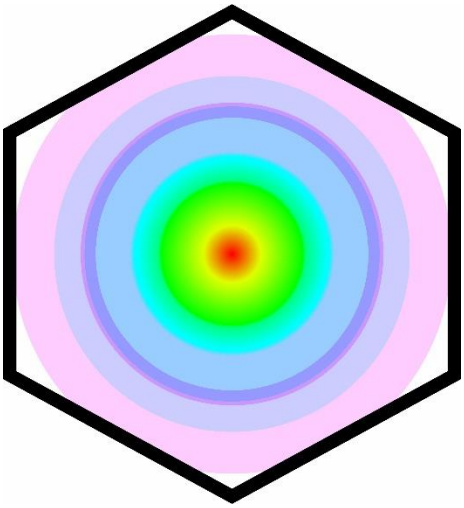
DIFFUSUP User's Guide

Software for Diffusion Simulation



2023.08 by Junxing Chen, Xu Chu

Version 1.13

DIFFUSUP is an advanced software solution specifically designed for performing diffusion modeling tasks. Its intuitive user interface and comprehensive toolbox enable users to simulate multi-component diffusion processes under a wide range of thermal and chemical conditions. Built on the MATLAB platform, DIFFUSUP employs the Crank-Nicolson algorithm to ensure accurate modeling results. As a stand-alone software available for free download, DIFFUSUP provides an accessible option for anyone intrigued by diffusion modeling.

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Please be aware that the creators of DIFFUSUP bear no responsibility for any damages or issues that may arise from the use or modification of the software. Users must take full responsibility for adhering to all relevant laws and regulations pertaining to their utilization of DIFFUSUP.

Acknowledgement

We would like to extend our heartfelt gratitude to Zhenhao Zhou, Yi Zou, Ozan Akca, and other contributors who offered invaluable guidance and recommendations throughout the development process. Their insights were instrumental in ensuring the success of this project. Furthermore, we gratefully acknowledge the support provided by the University of Toronto and the Discovery Grant from the Natural Sciences and Engineering Research Council of Canada.

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Menu

1. Before You Use DIFFUSUP:

1.1 General information

- DIFFUSUP is a specialized software package created for simulating diffusion profiles. It utilizes the finite difference Crank-Nicholson method (Crank & Nicolson, 1947) to calculate the modeled results.
- Developed in MATLAB, DIFFUSUP is a stand-alone software, allowing users to download, install, and operate it without requiring MATLAB or prior programming experience.
- MATLAB Runtime R2020b is necessary. If MATLAB Runtime R2020b is not already installed on your computer, the DIFFUSUP installer will assist you in automatically installing it (refer to Section 1.3).
- Please be aware that compatibility issues may arise with other versions of MATLAB Runtime when using DIFFUSUP.

1.2 System requirements

Operating System Supported:

- Windows® 7, 8, 10, 11 are all supported. Older versions such as Vista or XP are not tested.
- MacOS 10.12-11 and newer versions are also supported. For Macs with M-series chips, if you experience any issues while using Rosetta 2 to translate the software from X86 to ARM, please reach out to the author.
- A Linux version will be available soon.

Hardware Requirement:

- A minimum disk capacity of 2 GB is necessary for the server software installation and log files.
- At least 1 GB of RAM is required; however, for enhanced performance, we recommend having 2 GB of RAM or more.
- To achieve optimal performance, it is advised to allocate one processor core (or virtual core) per worker to be deployed.
- Superior hardware will lead to an improved user experience.

Developer's Computer Configuration:

- Operating System: Windows 11/Windows 10 Home
- CPU: AMD Ryzen 7 3700X or Intel Core i7-9700K

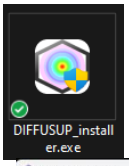
- RAM: 64 GB Kingston HyperX Fury RGB 3200MHz (8 GB is sufficient for smooth use)
- SSD: WD Blue SN550 NVMe M.2 1TB + WD Blue 1TB 3D NAND SATA III Internal Solid State Drive
- GPU: Single graphics card is NOT required, but the author uses an MSI GeForce RTX 3070 VENTUS 2X OC 8GB.

1.3 Download Installation & Running

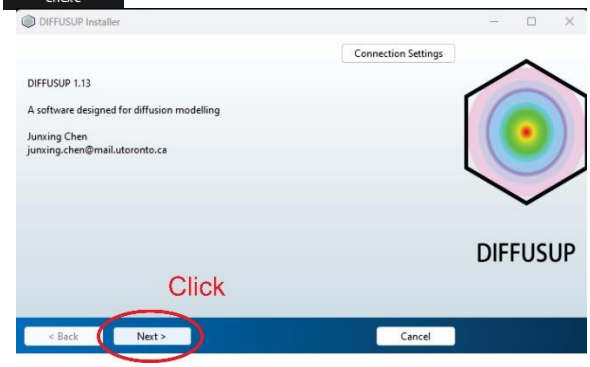
1.3.1 Where to download & future updates

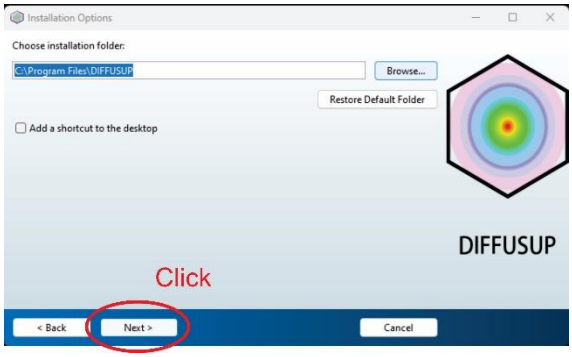
- The DIFFUSUP + MATLAB Runtime R2020b installation package can be obtained from the website: www.diffusup.org
- For the most recent version of the DIFFUSUP + MATLAB Runtime R2020b installation package, please contact the authors at junxing.chen@mail.utoronto.ca or yxzhhw@gmail.com.
- MATLAB Runtime R2020b can be downloaded for free from its official website: https://www.mathworks.com/products/compiler/matlab-runtime.html.
- Stay up-to-date with the latest enhancements by visiting www.diffusup.org. A summary of new features can be found in the "New Functions.txt" file within the installed DIFFUSUP folder.

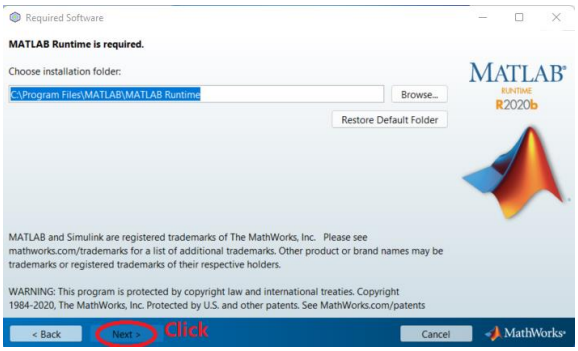
1.3.2 Windows installation



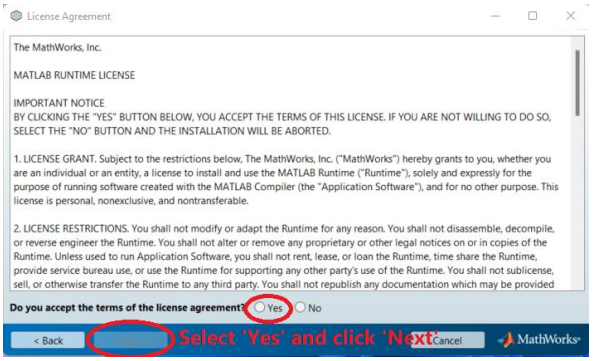
- To initiate the installation, double-click on "DIFFUSUP_installer.exe" and follow the Windows system settings until you arrive this window:

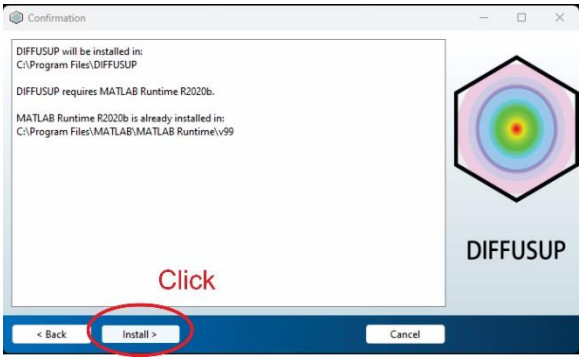


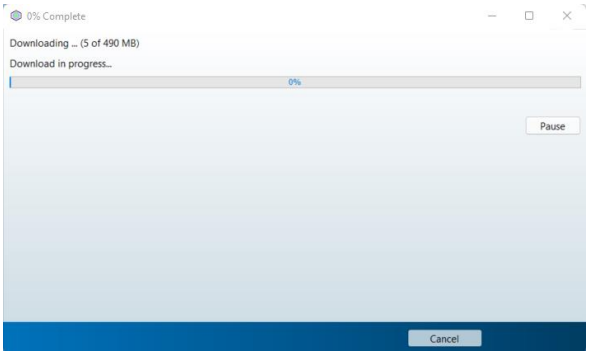




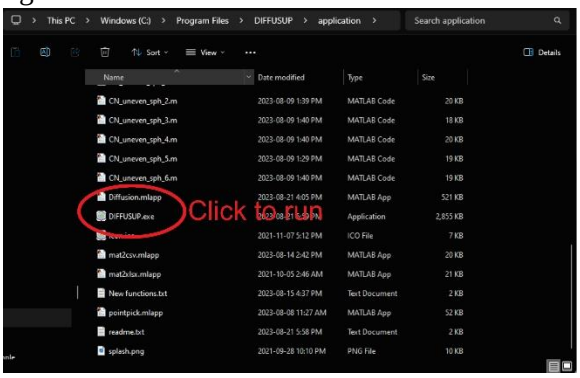
- Click "Next" to choose the installation location for DIFFUSUP, then click "Next" again.
- Select the installation location for MATLAB Runtime R2020b, and click "Next".
- Accept the agreement, and click "Next" to commence the installation.







- Proceed with downloading and installing MATLAB Runtime R2020b.
- Allow the installation process to finish.
- Click "Finish" to complete the installation, and begin using DIFFUSUP.
- The default folder location is C:\Program Files\Diffusion\application. Launch DIFFUSUP by clicking "DIFFUSUP.exe".



- Caution: Ensure that the folder path contains only Latin (English) characters.
- Default folder path (Window 10/11) : C:\Program Files\DIFFUSUP\application\

1.3.3 MacOS setup

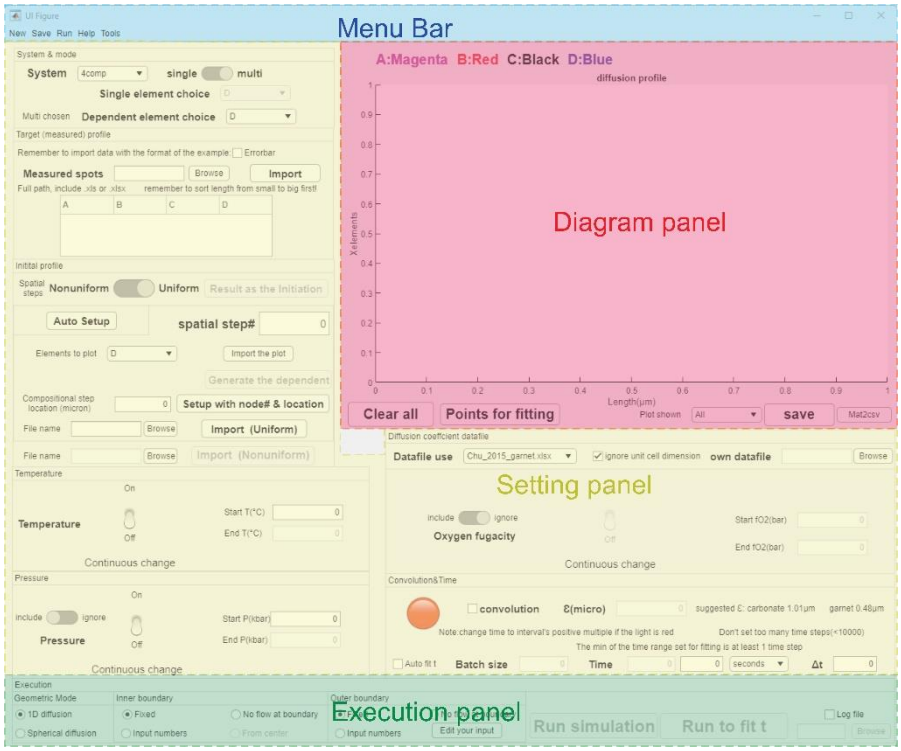
Similar steps as the Windows ones shown in 1.3.2.

- Double-click the DIFFUSUP package. Click "Continue" and accept the license agreement.
- Select the desired location for installing DIFFUSUP, then click "Install."
- Enter your Mac's administrator password and click "Install Software".
- Proceed with downloading and installing MATLAB Runtime R2020b.
- While waiting, feel free to enjoy a cup of coffee.

- Click "Close" and start exploring DIFFUSUP.
- The default folder is located at: Application\Diffusion\application. Click "Diffusion" to launch DIFFUSUP.
- Caution: Ensure that the folder location address contains only Latin (English) characters.

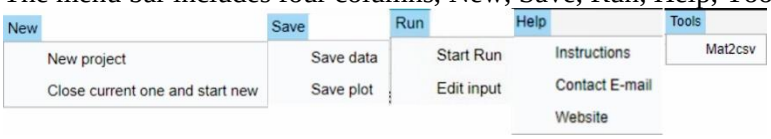
2. Interface

There are four main sections in DIFFUSUP: the menu bar, the setting panel, the execution panel, and the diagram panel.

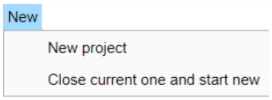


2.1 Menu bar

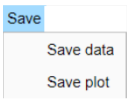
The menu bar includes four columns, New, Save, Run, Help, Tools.



- "New" - Start a new diffusion model project. You have the option to initiate a new project without closing the current one, or you can close the current project and then start a new one. The new project interface will appear at the default position. To avoid overlapping, be sure to move the old project interface before opening the new one, as the new interface will otherwise cover the previous one.

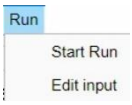


- "Save" - By clicking the "Save data" button, you can store crucial information used in the modeling process, such as modeled profiles, the initial profile, measured profiles, time steps, and spatial nodes (length steps + 1), among other data. This information can be utilized to verify and reproduce your modeled results. The "Save data" button serves the

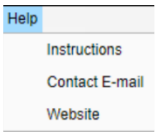


same purpose as the "Save" button found in the diagram panel. Additionally, you can directly export your modeled diagram results by clicking the "Save plot" button.

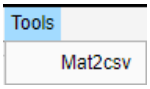
- "Run" - Begin the modeling process swiftly using the two options in the "Run" column. These options allow you to modify the boundary input or initiate the modeling. Unlike the buttons in the "Execution panel", the choices in the "Run" column are always clickable. Ensure that the settings are accurate before clicking on them, as selecting these options without completing the settings might lead to an error.



- "Help" - To report bugs or get in touch with the author, navigate to the "Help" column and click on the relevant option. This will allow you to access the instruction manual, visit the website, or send an email to the author. The "Help" column is self-explanatory and does not necessitate further clarification.



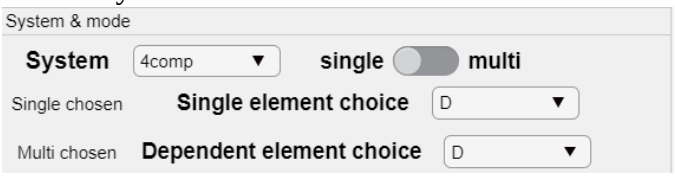
- "Tools" - Discover handy tools to enhance your experience with DIFFUSUP. At present, the sole available tool is "Mat2csv", tailored for users who do not have MATLAB. This tool enables you to convert the .mat output from DIFFUSUP into an .csv file, which can then be accessed and analyzed according to the specific requirements. Furthermore, you have the option to enable automatic saving of log files after each simulation, ensuring convenient record-keeping and documentation of their diffusion modeling processes.



2.2 Setting panel

The 8 subpanels cover setting of "System & mode", "Target (measured) profile", "Initial profile", "Temperature", "Pressure", "Oxygen fugacity", "Diffusion coefficient datafile", "Convolution & Time"

2.2.1 System & modes

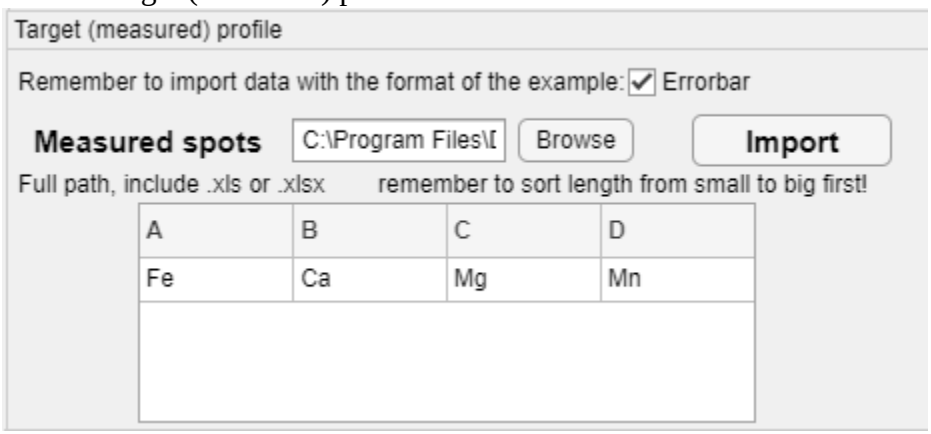


The "System & Modes" subpanel determines the diffusion system to model. The "single" - "multi" switch indicate whether the interactions between diffusion elements are considered. If you select "multi", the software takes into account the interactions among diffusion elements. The "System" dropdown is designed to define the number of elements considered in your system, allowing up to four elements. It is essential to declare the number of elements before modeling. In this case, it is necessary to import or generate the measured and initial profiles for all elements. When choosing "multi" for three or more

components, you need to specify the dependent element for modeling. In case of "single"-component, you must select the species to model.

For instance, if you want to model the multi-component diffusion of Ca, Mg, Fe, and Mn in garnet with Ca as the dependent element, select "4comp", "multi", and one of the "A", "B", "C", "D" as the dependent. Then, import the data file with Ca as the chosen alphabet in the subsequent "Target (measured) profile" subpanel. If you want to model Ca as the only single element diffusion in garnet using the same data file, choose "4comp", "single", and one of the "A", "B", "C", "D" as the single element choice, then import the data file with Ca as the chosen alphabet in the next "Target (measured) profile" subpanel. The same concept applies to a 3-component system. You can find detailed examples in section 3.

2.2.2 Target (measured) profile



The "Target (measured) profile" subpanel allows you to import measured data, which serves as the target profile to be fitted. Error bars are optional. To import the file, enter the complete file path, including the file name and extension, in the provided blank. Alternatively, click the "Browse" button to locate the file. Supported file formats include .txt, .dat, .csv, .xls, .xlsb, .xlsm, .xlsx, .xltm, .xltx, .ods, and .xml.

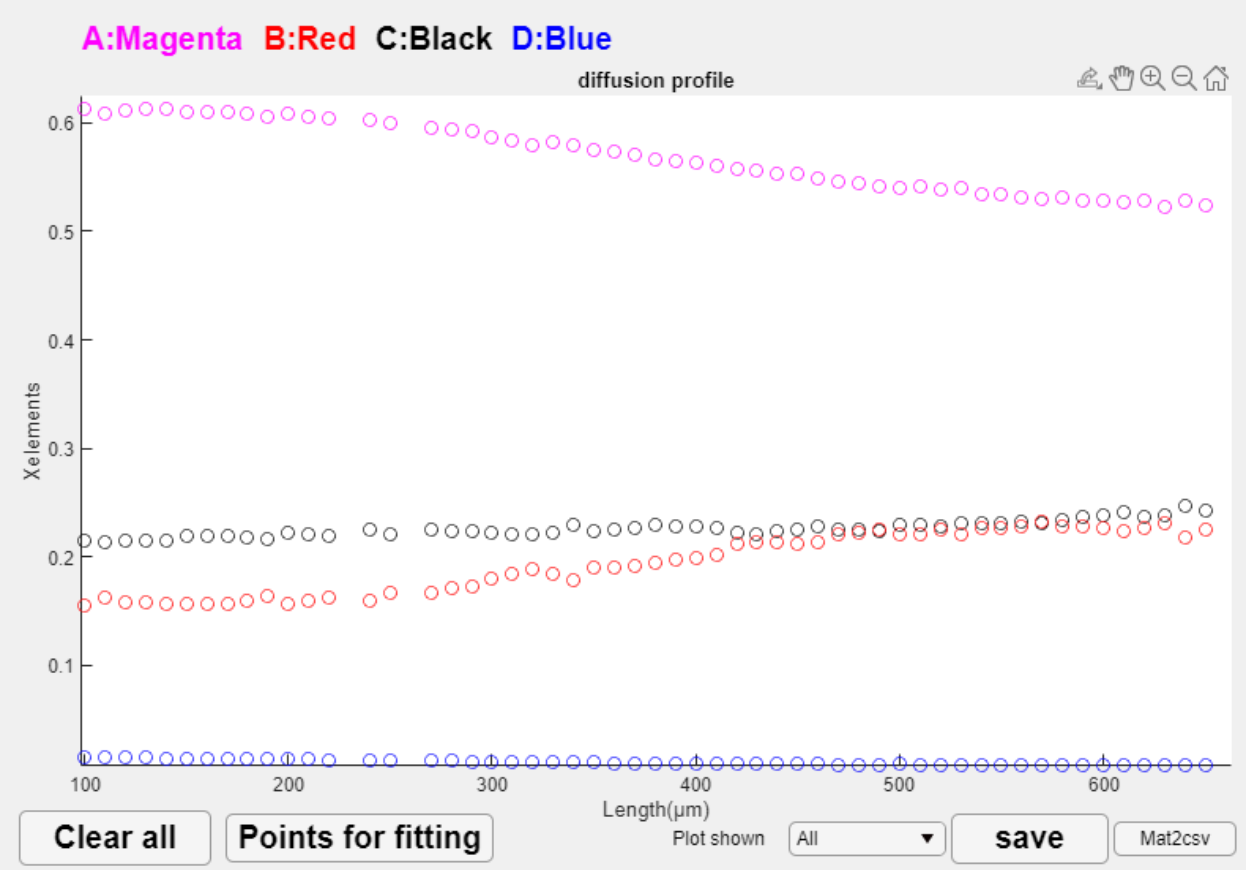
The data file requirements vary depending on the diffusion system you have selected:

- For all system types, the "distance" column must be included. The values in this column represent the position of your measured spot in micrometers (μm), ordered from the smallest to largest.
- The required number of columns depends on the chosen system. Each element needs five columns, including three concentration columns, one error column, and one column for the element name. For example, if you choose element "A", you will have three "A" concentration columns: "A", "A_start", and "A_end". The values under the "A" column represent the concentration of element A at the specific spot. The "A_start" and "A_end" columns contain numbers used to generate the initial profile, as discussed in section 2.2.3. The "A_Error" column represents the measurement

uncertainty of the A concentration, while the "A_content" column contains the actual name of the element represented by A, such as Ca. The three concentration and species columns of each element must not be empty. If you opt to include error bars, the error column must not be empty either.

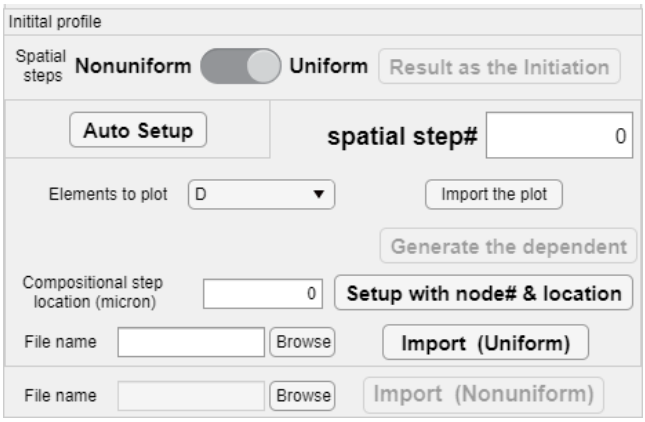
- If you select the "multi"-component system. The sums of the "X", "X_start", and "X_end" columns should all equal 1. For example, in a "4comp" system data file, the sum of A+B+C+D should be 1 for every row, and the sum of A_start + B_start + C_start + D_start should also be 1.

Example files with various configurations can be found in the "measured_profile_example" folder at the default installation location of your DIFFUSUP software. The example data are the one from Fan et al. (2022).



Upon importing the file and clicking the "Import" button, the measured data will be imported, and the spots will be plotted in the diagram panel. After a successful import, the element profiles will appear in the diagram panel, and the element names will be displayed in the table (as shown in the "4comp" example diagram above).

2.2.3 Initial Profile



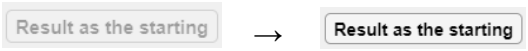
To create a model, you need a set of initial profiles. These profiles can be generated in various ways. The first step is to choose from "Nonuniform" or "Uniform" spatial steps. When selecting "Uniform", there are three methods to generate the initial profile for the modeling process:

- "Auto setup" creates a one-step profile with 100 spatial steps (101 nodes), using the "X_start" and "X_end" values imported. The location of the step is automatically chosen, and can be modified as well as the step number. This is applicable for all systems.
- You can import a file that provides the initial profile for the modeling process. Enter the full path of the file or click "Browse" to locate it. The file can be in .txt, .dat, .csv, .xls, .xlsb, .xlsm, .xlsx, .xltm, .xltx, .ods, or .xml format. The number of rows equals to the number of nodes (rows) equals to the number of spatial step number + 1. The columns for the elements not used in the system should remain empty.

- The initial profile for each species could be plotted in the display diagram using the cursor. In a "multi"-component system, one element is dependant and its profile is automatically calculated by

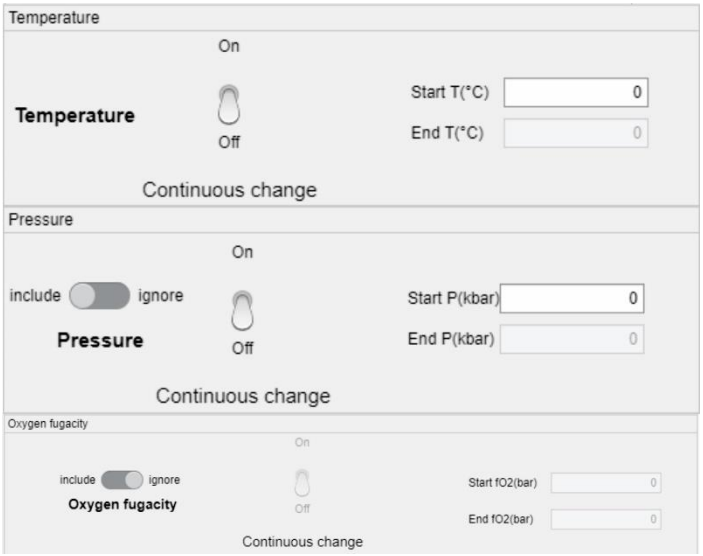
clicking "Generate the dependent". In most scenarios, the locations of compositional discontinuities should be the same for all species.

An example importing file for "Nonuniform" modeling is provided in the 'Initial_profile_example' folder. For "Nonuniform" spatial steps, The locations of the nodes ("distance" in fifth column of the input spreadsheet) must be included.



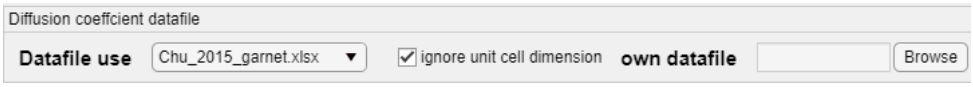
After completing one simulation, the "Results as the starting" button will become available. Simply click it to use the results from the last simulation as the new initial profile. Keep in mind that this button will become unavailable if you change the system or the "Uniform/Nonuniform" selection.

2.2.4 Pressure-Temperature-f_{O2} Setting



The pressure, temperature, and oxygen fugacity (f_{O2}) conditions are essential for diffusion simulation. The subpanels are similar. The temperature must be always specified, and you can choose to include pressure and oxygen fugacity as well. You can also set the conditions to change continuously during the modeling time, by turning on the linear change switch. Note that the default oxygen fugacity is buffered by carbon-carbon oxides (CCO).

2.2.5 Diffusion Coefficient

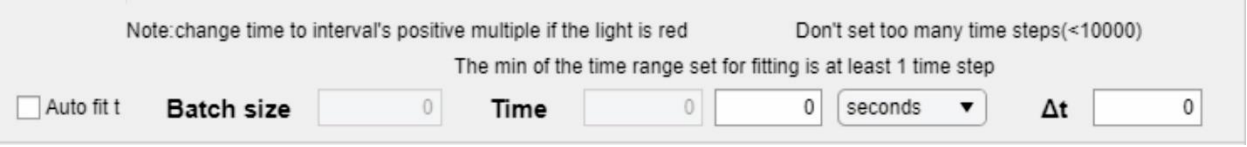


Diffusion models require diffusion coefficient parameters for the elements of interest. You have the option to use pre-built diffusion coefficient data files or create your own. Pre-built files currently available in DIFFUSUP include garnet models from Chu & Ague (2015), Carlson (2006), and carbonate parameters from Müller et al. (2012). The parameters for unit-cell dimension are located in the sixth column of the diffusion coefficient data file, and could be turned off by checking the "ignore unit cell dimension" box. To use a pre-built data file, simply choose the desired file from the dropdown list. If you prefer to use your own data file, ensure it adheres to the same format as the pre-built files, and select the file location by either

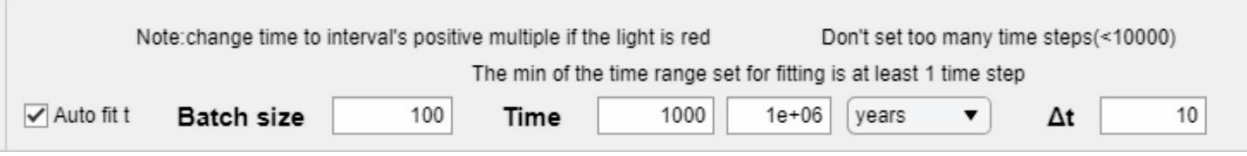
entering the full path or browsing for the file. The diffusion rates are then calculated using the specified diffusion model and P-T-f_{O2} conditions.

2.2.6 Convolution and Timescale Setting

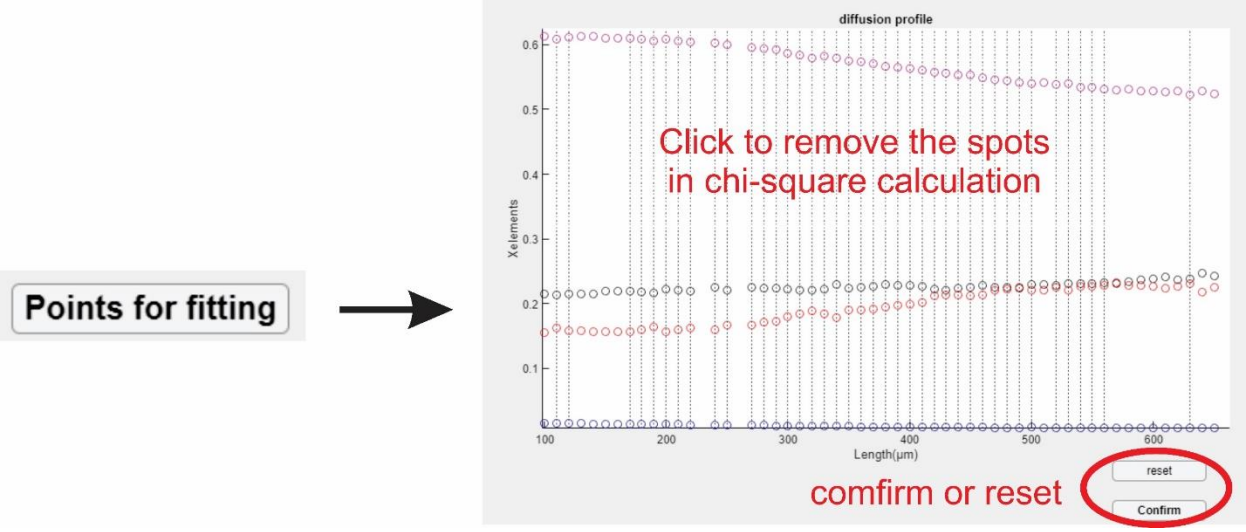
The finite resolution of analytical methods give rise to artificial spatial averaging effects, also known as convolution. Including the convolution effect in your model will account for the influence of the measurement resolution on the diffusion profile. This can be important for ensuring the accuracy and reliability of your modeling results, especially when dealing with high-resolution data or when the measured profiles exhibit rapid changes in concentration over short distances. The effect could be included by checking the box and specifying the convolution parameter ε (μm). Please consult this file for a more detailed explanation of the theory behind convolution and its effects on diffusion modeling:
https://diffusup.org/download/DIFFUSUP_SUPPLEMENTARY.pdf



To carry out the modeling, you need to specify the diffusion time, the time unit, and the time interval. The time interval should be a multiple of the step size used in the finite difference calculation method. Please note that the number of steps should not exceed 10,000, as this may lead to excessively long calculation times. By providing these parameters, you will enable the software to perform the diffusion modeling and generate results based on the input data and specified conditions.

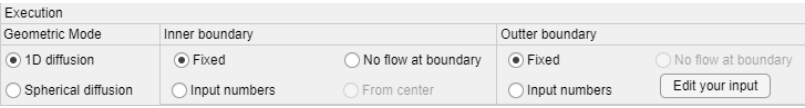


Furthermore, if you wish to automate the fitting process for time, you can do so by selecting the designated checkbox and inputting the desired time range and batch size. Through this approach, the software will carry out calculations by randomly sampling time and simulating accordingly. The resulting chi-square values will aid in determining the fitting time and associated uncertainties, enhancing the efficiency and accuracy of your simulations. The calculation of time mean and uncertainties are following the method in Chu & Ague (2015). Selecting the spots to be included for chi-square calculation is a straightforward process, as shown below.



2.3 Execution panel

Once you have completed the time settings, you are greenlighted to proceed with the modeling process. At this point, you can select between a spherical or 1-D situation and set the appropriate boundary conditions for your diffusion model.



Then, you can click the "Run simulation" or ‘Run to fit t’ button to initiate the diffusion simulation or time fitting. After running the model, the modeled profile will be displayed in the diagram panel alongside the imported measured data. This allows you to visually compare the modeled profile with the measured data and evaluate the fit. The details of the algorithm used in the modeling process, as well as the various boundary condition options, can be found in the theory document provided with the DIFFUSUP software.

2.4 Diagram panel

Once you have successfully imported, plotted, and generated your diffusion profile, you can view it in the diagram panel within the DIFFUSUP software. The Y-axis of the diagram will automatically adjust to display the chosen element's concentration. You can customize the Y-axis by selecting different elements from the provided options, allowing you to focus on specific parts of your diffusion system. The diagram panel offers tools in the top right corner that enable you to zoom in, zoom out, and adjust the view of the plotted data to your preference. If you wish to save the data represented in the diagram, click on the "Save" button. Keep in mind that this action saves the underlying data, not the visual diagram itself. If you want to

save the diagram, use the "Save plot" button. To clear all the data and the diagram from the panel, click on the "Clear all" button. This action will remove all the plotted data and allow you to start fresh with new data or modeling settings.

3. Workflow & Example

3.1 Units, Input, and Output Summary

In DIFFUSUP, the units are as follows:

- Temperature: Celsius (°C)
- Pressure: kilobar (kbar, 10^8 Pa)
- Oxygen fugacity: bar (10^5 Pa)
- Length: micrometer (μm, 10^{-6} m)
- Time (range for fitting) : customizable

You'll need to input, set, and choose the following content to complete your diffusion modeling:

Input/Import/Generation (it's recommended to use the full file path):

- Target profile to model
- Initial profile for the modeling
- Diffusion coefficient datafile

Choices:

- Modeling system (multi-component diffusion/single-component diffusion)
- Dependent elements (if multi-component diffusion)
- Ignore influence of unit cell dimensions or not
- Points picked for chi-square calculation/fitting (optional)

Settings:

- Pressure-temperature-oxygen fugacity-time for diffusion
- Convolution and parameters
- Time steps

It's recommended to keep all input files in the same folder where DIFFUSUP is installed.

3.2 General Steps

Here are the typical steps to follow when using DIFFUSUP:

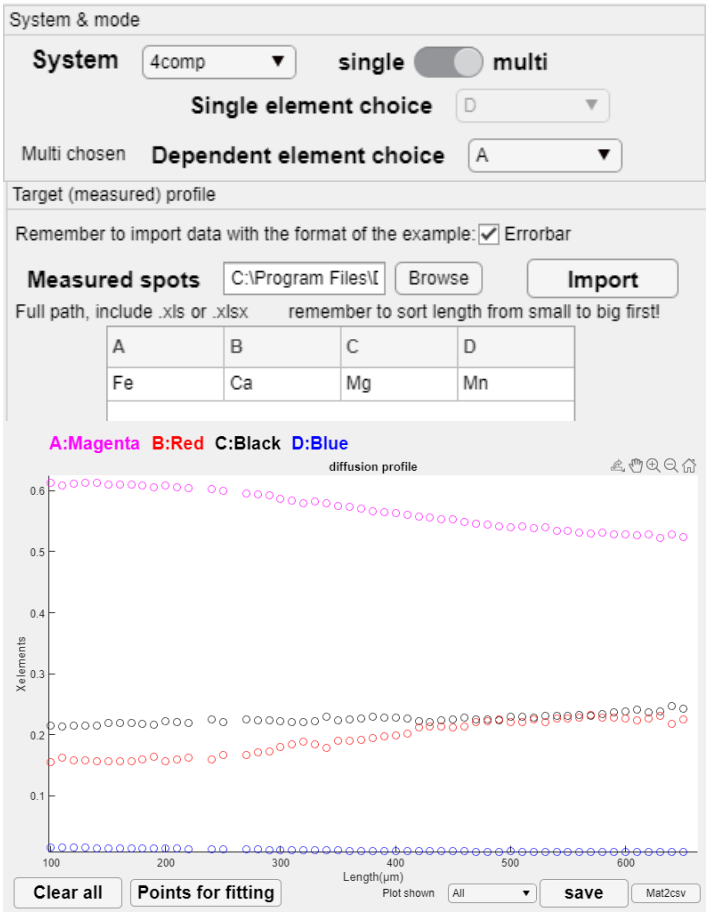
- Choose the system situation (spherical or 1-D)
- Import your target profile to fit (mostly experimental measured profile)
- Import, plot, or auto setup the initial profile of your model

- Set the pressure, temperature, and f_{O_2} conditions
- Choose or import the diffusion coefficients
- Set the convolution parameters
- Set the time (range) and time steps
- Run the model
- View the results
- If necessary, adjust the input settings and repeat steps 4-9 until you achieve a satisfactory result
- Save the results

DIFFUSUP is designed to follow these steps in a logical sequence from top to bottom and from left to right of the user's interface. In the next section, we provide examples of common diffusion modeling cases.

3.3 Example

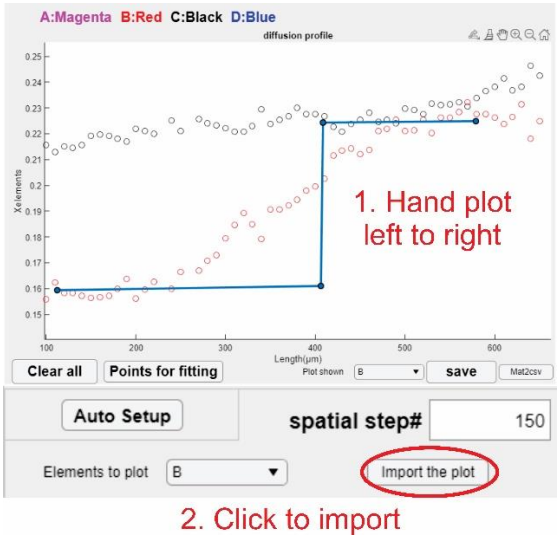
To illustrate how to use DIFFUSUP, we will provide an example using the "4comp" files from Fan et al. (2022) included with the software. The simulation of other diffusion scenarios are similar, please follow the steps outlined in Section 3.2.



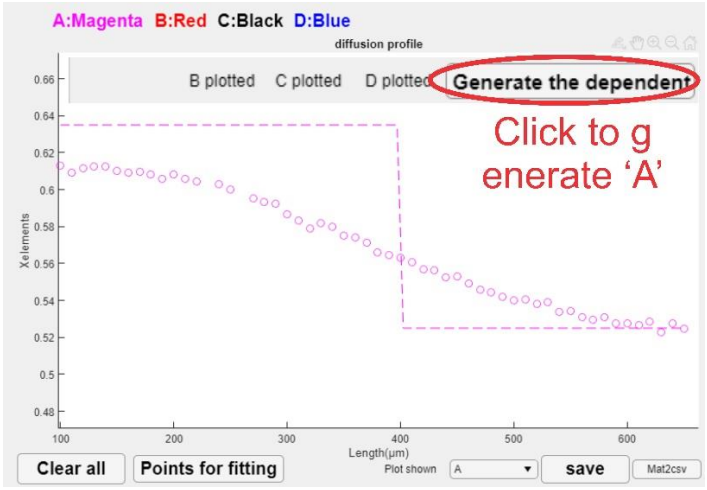
- Step 1: Choose the system configuration from the dropdown menu. For this example, we will be using a four-component system, so we select "4comp". Next, select "multi"-component for this example. If you select "single", only the elements you select will be used in the modeling.

- Step 2: Load your datafile for measured spots. Consult Section 2.2.2 for the format and requirement of input spreadsheet. If the input datafile is consistent with your system configuration, the corresponding elements A, B, C, and D will appear in the table, along with the information from your imported file. The spots will also be plotted in the diagram panel. If the uncertainties are included in the input spreadsheet and the "Errorbar" box is checked, errorbars will appear in the display diagram.

- Step 3: In this example, we input the initial profiles by plotting them in the display diagram. Choose one element as dependent in the "System & Modes" subpanel, for example, let's select element "A" as dependent. In the "Initial profile" subpanel, choose the "Uniform" option and then click the "Import the plot" button. Specify the number of steps, for example, 150. Pick one species from the drop-down menu of independent elements, for instance, element "B". Manually plot the initial profile for element "B" by clicking on the display diagram to create points. You can adjust the points by dragging them if necessary. Once you have plotted the initial profile for element "B", proceed to the other independent species (in this case, elements "C" and "D") and repeat the manual plotting process.



After plotting the initial profiles for all independent elements, click the "Generate Dependent" button in the "Initial profile" subpanel. This will automatically generate the initial profile for the dependent element (in our example, element "A"). All your initial profiles will be displayed in the diagram panel as dashed lines. You can differentiate them from the measured profiles (solid lines) and the modeled profiles (which will be displayed after running the diffusion model).

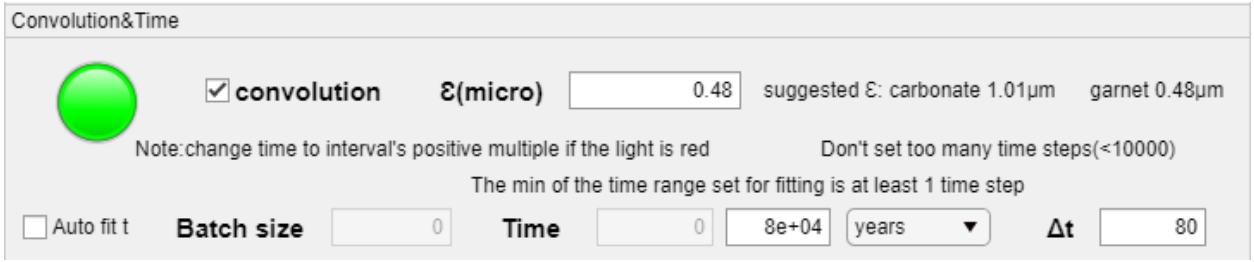


Now you have set up the initial profiles for all elements in the system, and you're ready to proceed with running the diffusion model and analyzing the results.

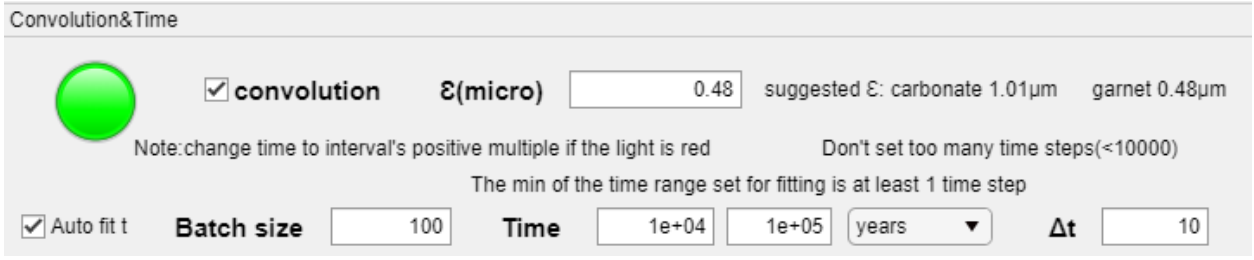
- Step 4: Follow the instructions in section 2.2.4 to set your *P-T-*f_{O2} condition(s). A linear change of the conditions is also available by turning up "continuous change". Nonlinear variations can be approximated by descretization to a series of linear steps. In this example, we'll use a the conditions from Fan et al. (2022) 860 °C with linear change from 20 kbar to 12 kbar, and CCO oxygen fugacity.

- Step 5: To use the appropriate diffusion coefficient datafile for your system, go to the "Diffusion coefficient parameter" subpanel in the software. Make sure the datafile includes the "A", "B", "C", "D" elements for your system. In this example, we will use the garnet diffusion datafile from Chu & Ague (2015). Select this file from the pre-built datafile dropdown list in the "Diffusion coefficient parameter" subpanel. If you want to use your own datafile, ensure it follows the correct format and either type in the full path or browse to find the file.

- Step 6: Set up the convolution factor ε = 0.48 μm for garnet EPMA profiles (Ganguly et al., 1998). Set the total time length (and unit) for the modeling. We recommended time steps within the range of 1/10 to 1/10000 of the duration to ensure accurate and efficient modeling. In this example, we set the total time length to 80000 years and choose a time step of 80 years.

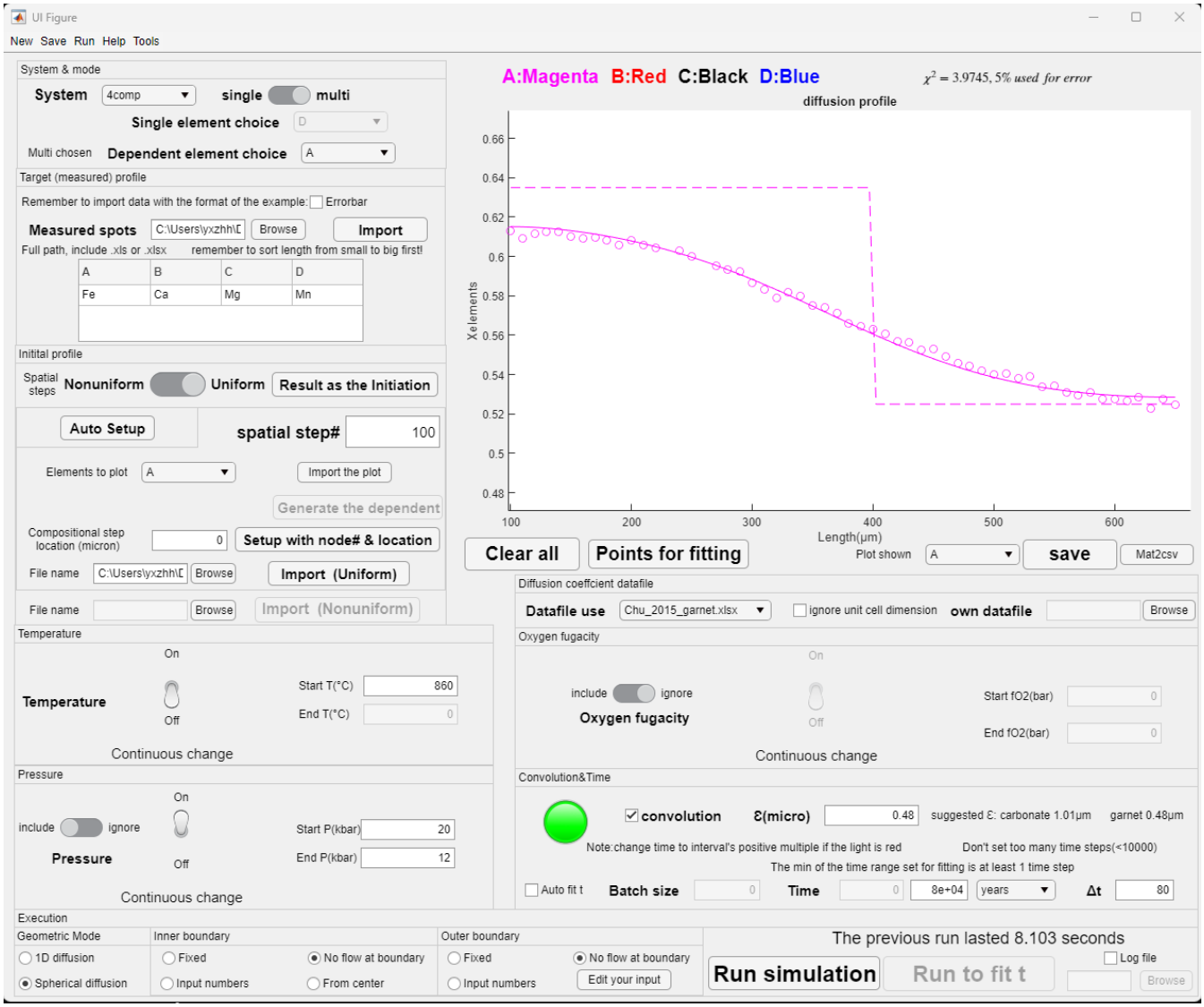


- Step 8: you are now ready to input the time settings and run the simulation. In this example, we will use the spherical model with zero-net-flow boundary diffusion mode. After the loading bar reaches the end, the results are displayed.



You can then repeat the process by modifying the inital profile (Step 3), changing the physical conditions (Step 4), selecting a different diffusion coefficient dataset (Step 5), or adjusting the time and time steps (Step 7). Through iteration, you can refine your model to achieve a better fit. Once you are satisfied by the model results, save the diagram and data. If you want to automatically fit time, you can click one the ‘Auto fit t’ and add the batch size and time range for fitting.

The diagram can be saved as .eps, .jpg, .png, .tif, or .pdf files. The data can be saved as a .mat file, to be opened in MATLAB. The Mat2CSV tool provided converts the .mat file to .csv format. The output data could be modified to incorporate garnet growth or resorption, for the initial profiles of the next modeling step. The model result could be directly transferred to the next step by clicking "Result as the starting" in the initial profile subpanel.



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