 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 out to investigate its potential usage.

- **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, U-series and Th-series (series at secular equilibrium). The “Ud” means a user defined spectrum, and this file is in the folder DosiVox-2D/data/spectra. You can implement it to create your own spectrum in a similar way as other available spectra, which can be used for simulating a disequilibrium environment.

- **Particle average range (in mm):** The average range of the chosen particle in simulation (usually few millimeters for beta particles), which is used for determining the area with potential edge effects (edge effect zone, EEZ). The edge 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 (proportional to their remaining energy). The accuracy of the simulation can be increased with a smaller value, but the simulation speed can be slow down (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. For beta particles, the cut in range value is recommended to be no smaller than 0.001 mm.

- **Material for dose mapping:** This option allows selecting at least one material for the dose mapping (see part 5). It simplifies the processing of the dose rate mapping if you are only interested in a particular material. The average
dose rates and dose distribution histogram of all materials are still provided in the main result file, but these phases will not show in the dose rate mappings. If you prefer to get the mapping of all materials, just let the option to be “All materials”. You will be able to separate the dose rate mapping for each material by post 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 file. 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 (when the statistical isotropy of the modelling is respected), uncheck this box.

- **Voxel description:** The sizes of the voxel in X and Y direction, corresponding to the resolution of the 2D image in these directions, are required here. The voxel value is automatically generated when loading the 2D geometry from an image, or can be set when manually creating the geometry.

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 before loading a 2D image. Otherwise, the saved file will be too heavy and reloading it may take a long time and cost large memory. 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**

For building the geometry, a 2D 8bit image with grey scale in TXT format (available in standard spreadsheet software or the image processing software ImageJ) is required. Each material/mineral has to be segmented, corresponding to a specific grey shade.

When 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 will appear in the interface displaying all images available in the folder (Fig.6). From it, you can select the image (Fig.1) by clicking on it and the “Validate the select image” button at the top of the window.

Figure 6: Image selection window
Another window will appear displaying the created materials and the shades of grey of the image. From it, you can associate each grey value (Fig.7) with a material (select them both) and input its K, U, Th and Ud (representing the element associated with the user defined spectrum) concentrations in the boxes. If you do not know the concentration of any radioactive elements or do not want to simulate it, set the value to be “0”. 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. The current window and image will be closed then, and associations will be displayed in the “Editor” tabulation (Fig.8). One should be noticed that a material can be associated to different grey shades, but a shade can only be linked to one material. If necessary, a material can be created in this window as well, but its properties needs to be specified in the “Forge” tabulation. Additionally, you can clear any association of shade/material/radioactive element concentration by selecting it in the list on the right, and clicking on the “clear the selected association” button.

Figure 7: Association window

The interface provides various tools for modifying the material and the concentrations of radioactive elements loading the image. To do that, you can select a material in the list at the right bottom of the Editor tabulation (Fig.5), and set the requested concentrations 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 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 modifying all the voxels in a selection square. Be careful: there is no “undo” button. Besides, it is also possible to modify the content of radioactive elements directly 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 concentrations of these elements in all voxels filled with 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 in 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 concentrations of radioactive elements/series can be set in the “Radioactive Element Contents” boxes (Fig.5).
Create the PTF

DosiVox-2D uses a system of pilot text file (PTF) to run the simulation. To create the PTF corresponding to your 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).
Figure 9 Generate the PTF

![PTF Generation](image)

Figure 10 PTF checking

![PTF Checking Alert](image)
The Pilot Text File (PTF)

The PTF is an ASCII format text file containing the information of the sample and parameters for simulation. This file is read by the DosiVox-2D software when running a simulation. The concept is inherited from the DosiVox software (Martin et al., 2015a), and allows modifying the simulation parameters (e.g., the number of particles simulated, or the moisture of a material) easily with any text editor software without reloading the entire project into the interface. It is also a convenient way to transfer a modelling from a computer to another since PTF can be easily sent in attachment of an email or by SSH connection. It is also possible to create a modelling by directly writing or editing a PTF, but one should follow its layout rules, otherwise DosiVox-2D cannot read the file.

The simulation data are represented by numbers in the PTF (integer or floating-point numbers) organized in different lines and different blocks. The description of the data of each line (seen as a comment by the software, and then not interpreted) is given at the end of the corresponding line after the symbol « # ». An example of PTF was presented in Fig.11, followed by the description of the different blocks:

- The first line (1) is the name for the results file (or RTF, see part 5).
- The first block contains general parameters of the simulation (2), e.g., the number and type of the particles to generate, and the radioactive element and/or series to simulate.
- The following series of blocks describes the new components created for this case (3). Each component is characterized by an index (start with 18, the indexes 0 to 17 correspond to the basic components available in the interface), its name, its, the number of elements it contains, and the element composition data (symbols and numbers of atoms).
- The second series of blocks describes the different materials filling the voxels (4). Each one is characterized by an index, which is used to create the geometry. The detailed material information is present, including material name, density, moisture content, and the properties of each component.
- After the material description, a data block defines the voxel grid, including voxel sizes and numbers in X and Y directions (5).
- The first matrix below (6) represents the material in each voxel of the grid. The size of the matrix is that of the grid, and the number is the material index which represents a material in a voxel.
- The four following matrices, sharing the same layout as the material mapping matrix, representing the map of the radioactive element concentrations. The order of the matrices is $^{40}$K, 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. The main rules and advices are:

- You must follow the layout and the order of the data blocks presented above.
- The data blocks, the components and the materials must be separated by 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 index of the new components starts at “18” (because 0-17 are attributed to pre-created components), those of the created material at “0”.
- The unit of the U, Th and Udef mapping is ppm. The unit of the K mapping is %.
Figure 11: Example of Pilot Text File
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. The terminal must be opened under the DosiVox-2D/ folder (Fig.12), by right-clicking the folder and selecting “Open in Terminal” (Fig.13). You can open as many terminals as you need to launch several simulations in parallel. If a terminal is opened a different address other than 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 Linux command, see the Linux documentation.

WARNING: The DosiVox-2D_0.9 version cannot 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 the command “build/DosiVox2D” 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 are 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 limit 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 (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

![Terminal](image)

The progression of the simulation is displayed in the terminal, at a frequency (in percent of the total number of particles to emit) depending on 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 simulation time (depending on the energy, the cut in range asked, the materials crossed, the proximity of the edges of the modelling, etc.). The simulation ends when the particles requested in the PTF have been simulated. The message “end of the simulation” will be displayed in the terminal (Fig.16).

Figure 16: End of the simulation

![Terminal](image)
5 – Result processing

The Result Text Files (RTF)

DosiVox-2D provides 3 types of Results Text Files (RTF) in the end of each simulation, created in the folder DosiVox-2D/results (Fig.17). The first file, with the same name as 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, which can be recognized by the RTF name followed by the “DoseMapping” and the letter followed indicates the simulated beta spectra (K for the potassium 40, U for the U-series, Th for the Th-series and Udef for a user defined spectrum). 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), while it is usually easier to read 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 bulk of the modelling (average content of radioactive element/series, average content of water, average density, etc.) and dosimetric results (average dose rates of the bulk). It is preceded by a description line detailing the nature and unit of each data.

(2) The second data block retakes the same layout, but gives the data for each material. It allows getting 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 provide 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 additional information).

(5) The last data block is the calibration values 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:

\[
\text{Dr}_x = \frac{\text{Dose}_x}{\text{EmMass}_{\text{bulk}}} \times \text{Content}_{\text{bulk}} \times F_c
\]

Where \(\text{Dr}_x\) (Gy/ka) is the dose rate of the material \(x\), \(\text{Dose}_x\) (Gy) is the dose recorded during the simulation by the voxel containing the material \(x\), \(\text{EmMass}_{\text{bulk}}\) (Gy) is the quantity of kinetic energy by unit of mass simulated, \(\text{Content}_{\text{bulk}}\) (in ppm or percent) is 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 DosiVox-2D/data/spectra), is by default from (Guérin et al., 2011), but user is free to replace it with the preferred factor.

Figure 18: The main Result Test File (open in a spreadsheet)
If the objects of interest are grains included in one of the material/mineral phases of the modelling, the dose rate calculated for this specific phase can be considered as the dose rate of the environment of 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 as the 2D image used for the model creation. Each value of the matrix represents the dose rate recorded by the voxel at its location. The results provide mapping files for each simulated radionuclide, and 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 16 bit image, corresponding to the maximum dose rate of a voxel). The value “0” may correspond to the EEZ (Edge Effect Zone) when it is excluded from the results or the materials not selected for dose mapping (see part 3). To calibrate the dose mapping files in Gy/ka (linear calibration), use the values of the last data block in the main result file.

In addition to the visualization of the dose rates, the dose mapping files, once calibrated, can be used to investigate the dose rates distribution. Therefore, it is possible to obtain histogram of dose rates distribution from different areas of the sample. You can also isolate the dose rate of any material/mineral phase using the original segmented image by creating a ROI (Region of Interest) or a binary mask of that phase, and then apply to the dose mapping (https://imagej.nih.gov/ij/). Additionally, it is 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 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 to convert the image to 32bit images once the dose mappings were calibrated as 16bit images.
6 – References


Martin, L., Incerti, S., Mercier, N., 2015c. Comparison of DosiVox simulation results with tabulated data and standard calculations. Ancient TL 33 n°2, 1-9


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