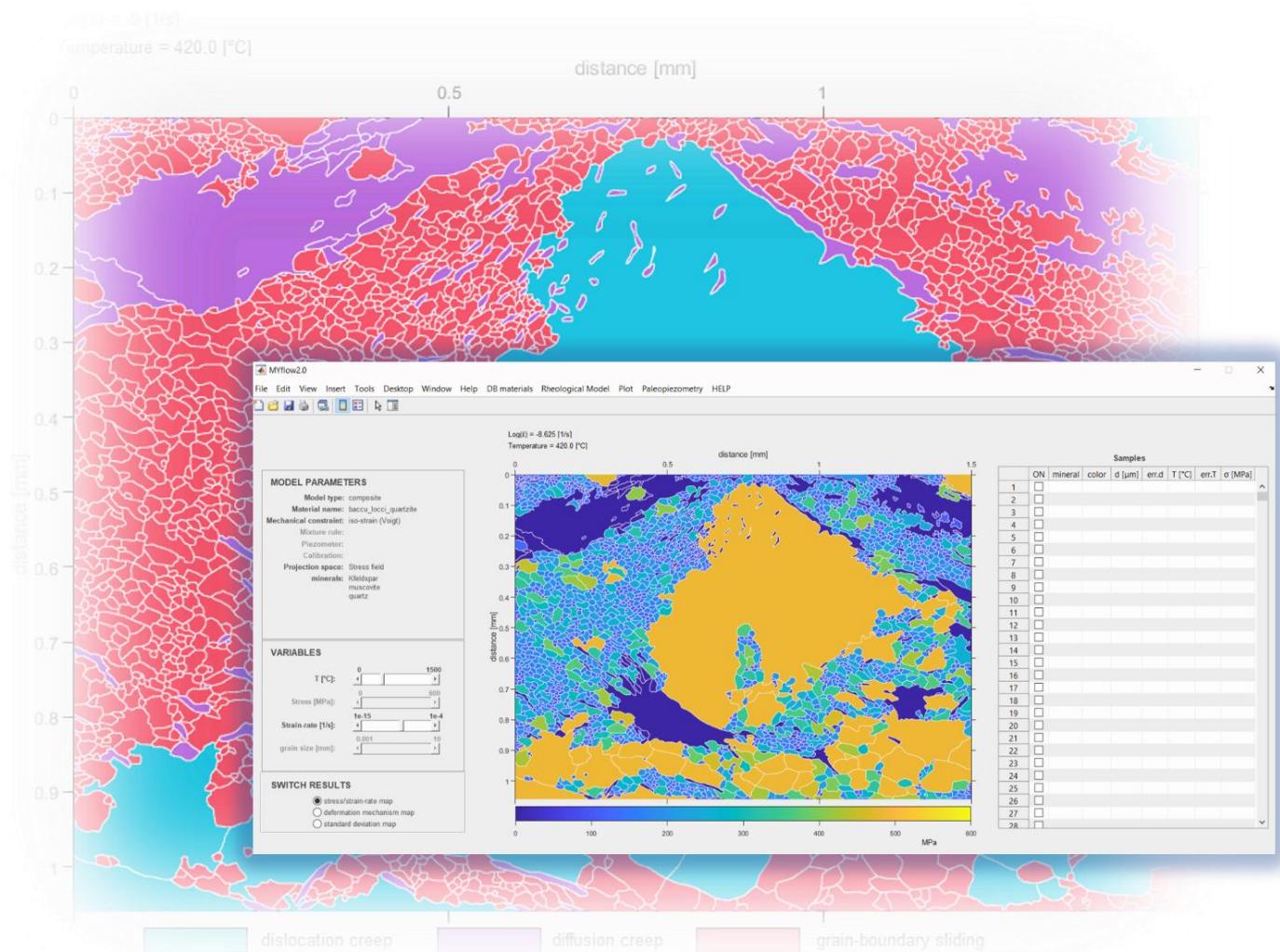


MYflow

User guide



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1. Introduction

MYflow is a Matlab® derived software that allows calculating the flow strength of mylonite (MYlonite flow) as well as doing rheological modelling using either compositionally homogeneous rocks or composite materials, or single minerals. This implies that MYflow can handle both 0th dimensional rheological models that evaluate the stress or strain-rate dependency of pure single phases, or 2D models evaluating the flow strength of compositionally homogeneous rocks with spatially variable grain size and grain size distribution, or compositionally heterogeneous rocks made of grains of variable composition and grain size. These latter models are derived from 2D phase maps and phase-boundary maps and show the stress/strain-rate pattern that result from a given microstructure with specified spatially variable grain size and composition. The results obtained from modelling could be displayed in various projection spaces showing the mutual sensitivity of stress, strain rate, temperature and grain size for different rock composition and rock microstructure. Besides, MYflow can be used to calculate deformation mechanism maps of several of the major rock-forming minerals, eventually combined with independently constrained paleopiezometric data. The software is designed as a simple all-in-one platform to perform several routine microstructural analyses including average grain-size, grain-size distribution, phase mixing intensity, as well as inverse rheological modelling. In spite of this great analytical flexibility, the program is intended for users that have minimal confidence with the Matlab language or computer programming overall, thus MYflow is provided along with an easy-to-use graphical user interface that allow doing calculation, modelling, and update or customize the databases. Finally, the software returns exportable figures, graphic objects, and data in several widely distributed formats.

1.1. Installation, OS and hardware requirements

MYflow can run in two ways depending on user's personal preferences and the availability of supporting software. The first option, warmly recommended if you are already a Matlab user, is to install MYflow by copying the folder 'MYflow2' and all the sub-folders ('DB_composites', 'DB_mineral_parameters', 'help', 'paleopiezometry', 'plotting_functions', 'rheological_functions', 'SiiEii_map', 'thermodynamic_functions') and the mainscript (MYflow2.m) into a directory on a PC or Mac that has Matlab® already installed. Once the files have been copied, you can launch the software the usual way, that is, executing the function 'MYflow2' from the Matlab's command window. This action opens the Graphical User Interface that controls all the operations that can be done in MYflow. The requirements are the same recommended for Matlab R2021a, that is:

PC

Operating System: Windows 11

Windows 10 (version 20H2 or higher)

Windows Server 2019

Windows Server 2022

Processor: Any Intel or AMD x86–64 processor with four logical cores and AVX2 instruction set support

RAM: 4 GB/core (recommended), minimum is 4GB

Storage: >32 GB, an SSD is strongly recommended

Graphic: No specific graphics card is required, but a hardware accelerated graphics card supporting OpenGL 3.3 with 1GB GPU memory is recommended.

Mac

Operating System: macOS Ventura (13)

macOS Monterey (12)

macOS Big Sur (11.6)

Processor: Any Intel or AMD x86–64 processor with four logical cores and AVX2 instruction set support

Any Apple Silicon M-series chip

RAM: 8 GB

Storage: >25 GB, an SSD is strongly recommended

Graphic: Any Mac able to run macOS Big Sur has a GPU able to run MATLAB.

Linux

Distribution: Ubuntu 22.04 LTS

Ubuntu 20.04 LTS

Ubuntu 18.04 LTS

Debian 11

Debian 10

Red Hat Enterprise Linux 9

Red Hat Enterprise Linux 8 (minimum 8.4)

Red Hat Enterprise Linux 7 (minimum 7.9)

SUSE Linux Enterprise Desktop 15

SUSE Linux Enterprise Server 12 (minimum SP2)

SUSE Linux Enterprise Server 15

The second option requires installing MYflow as a standalone software and does not require to have Matlab® installed in your computer. If you want to go this way, double click on the executable file MY_installer.exe and wait until installation is complete. For the moment, MYflow can be installed as a standalone software only on windows OS.

1.2. Getting started with MYflow

The MYflow Graphical User Interface (Fig. 1) controls the various functions used for rheological modelling and visualize the results into the main plot. All the operations required to build and show a rheological model can be accessed by selecting the appropriate choices in the menus 'Rheological Model' and 'Plot'.

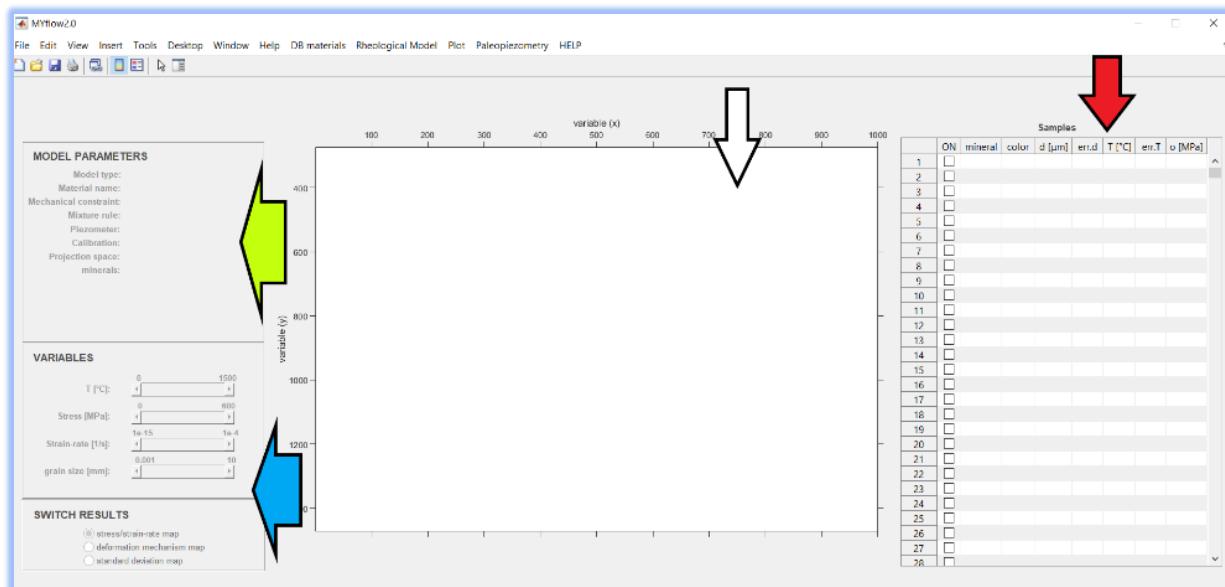


Fig. 1. MYflow Graphical User Interface: the green arrow indicates the 'MODEL PARAMETERS' panel, the blue arrow indicates the interactive controls panels, the white arrow indicates the main plot, the red arrow indicates the paleopiezometry (Samples).

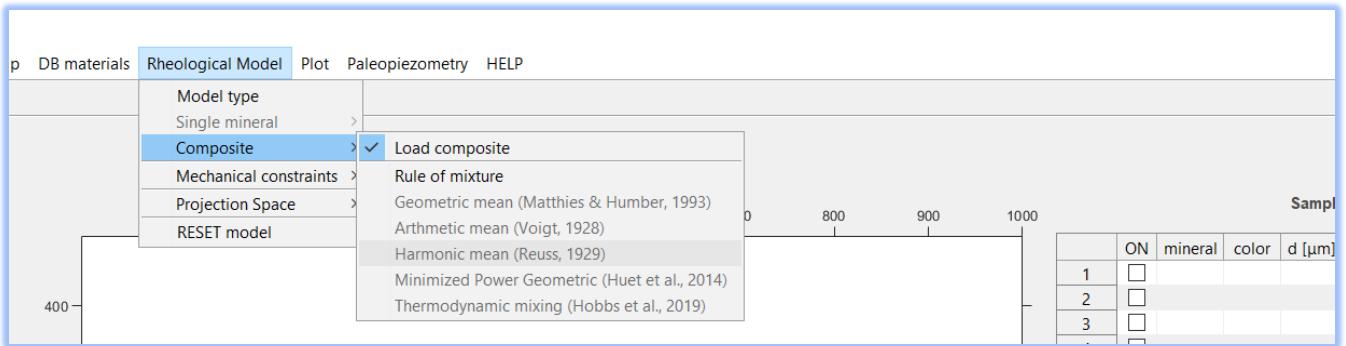


Fig. 2. Menu ‘Rheological Model’ with check next to the selected model type (composite). Note that the alternative model type option ‘Single mineral’ is not available due to the selected ‘composite’ model.

The menu ‘DB materials’ provides access to the databases of mineral phase and composite materials, and eventually allow to modify the parameter of a given mineral/composite, or to create new mineral phases/composites. The menu ‘Paleopiezometry’ controls all the operations needed to calculate paleostress from grain size data, as well as the database of paleopiezometric calibrations. The latter menu ‘Help’ opens the manual. Once an active (dark grey) menu item is selected from a menu, a small check appears in the menu next to the item, and eventually other options may become not available (Fig. 2). In this latter case, the deactivated options become light grey. Selecting any items of the ‘Rheological Model’ menu generally results into an update of the ‘MODEL PARAMETERS’ panel, which shows in real time the currently active settings of the rheological model (Fig. 3).

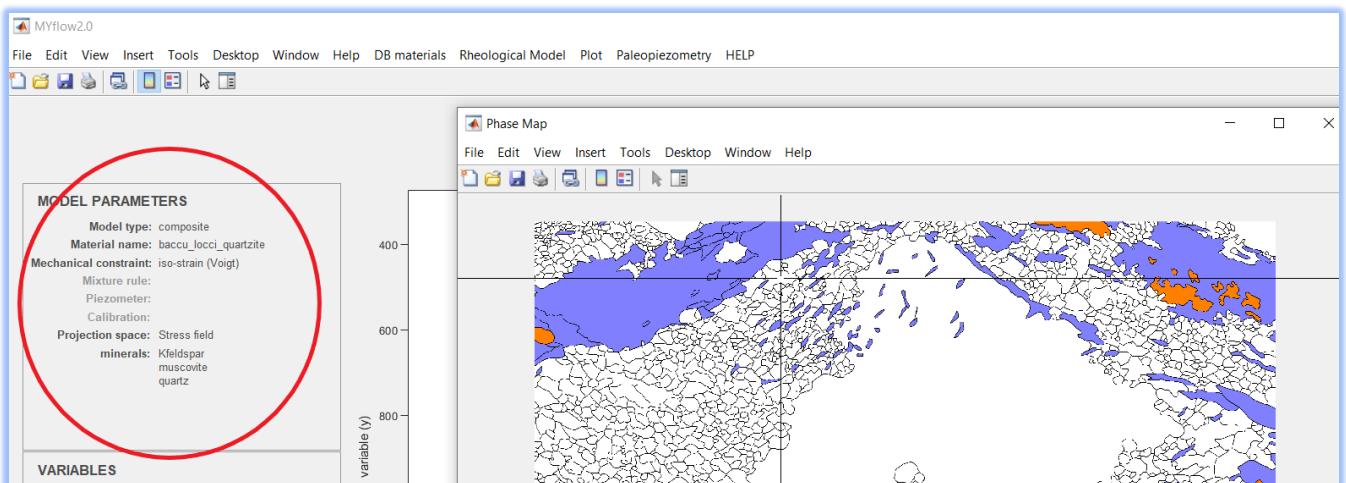


Fig. 3. MODEL PARAMETERS panel showing the settings of current rheological model (red circle). The field ‘Material name’ could indicate either the name of a mineral phase or the name of a composite. In this latter case, the list of constituent mineral phases is also shown in the field labelled ‘minerals’.

Any selection remains active as long as the user close the MYflow session or decide to reset the rheological model by clicking on the ‘RESET model’ item at the end of ‘Rheological Model’ menu. This latter action will cancel any setting chosen by the user, restoring the initial configuration of MYflow. Resetting the model is required whenever the user wants to build a new model using a different material (i.e., from single phase materials to composites, or the contrary), or if the user wants to change the mineral phase of single phase materials (i.e., from ‘anorthite’ to ‘quartz’ or whatever). Resetting the model is also required to change the type of mechanical constraint, or the projection space.

1.3. Software development & debug

The first version of the software MYflow (version 1.0, Database mineral dbm13_2022, Database piezometric calibration dbpc5_2021) was released in 2023. The software has been developed by Leonardo Casini, University of Sassari, and Matteo Maino, University of Pavia (Italy). Inputs and feedbacks from Stefania Corvò, Luca Menegon, Davide Zanoni and Michele Zucali helped us improving the software capability and usability and are thus greatly acknowledged. Programming, debug, and maintenance of the routines and the databases are performed by Leonardo Casini. Should you find any bug causing crash or unwanted behaviour of the software, please send a report to [casini@uniss.it](mailto:cavini@uniss.it). Your help to improve the stability of the software and the performances is greatly appreciated.

2. Databases

MYflow stores the physical parameters of minerals and composites, and several piezometric calibrations, in three databases. The first database of mineral parameters (version: dbm13_2022) contains the flow parameters of several rock-forming minerals including: 1) quartz, 2) K-feldspar, 3) calcite, 4) wet/dry anorthite, 5) jadeite, 6) diopside, 7) magnetite, 8) muscovite, 9) biotite, 10) hornblende, 11) garnet, 12) wet/dry olivine. The second database contains the parameters of composite materials. This database is provided with three composites that serve to demonstrate the applicability of the code; however, it is generally implemented by the users adding new composites if they need to perform new simulation using custom compositions. Deleting or modifying any of the composites has no effect on software functionality unless they won't be used anymore. The last database (version: dbpc5_2021) includes several piezometric calibrations empirically determined for some of the mineral phases included in the database of minerals.

2.1. Mineral phases

2.1.1. Load mineral phases

This option implies selecting 0th dimensional model composed of a single mineral phase; thus, 2D stress and strain-rate maps are not available (Stress/x,y and Strain-rate/x,y projection spaces). To load any mineral phase, already included in the mineral database, enter the menu ‘Rheological model’ and then select the sub-menus ‘Single mineral’ and ‘Load mineral’. This action first opens a list box that allow selecting one of the available minerals from the mineral databases, then a message box confirm model selection and remind the user the next step (Fig. 4).

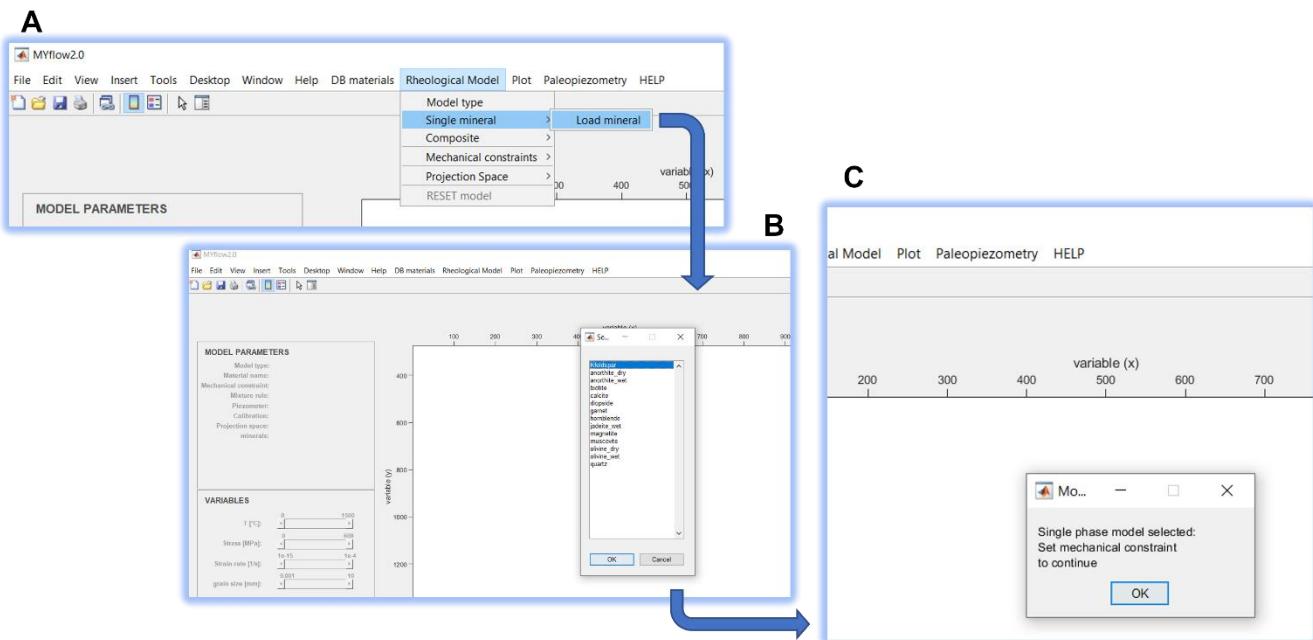


Fig. 4. Load mineral phase: a) Menu selection required to work with single-mineral 0th dimensional rheological models, a) list box showing the database of currently available (selectable) mineral phases, c) message box that appear at the end of selection whenever.

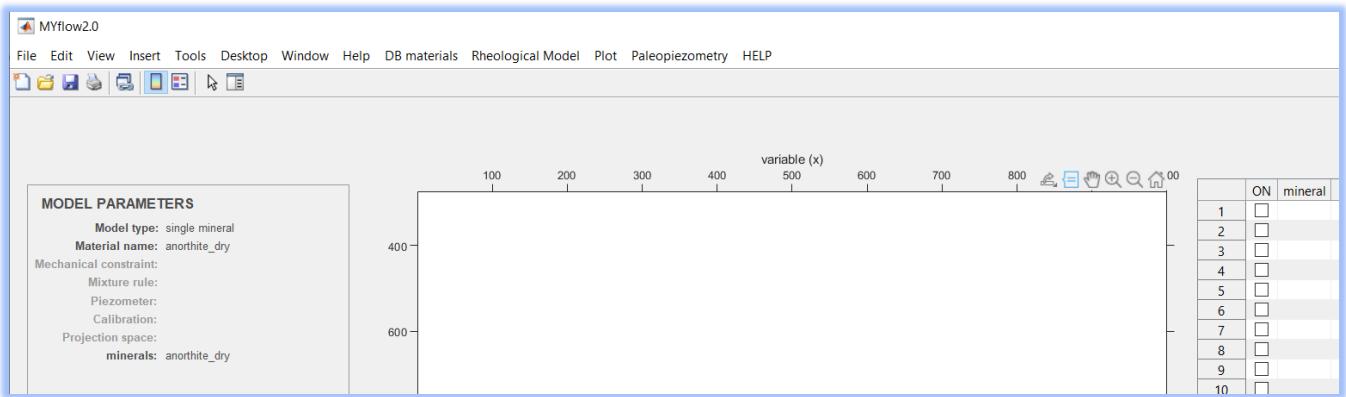


Fig. 5. Change of MODEL PARAMETERS properties ‘Model type’, ‘Material name’ and ‘Minerals’ as a single mineral is selected

Once the mineral phase has been selected, the MODEL PARAMETERS section is being updated modifying the value of the fields ‘Model type’ and ‘Material name’, as well as the field ‘Minerals’ (Fig. 5). The ‘Mechanical constraints’ menu, a sub-menu of ‘Rheological model’ menu, is activated.

2.1.2. Edit/Add new mineral phase

The mineral database is designed to be easily implemented and expanded by the users. New mineral phases can be added to the database from the menu ‘DB materials’ by selecting ‘Edit mineral DB’ and then ‘Add new phase’ submenu. This option first opens an input dialog box that requests the name of the new mineral phase being added to the database, then it opens two input dialog boxes that could be used to set the physical parameters of the mineral (Fig. 6).

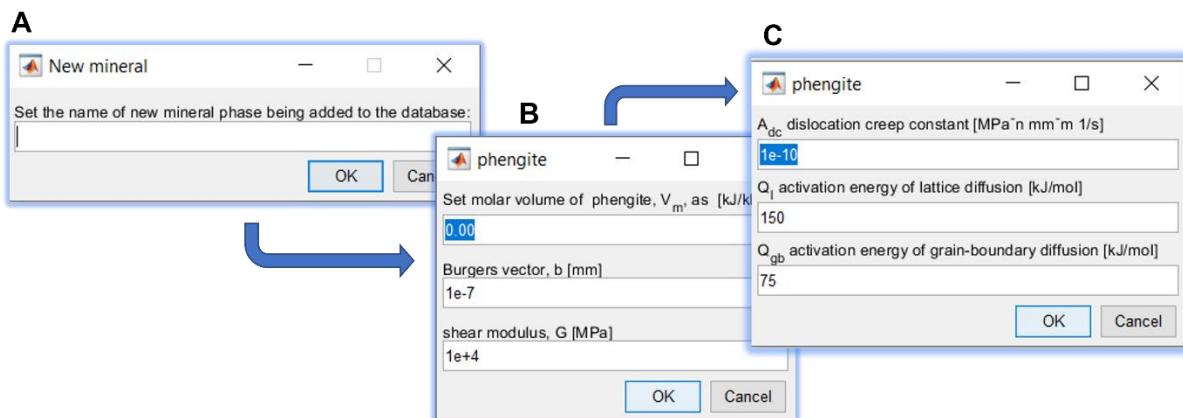


Fig. 6. Input dialog boxes opening whenever a mineral phase is created or modified: a) first dialog box to set the mineral name; this one opens only whenever a new phase is being created, b) set molar volume, Burgers vector and shear modulus, c) set dislocation creep pre-exponential constant, and activation energies of dislocation/diffusion creep

The physical parameters required to set up a new mineral phase are: 1) molar volume [kJ/kBar], 2) the Burger’s vector [mm], 3) shear modulus [MPa], 4) pre-exponential constant of dislocation creep [$\text{MPa}^{-n} \text{ mm}^{-m} \text{s}^{-1}$], which is usually available from creep experiments, 5) activation energy of lattice diffusion [kJmol^{-1}], and 6) activation energy for grain boundary diffusion [kJmol^{-1}].

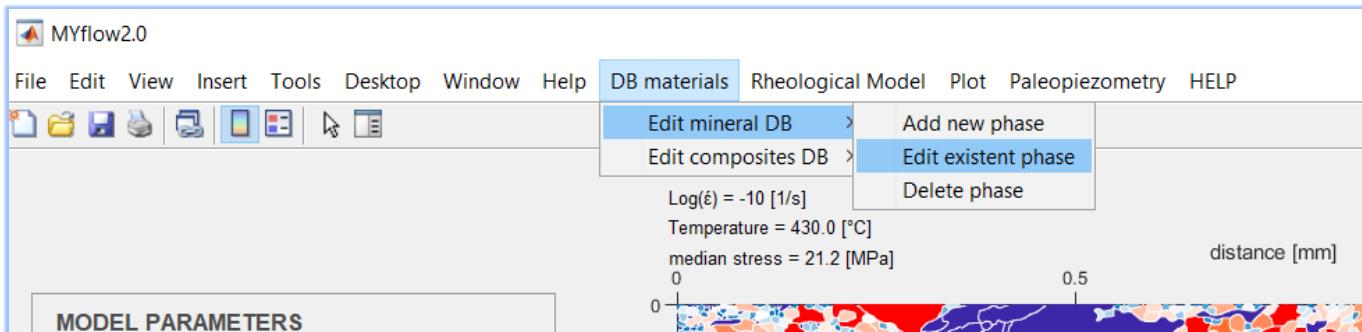


Fig. 7. Add/Edit mineral phase. Menu selection required to modify the physical parameters of a mineral already included in the mineral database.

Similarly, the physical parameters of a mineral which is already included in the database can be modified from the ‘DB materials’ menu by selecting ‘Edit mineral DB’ and then ‘Edit existent phase’ submenus (Fig. 7). This action first opens a listbox that allow to select the mineral to be modified, then opens the same input dialog boxes used to set up the parameters of a new mineral, except the first one for the name. This time, however, each field in the dialog boxes already contains a value of the relevant parameter so that the user can modify all the parameters or only a few of them. Clicking the ‘OK’ button without changing any value has no effect on MYflow functionality as the existent material parameters remain unmodified.

2.2. Composite materials

2.2.1. load existent composite

You can upload any composite material already included in the database of composites simply by selecting ‘Composites’ and ‘Load composite’ from the menu ‘Rheological model’ (Fig. 8). This action will load a composite material characterized by a given number of different mineral phases, each with an average grain size expressed in mm. Composite materials should be formed by a minimum of one mineral phase.

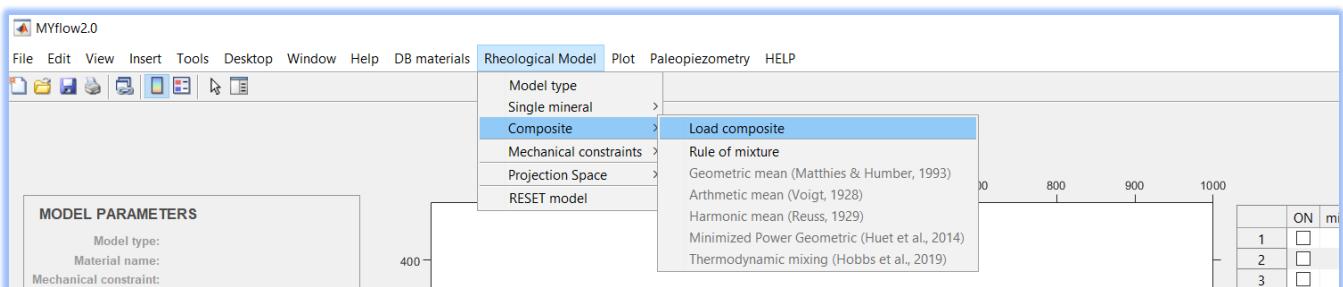


Fig. 8. Menu selection to upload one existent composite material.

2.2.2. add/modify composites

New composites can be created by selecting ‘Edit composites DB’ and ‘NEW composite’ from the menu ‘DB materials’ (Fig. 9). This option first opens an input dialog box that requests specifying the number of phases that constitute the new composite (N). The minimum accepted value of N is 1, this option obviously does not correspond strictly to a composite rock, however it should be used to model the rheology of compositionally homogeneous rocks characterized by spatially variable grain size (see [par. 3.3.2 ‘2D projections’](#)). This version of MYflow does not account for any effects of variable Crystallographic Preferred

Orientation (CPO) nor Shape Preferred Orientation (SPO), that will be implemented in a future release. Once the number of phases is set, MYflow opens sequentially N input dialog boxes that allow setting the volume proportion and the mean grain size of each phase in the composite (Fig. 10).

Volume proportions should be defined in the range 0.00 to 1.00, and the sum of all phases must equal 1.00. Once the volumetric proportions are set up, the new composite is saved in the ‘MYflow\DB_composite’ directory and is readily available for rheological modelling (see [chap. 3. Rheological modelling](#)).

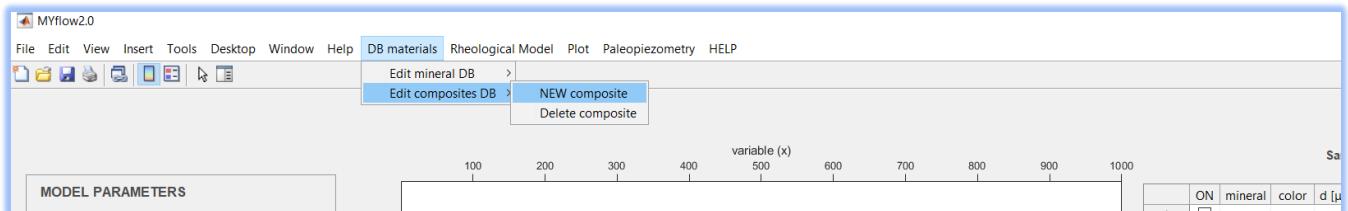


Fig. 9. Menu selection to create a new composite material.

Existing composites may also be deleted programmatically entering the menu ‘Edit composites DB’ and selecting ‘Delete composite’, which opens a list box that allow selecting the composite to be eliminated. Alternatively, for non-standalone installation, composites can be also eliminated manually from the DB_composite folder.

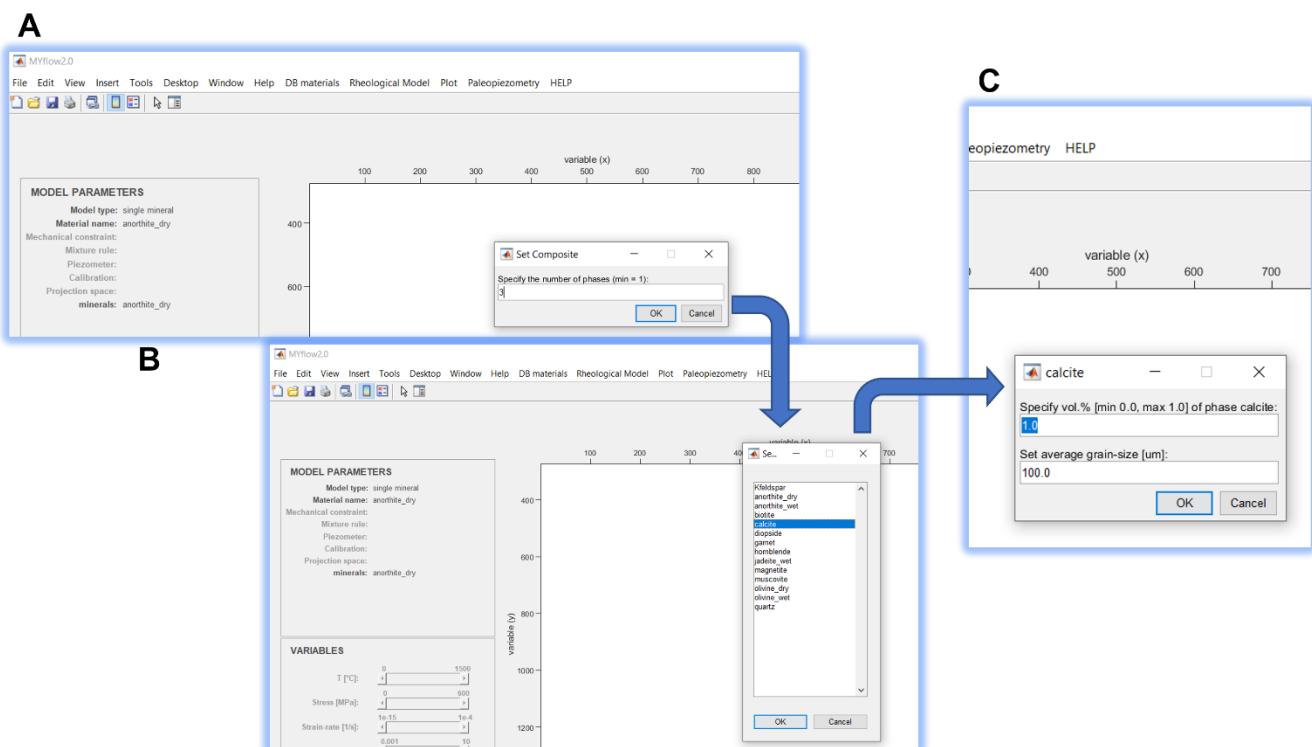


Fig. 10. Input dialog boxes that allow setting up a new composite: a) the first box request specifying the number of phases in the composite (minimum value is 1), b) the list box opens -as many times as the number of phases in the composite – and allow selecting the various phases, then c) another input dialog box opens to specify the volume proportion and average grain size of each phase.

2.3. Paleopiezometric calibrations

2.3.1. Load calibration

MYflow allow to calculate paleostress data from grain-size/T pairs using several empirical calibrations derived for major rock forming minerals such as quartz, calcite, olivine, plagioclase, and orthopyroxene. The current version of the database includes a total of 17 paleopiezometric calibrations parametrized using the general expression:

$$\left\{ \begin{array}{l} \sigma = A^0 \beta^0 d^p \\ \sigma = \left(\frac{d}{A \exp \left(\frac{\beta}{T} \right)} \right)^{\frac{1}{p}} \end{array} \right. \quad (1)$$

With the following equivalences:

$$\left\{ \begin{array}{l} A^0 = \frac{1}{A} \\ \beta^0 = \frac{1}{\exp \left(\frac{\beta}{T} \right)} \end{array} \right. \quad (2)$$

Where σ is differential stress [MPa], A is an empirical constant that characterize the stress-grain size response of the mineral [MPa mm^{-p}], β is a temperature-dependent term [K] that is usually 1 in most calibrations except some developed for quartz (i.e., [Shimizu, 2008](#)), d is grain size expressed as the diameter of the circle of equivalent area [mm] and p is the grain size exponent.

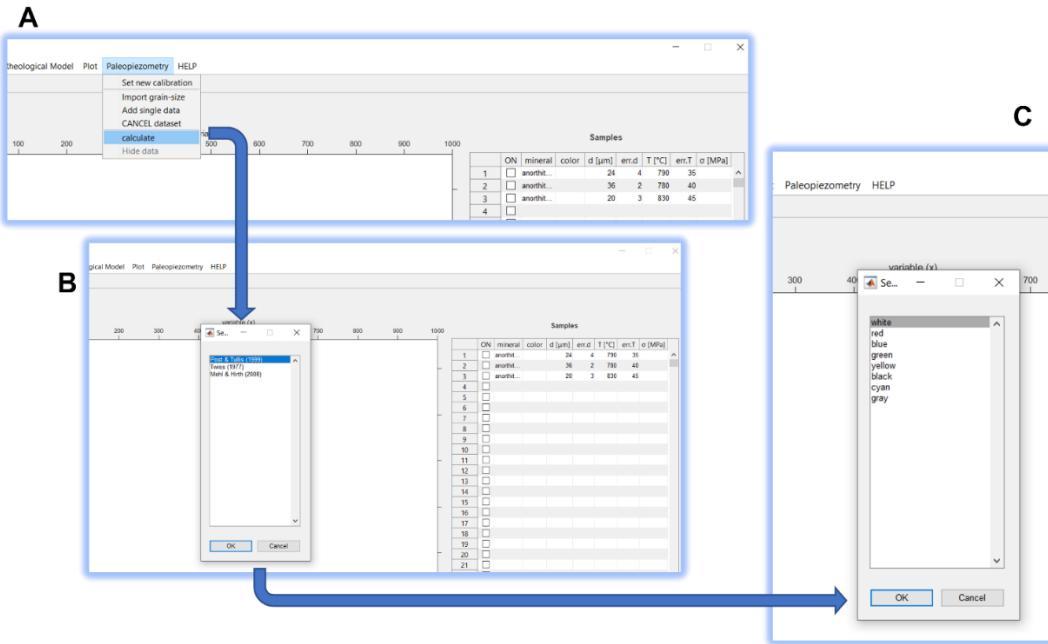


Fig. 11. Input dialog boxes that open to apply a given piezometric calibration already uploaded in the database: a) in the ‘Paleopiezometry’ menu, the sub-menu ‘calculate’ become active whenever at least one grain-size/T data pair has been uploaded and appear in the data table right to the main plot (i.e., table ‘samples’), b) just on click the ‘calculate’ sub-menu, a list box opens showing the piezometer(s) available for the current mineral phase (see second column of ‘samples’ table), then 3) after a calibration has been selected, a last list box allow setting the colour of the marker for the paleostress data being displayed.

The 17 calibrations included in the database of piezometers (version dbpc5_2021) provide stress/grain size relationships for quartz (Twiss, 1977; Stipp & Tullis, 2003; Stipp & Tullis 2003 corrected after Holyoke & Kronenberg, 2010; Shimizu, 2008), olivine (Twiss, 1977; Karato et al., 1980; van der Waal et al., 1993), calcite (Twiss, 1977; Schmidt et al., 1980; Rutter et al., 1995), plagioclase (Twiss, 1977; Post & Tullis, 1999; Mehl & Hirth, 2008) and pyroxene (Bruijn & Skemer, 2014). Paleostress analysis requires to upload at least one grain size/T pair, either by manually entering the values using the sub-menu ‘Add single data’ from the ‘Paleopiezometry’ menu, or by uploading a dataset from an excel spreadsheet. This last action should be done using the ‘Import grain-size’ sub-menu from the menu ‘Paleopiezometry’ (Fig. 11a). Once grain size/T data appear in the data table next to the main plot (table ‘Samples’), the sub-menu ‘calculate’ switch on (Fig. 11a), and the user can select from a list box one of the available piezometric calibrations for the current mineral phase (Fig. 11b). After a calibration is selected, another list box allows selecting the colour of the marker(s) that will be used to show the current dataset in the main plot, in a stress/T space. Adding new grain size/T pairs require repeating the procedure

2.3.2. Add new calibration

New piezometric calibrations could be add to the datatase following a simple procedure: first, click on the ‘Set new calibration’ sub-menu of the ‘Paleopiezometry’ menu (Fig. 12a). This action will open in sequence two input dialog boxes that allow first to specify the name of the new piezometer, and finally to set up the mineral the new calibration is designed for and its parameters, formulated as material constant A, T-dependent term and stress exponent (Fig. 12b,c).

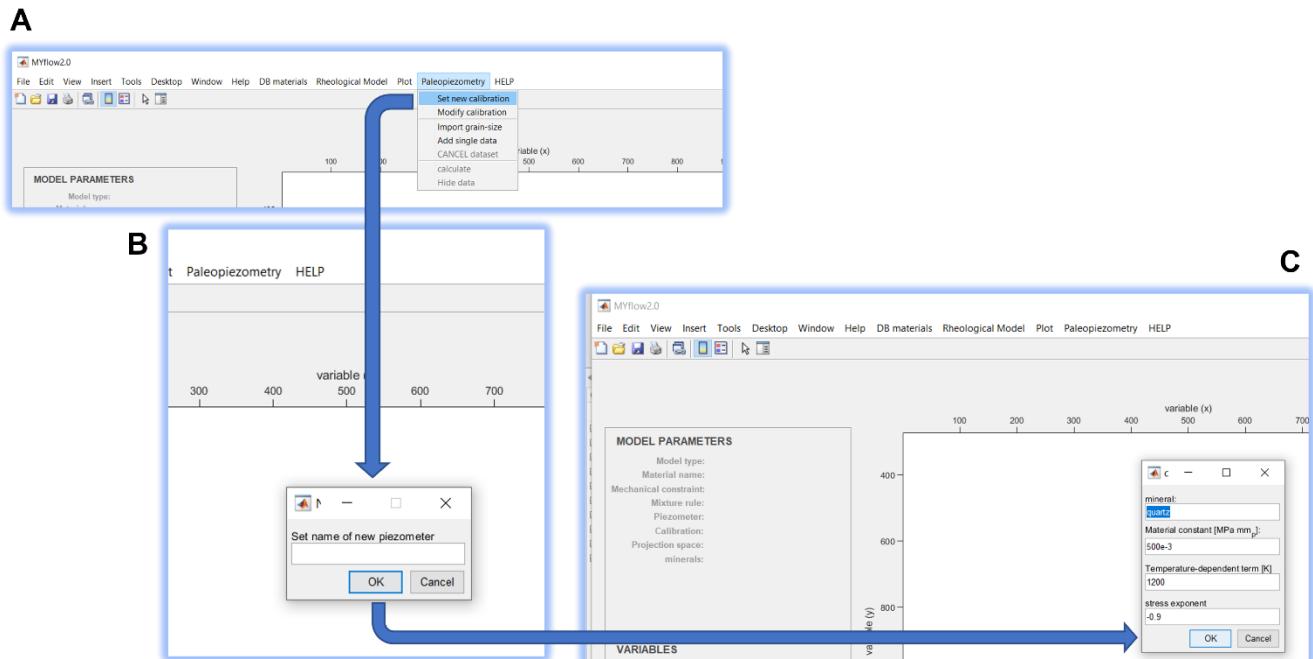


Fig. 12. Input dialog boxes that open to add a new piezometric calibration to the current database: a) in the ‘Paleopiezometry’ menu, the sub-menu ‘Set new calibration’ is always active regardless of grain-size/T data pair has been uploaded or not , b) just on, an input dialog box opens and request to set up the new piezometer’s name , then c) another input dialog box allow setting the parameter of the new calibration, and the mineral phase the calibration is designed for.

The new piezometer is automatically saved and added to the database at the end of procedure, so is readily available for modelling.

3. Rheological modelling

MYflow automatically computes the flow law parameters of dislocation creep, diffusion (Coble) creep and grain-boundary sliding of both single-phase and composite materials. Single-phase models can be created by selecting the submenus ‘Single mineral’ and ‘Load mineral’ from the ‘Rheological model’ menu (Fig. 13a). This action will open a list dialog box that allow selecting one of the existent mineral phases in the database (Fig. 13b). The current selection is displayed in the data zone to the left of the main plot just on click the OK button (Fig. 13c).

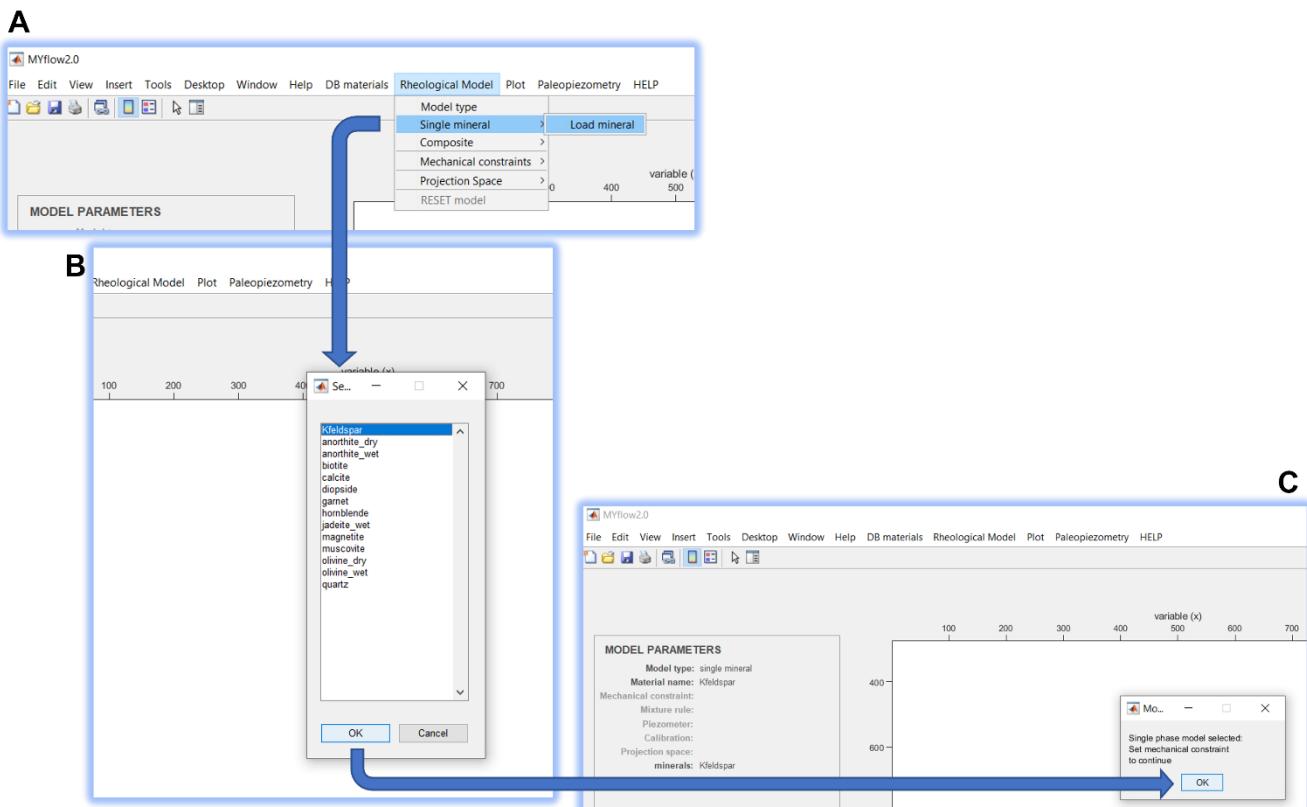


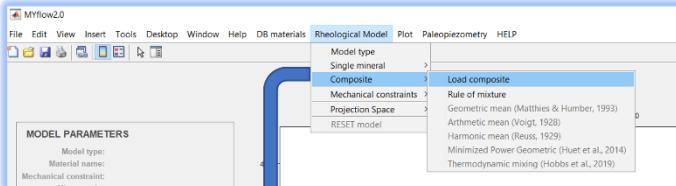
Fig. 13. Set single phase models: a) select ‘load mineral’ from ‘single mineral’ menu, b) select one of the available mineral phases from the mineral database, c) confirm model type and display current selection in the data zone to the left of the main plot.

Composite models (i.e., rocks composed of two or more mineral phases) can be selected in a similar way by clicking on the ‘Composite’ and then ‘Load composite’ submenus from the ‘Rheological model’ menu (Fig. 14a). A list dialog box opens allowing to select one of the available composite models stored into the ‘DB_composite’ folder (Fig. 14b). As for the single-phase models, after click on the OK button, the model type, composite name, minerals (within the composite) properties are updated in the data zone to the left of the main plot (Fig. 14c). Rheological modelling allows to upload only single minerals or composites already included in the respective databases; thus, the users should add/modify their own materials before going to rheological modelling.

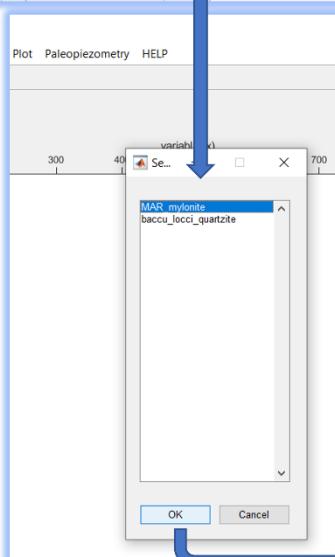
The flow law parameters of dislocation creep (DC), diffusion creep (Diff) and grain boundary sliding (GBS) of each mineral phase are calculated from six independent physical constants according to the theoretical model proposed by [Langdon & Mohamed \(1976\)](#) and modified by [Hobbs et al. \(2019\)](#). The constants include the pre-exponential constant of dislocation creep A_{DC} [Mpa⁻ⁿ s⁻¹], the molar volume V_m , [kJ/kBar], the Burger’s vector b

[mm], shear modulus G [MPa], the activation energy of lattice diffusion Q_L [kJmol $^{-1}$], and the activation energy of grain boundary diffusion Q_{GB} [kJmol $^{-1}$].

A



B



C

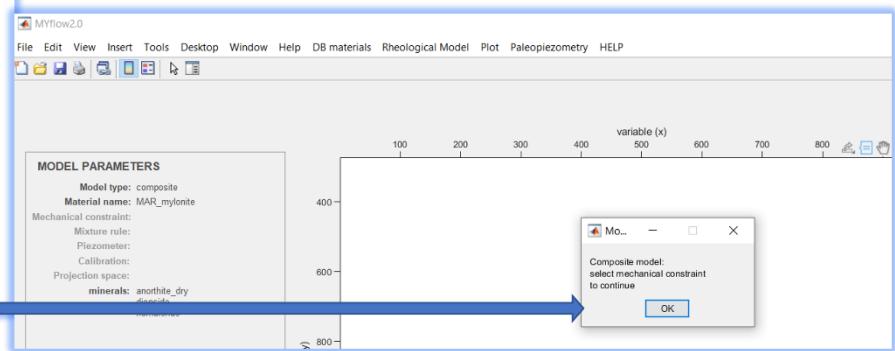


Fig. 14. Set composite models: a) select ‘load composite’ from ‘composite’ menu, b) select one of the available composites from the composite database, c) confirm model type and display current selection in the data zone to the left of the main plot.

The flow law parameters of pure minerals are formulated assuming a general flow law of the form:

$$\dot{\varepsilon} = A\sigma^n D \exp\left(\frac{-Q}{RT}\right) \quad (3)$$

$$D = d^{-m}$$

where $\dot{\varepsilon}$ is strain rate [s $^{-1}$], A is the pre-exponential constant that characterizes the material [MPa $^{-n}$ mm $^{-m}$ 1/s], σ is flow stress [MPa], d is the grain size [mm], Q is the activation energy of the specific deformation mechanism [kJ/mol], R is the gas constant [JK $^{-1}$ mol $^{-1}$], T is temperature [K], n and m are the stress and grain-size exponent, respectively. The various flow law parameters are calculated from Eq. 3 and the physical parameters of the given mineral parameters based on the following equivalences ([Langdon & Mohamed, 1976](#); [Hobbs et al., 2019](#)):

$$\begin{cases} A_{dc} = 3D_0G^{-3}b/kT \\ A_{diff} = \frac{82D_0b^4}{kT} = (82G^3b^3/3)A_{dc} \quad (4a) \\ A_{gbs} = \frac{10D_0G^{-1}b^3}{kT} = (10G^2b^2/3)A_{dc} \end{cases}$$

$$\begin{cases} m_{DC} = 0 \\ m_{Diff} = 3 \text{ (4b)} \\ m_{GBS} = 2 \end{cases}$$

$$\begin{cases} n_{DC} = 4 \\ n_{Diff} = 1 \text{ (4c)} \\ n_{GBS} = 2 \end{cases}$$

Where D_0 is a reference diffusion coefficient ([Zener, 1951](#)), G is shear modulus [MPa], k is the Boltzmann constant, b is the Burgers vector [mm], A_{diff} , A_{gbs} and A_{dc} are the pre-exponential constants of diffusion (Coble), grain-boundary sliding and dislocation creep, respectively [$\text{MPa}^{-n} \text{mm}^{-m} \text{s}^{-1}$]. The average flow law parameters of composite rocks are calculated from [Eq. 3](#), upon selecting one of the available mixing rules (see [par. 3.2 Mixing rules](#)).

3.1. Mechanical constraints

Once the model has been set up, either single mineral or composite, the user is requested to specify the mechanical constraint that control the rheological behaviour of the material ([Fig. 15](#)). MYflow implements two options that corresponds to the Voigt and Reuss elastic bounds ([Voigt, 1928](#), [Reuss, 1929](#)). Although both mechanical constraints are potentially applicable to any mylonite regardless of its composition and microstructure, the choice of one of the two limits strongly influence the results, particularly whenever the investigated mylonite does not represent steady-state deformation (i.e., its microstructure is far away from a energetically stable configuration). In these cases, the selection of one or the other elastic limit should be based on general considerations, as explained more in details in the next sections.

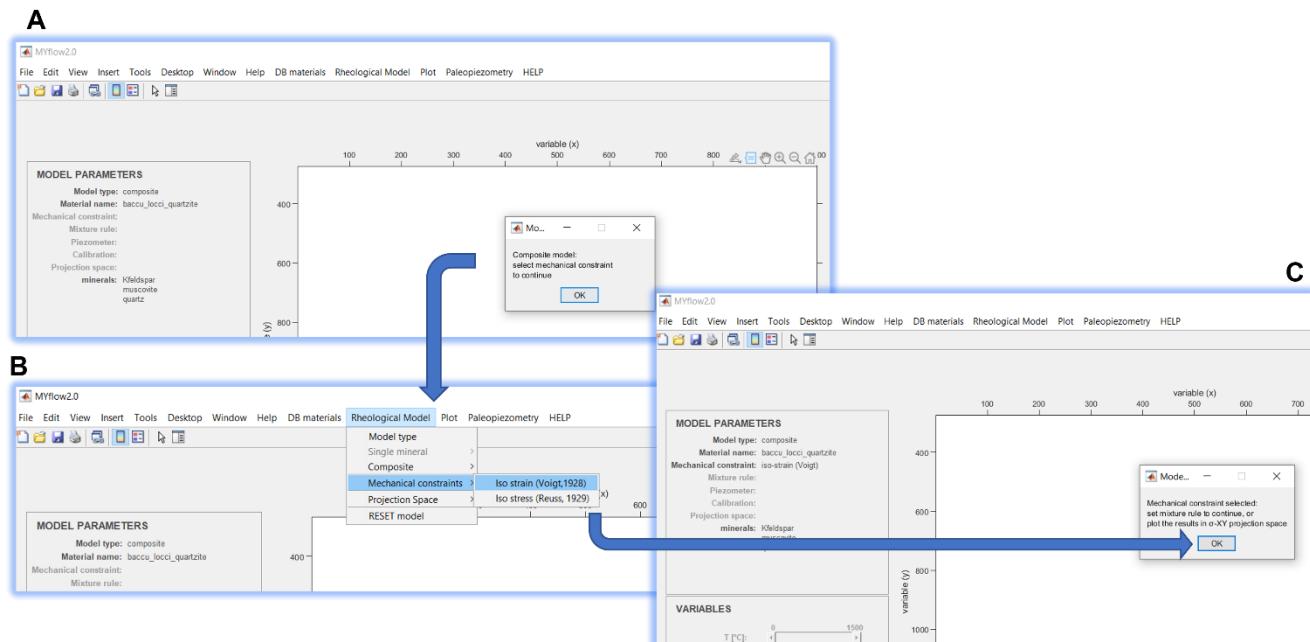


Fig. 15. Steps to select a mechanical constraint: a) dialog box requesting to select the mechanical constraint automatically opens upon model selection, b) menu allowing to select one mechanical constraint, c) the data zone is updated just on selection.

3.1.1. Voigt elastic bound

The Voigt elastic bound (Fig. 16a) describes the strength of an elastic composite material as the ratio of average stress to average strain provided that all the components of composite deform to the same strain ([Voigt, 1928](#)). For that reason, the Voigt bound is frequently identified as an iso-strain condition. The strength of viscous composite materials could be described similarly as effective viscosity, or the ratio of average stress to average strain-rate expanding the Voigt condition and assuming that all grains in the composite deform at the same velocity. Composite rocks can in no way be stiffer than the simple arithmetic average of the respective viscosities of their components provided by the Voigt bound through:

$$\eta_V = \sum_{i=1}^N \phi_i \eta_i \quad (5)$$

where η_V is the effective viscosity of the composite made of N components each characterized by a given volume proportion ϕ_i and specific viscosity η_i . [Eq. 5](#) implies that heterogeneous rocks composed of different mineral phases record spatially variable stresses, being largest in the phases with higher viscosity to keep their strain rate equivalent to that of weaker phases. Effective viscosity is expected to depend not only on composition, but also on grain size in minerals of identical composition.

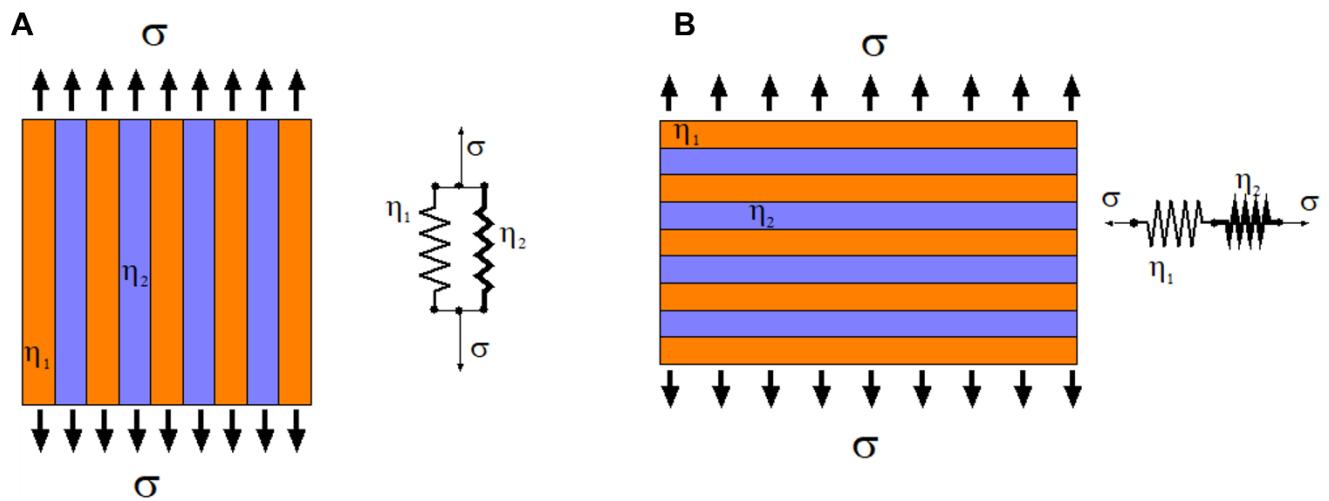


Fig. 16. Simplified geometrical model of Voigt and Reuss elastic bounds: a) Voigt bound describes a composite made of two different materials characterized by different viscosities (η_1 and η_2 , respectively). The fibres (particles) are connected in parallel, so they deform to the same extent, b) Reuss bound describe a composite where the fibres (particles) are connected in series so that stress is homogeneously distributed through the composite.

Crystals, in fact, may deform either by dislocation creep which is independent on grain-size, or by grain-size sensitive processes which could be either linear (diffusion creep) or non-linear in stress (grain-boundary sliding). Each deformation process is expressed by [Eq. 3](#) using mechanism-specific pre-exponential constants, activation energies, stress and grain-size exponents ([Eqs. 4a-c](#)). This implies that a given mineral will record different effective viscosity depending on the effective deformation mechanism.

3.1.2. Reuss elastic bound

The Reuss elastic bound (Fig. 16b), also identified as the iso-stress condition, describes the strength of an elastic composite material as the ratio of average stress to average strain provided that all the components of composite are loaded in the same way (Reuss, 1929). By analogy to the Voigt bound, composite rocks can in no way be softer than the harmonic average of the respective viscosities of their components provided by the Reuss bound through:

$$\frac{1}{\eta_R} = \sum_{i=1}^N \frac{\phi_i}{\eta_i} \quad (6)$$

where η_R is the effective viscosity of the composite provided by the isostress condition, and the other terms are the same introduced in Eq. 5. The Reuss model implies that heterogeneous rocks composed of different mineral phases might record spatially variable strain rates, being largest in the phases characterized by lower viscosity. Also, assuming a Reuss condition, effective viscosity is strongly dependent on both the composition and grain size of the various grains the composite is made of.

3.2. Mixing rules

Unless rheological modelling targets inversion of microstructural data to calculate stress or strain-rate/xy maps (see par. 3.3.2 ‘2D projections’), derivation of the averaged flow law parameters of composite materials requires setting an appropriate mixing rule. The current version of MYflow implement 5 different mixing models based on distinct theoretical approaches. Noteworthy, selection of Voigt or Reuss mechanical constraint precludes application of the harmonic or arithmetic average, respectively, which are based on opposite assumptions (Fig. 17).

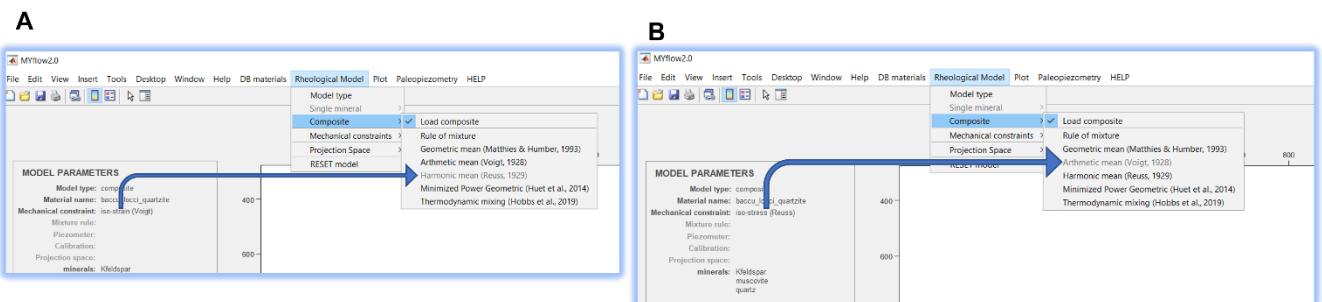


Fig. 17. Menu path to select one of the available mixing rules: a) list of the mixing rules available for Voigt mechanical constraint, b) list of the mixing rules available for the Reuss mechanical constraint.

3.2.1. Arithmetic average

The arithmetic average coincides with the Voigt model for composites deforming at uniform strain rate. By selecting this option, the flow law parameters of the composite are simply calculated from Eq. 5, volume-averaging each parameter over the N phases of the composite. This mixing rule is not available selecting Reuss as mechanical constraint.

3.2.2. Geometric average

The geometric average – a simple approximation of the Voigt-Reuss-Hill average - is based on a geometric averaging procedure which has no physical meaning although it reproduces satisfactorily the strength of two-phase composites ([Ji, 2004](#)) and the elastic properties of most aggregates composed of N different phases ([Matthies & Humbert, 1993](#); [Mainprice & Humbert, 1994](#)). The effective viscosity of a composite rock is estimated as:

$$\eta_{GM} = \sqrt[N]{\phi_i \eta_i \cdot \phi_{i+1} \eta_{i+1} \cdot \dots \phi_N \eta_N} \quad (7)$$

where η_{GM} is the bulk effective viscosity calculated by volume-averaging the geometric mean of the effective viscosities of the components. Obviously, the geometric average provides intermediate values of effective viscosity and other physical parameters, which are between the lowest values obtained from harmonic average ([see par. 3.2.3.](#)) and the highest resulting from arithmetic average ([see par. 3.2.1.](#)).

3.2.3. Harmonic average

The harmonic average coincides with the Reuss model for composites deforming under uniform stress. By selecting this option, the reciprocals of flow law parameters of the composite are simply calculated from [Eq. 6](#) by volume-averaging the reciprocal of each parameter over the N phases of the composite. Of course, the harmonic average mixing rule is not available by selecting Voigt as mechanical constraint.

3.2.4. Minimized Power Geometric Model (MPGM)

The Minimized Power Geometric Model assumes that rocks spontaneously tend to minimize the mechanical power dissipated during deformation. The model calculates effective viscosity and flow law parameters of composite materials made of an arbitrary number of phases using the Lagrange multipliers method ([Huet et al., 2014](#)). The MPGM has been developed based on the assumptions that the various phases are evenly distributed in the composite and do not have any SPO or CPO; this allow avoiding theoretical problems arising from anisotropic viscosity. The model also assumes that all phases deform by incompressible viscous creep according to an Arrhenius-type equation similar to [Eq. 3](#) unless the grain-size exponent is assumed to be zero, and that elastic deformation is negligible. Finally, all the grains from the same phase record the same strain rate and stress (i.e., problems related to local, grain scale, switch from grain-size insensitive to grain-size sensitive processes are not accounted for). The MPGM uses two types of mechanical constraints, conceptually equivalent to the Voigt and Reuss elastic bounds. The first type of mechanical constraint assume that strain rate is partitioned between the N phases of the composite so that the bulk strain rate is the volume-averaged mean of the phase strain rates (Voigt-type constraint). Alternatively, the bulk stress can be obtained by volume-averaging the mean of the phase stress (Reuss-type constraint). The type of mean that is used in the mechanical constraints provide a further distinction between models using a geometric mean ([Eqs. 8](#)) and models using the arithmetic mean ([Eqs. 9](#)):

$$\begin{cases} \sigma_G = \prod_i \sigma_i^{\phi_i} \\ \dot{\varepsilon}_G = \prod_i \dot{\varepsilon}_i^{\phi_i} \end{cases} \quad (8)$$

$$\begin{cases} \sigma_A = \sum_i \phi_i \sigma_i \\ \dot{\varepsilon}_A = \sum_i \phi_i \dot{\varepsilon}_i \end{cases} \quad (9)$$

Where $\dot{\varepsilon}_A$ and $\dot{\varepsilon}_G$ are the bulk strain rates derived from arithmetic and geometric averaging the local strain rates, respectively, and σ_A and σ_G are the bulk stresses obtained from similar principles. The first two mechanical constraints are used to extrapolate the bulk flow parameters from end-members flow law as the arithmetic mean of the phase parameters weighted by the factor $\phi_i a_i$ ([Huet et al., 2014](#)). These results into two sets of bulk flow parameters of composite that assume a Voigt-type condition of uniform strain-rate (MPGe model, [Eqs. 10](#)), or a Reuss-type condition characterized by uniform stress (MPGs model, [Eqs. 11](#)):

$$\begin{cases} \bar{n} = \frac{\sum_i \phi_i a_i n_i}{\sum_i \phi_i a_i} \\ \bar{Q} = \frac{\sum_i \phi_i a_i Q_i}{\sum_i \phi_i a_i} \\ \bar{A} = \prod_i A_i^{\phi_i a_i / \sum_i \phi_j a_j} \left(\sum_i \frac{\phi_i n_i}{n_{i+1}} \right)^{-\bar{n}} \prod_i \left(\frac{n_i}{n_{i+1}} \right)^{\phi_i a_i n_i / \sum_i \phi_j a_j} \end{cases} \quad (10)$$

$$\begin{cases} \bar{n} = \frac{\sum_i \phi_i a_i n_i}{\sum_i \phi_i a_i} \\ \bar{Q} = \frac{\sum_i \phi_i a_i Q_i}{\sum_i \phi_i a_i} \\ \bar{A} = \prod_i A_i^{\phi_i a_i / \sum_i \phi_j a_j} \sum_i \frac{\phi_i}{n_{i+1}} \prod_i (n_i + 1)^{\phi_i a_i / \sum_i \phi_j a_j} \end{cases} \quad (11)$$

where the term ϕ_i is the volume proportion of i^{th} phase, \bar{Q} , \bar{n} and \bar{A} are the bulk exponential term, stress exponent and pre-exponential constant, respectively. The term a_i is a product of flow parameters computed as:

$$a_i = \prod_{j \neq i} (n_j, A_j, Q_j + 1)$$

3.2.5. Thermodynamic Mixing Rule

The thermodynamic mixing rule assumes that the enthalpy difference for the process that controls the bulk viscosity of a composite (and hence its flow laws parameters) is the sum of the molar volume weighted enthalpy differences for the individual mechanisms in the aggregate ([Hobbs et al., 2019](#)). The mixing model accounts for both compositional and topological heterogeneities, so that it can be used to estimate the bulk strength of both compositionally heterogeneous aggregates made of N phases with distinct rheology, monomineralic rocks with variable grain-size, or a combination thereof. As for the MPGM models, the thermodynamic mixing rule allows derive mixing models using either an iso-strain-rate or iso-stress mechanical constraint ([par. 3.1 ‘Mechanical constraints’](#)). Using the first assumption, as always, implies that the composite deforms under uniform strain rate, so that

different deformation mechanisms operate in parallel. This gives the following average flow law parameters of the composite:

$$\begin{cases} \bar{n} = \frac{\prod_i n_i}{\sum_i \alpha_i \prod_{j \neq i} n_j} \\ \bar{A} = \prod_i A_i^{\alpha_i \bar{n}/n_i} \\ \bar{Q} = \bar{n} \sum_i \frac{\alpha_i Q_i}{n_i} \\ \bar{D} \end{cases} \quad (12)$$

and:

$$\alpha_i = \frac{\phi_i \prod_{j \neq i} V_j^m}{\sum_i \phi_i \prod_{j \neq i} V_j^m} \quad (13)$$

where the term α_i is the molar volume proportion of the i^{th} phase, defined based on the volume proportion ϕ_i and molar volume V_m of phases. On the other hand, using the second mechanical constraint ([Reuss, 1929](#)) gives the following bulk flow parameters:

$$\begin{cases} \bar{n} = \sum_i \alpha_i n_i \\ \bar{A} = \prod_i A_i^{\alpha_i} \\ \bar{Q} = \sum_i \alpha_i Q_i \\ \bar{D} = \prod_i d^{-\frac{\alpha_i}{m_i}} \end{cases} \quad (14)$$

The thermodynamic mixing rule has been developed based on the principles of statistical thermodynamics and is particularly suited to evaluate the strength of composite mylonite made of two or more phases deforming by different, cooperative, deformation mechanisms ([Hobbs et al., 2019](#)).

3.3. *Projection spaces*

MYflow display the results obtained from [rheological modelling](#) on both monomineralic 0^{th} [dimensional](#) and composite [2D models](#) in the main plot that is already initialized at the opening of the program ([Fig. 1](#)). Seven different projection spaces, described below in the following paragraphs, can be accessed based on the type of selected model (i.e., [single phase VS composite](#)) and [mechanical constraint](#) ([Fig. 18](#)).

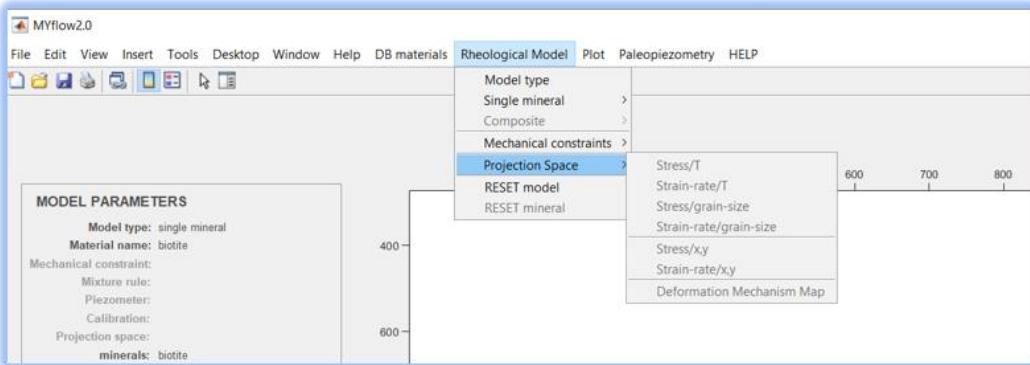


Fig. 18. Menu path to select one of the available projection spaces.

3.3.1. 0th dimensional projections

The results of both single-phase and composite models can be shown in different 0th dimensional projection spaces that uses stress, strain-rate, temperature, and grain-size as independent variables. Activation of one or more of these spaces depend on the choice of mechanical constraint. The iso-strain-rate condition (Voigt, 1928), in fact, enable plotting the results into either stress/temperature or stress/grain-size spaces. On the other hand, the iso-stress condition (Reuss, 1929) activates the strain-rate/temperature and strain-rate/grain-size projection spaces (Fig. 19). Any of these projection spaces requires setting the two independent variables not projected in the current reference system.

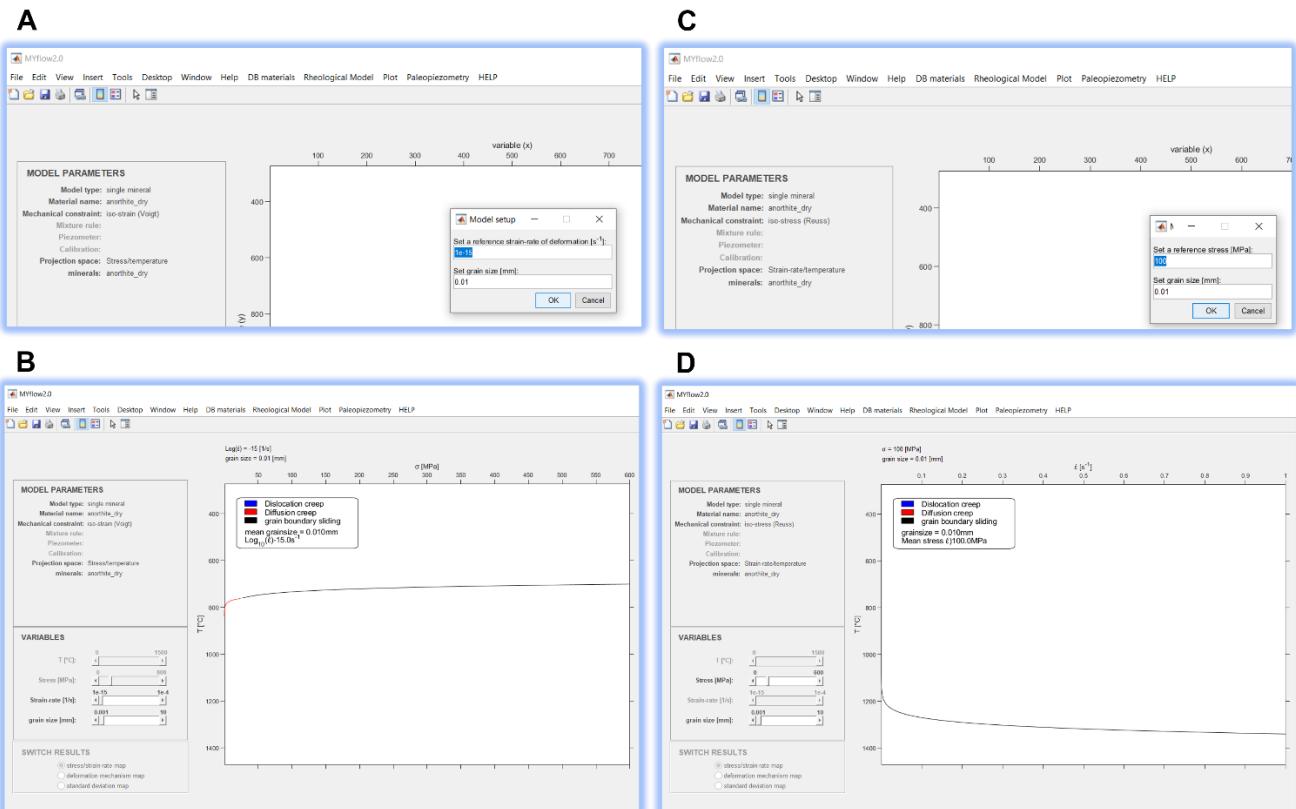


Fig. 19. Setting up projection spaces: a) set up of background (average) strain-rate and grain-size is requested after selecting Stress/T as projection space, b) 0th dimensional plot showing the stress/temperature relationship for anorthite. The value of the two independent variables assumed in the model (strain-rate and grain-size in this example) are shown in the upper left corner above the main plot. Note that segments of the curve take different colours in relation to the stable deformation mechanism that accommodate

deformation in the respective range of stress(strain-rate)/grain-size, c) set up of background (average) stress and grain-size is requested after selecting Strain-rate/T as projection space, d) 0th dimensional plot showing the strain-rate/temperature relationship for anorthite.

After selecting the projection space, MYflow request setting the appropriate independent variables ([see Fig. 19a,c for an example](#)) and then shows the results in the main plot ([Fig. 19b,d](#)). The rheology of either composite rocks or single-phase materials is shown as colour-coded curves where each colour corresponds to a different deformation mechanism, which is considered stable under the given range of temperature, stress, strain-rate and grain-size conditions based on the selected mechanical constraint. As the models are 0th dimensional (i.e., they correspond to just one mineral grain, or infinitesimal volume of ideally isotropic composite), we assume that various deformation mechanisms including dislocation creep (DC), diffusion creep (Diff) and grain-boundary sliding (GBS) compete to accommodate strain. Thus, assuming the principle of least action, we use two different stability criteria. The first criterion follows from the iso-strain-rate mechanical condition and implies that the effective deformation mechanism maximizes strain-rate ([Eq. 15](#)). The second criterion is related to the iso-stress mechanical condition and implies that the effective deformation mechanism minimizes stress ([Eq. 16](#)).

$$\dot{\varepsilon}_{bulk} = \max(\dot{\varepsilon}_{DC}, \dot{\varepsilon}_{Diff}, \dot{\varepsilon}_{GBS}) \quad (15)$$

$$\sigma_{bulk} = \min(\sigma_{DC}, \sigma_{Diff}, \sigma_{GBS}) \quad (16)$$

The switch from one to another of the 0th dimensional projection spaces is not allowed, unless resetting the rheological model through the related menu at the end of the ‘Rheological model’ menu. This implies repeating the procedure from the very beginning (i.e., selecting the model type as either ‘single phase’ or ‘composite’, selecting the mechanical constraint and so on).

3.3.2. 2D projections

Besides 0th dimensional MYflow allows evaluating the rheology of either single-phase or composite mylonite taking in stress/xy and strain-rate/xy maps. These models consider most geometrical parameters related to microstructure, such as grain-size and grain-size distribution, phase mixing, and phase-boundary topology, providing maps that show the theoretical spatial variation of stress or strain-rate as function of mylonite microstructure. Obviously, also using these projection spaces there will be two distinct types of plots based on the mechanical constraint. The distribution of stress is calculated from the [iso-strain-rate condition](#), whereas the strain-rate pattern requires selecting the [iso-stress condition](#). Both stress/xy and strain-rate/xy maps require uploading a microstructural phase map ([Fig. 20](#)).

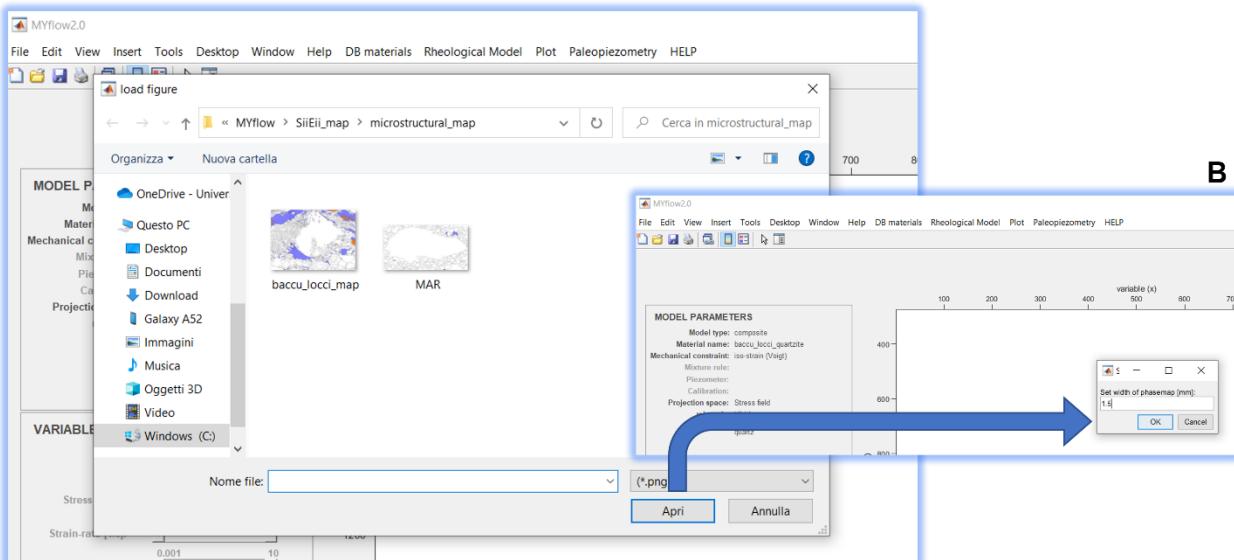
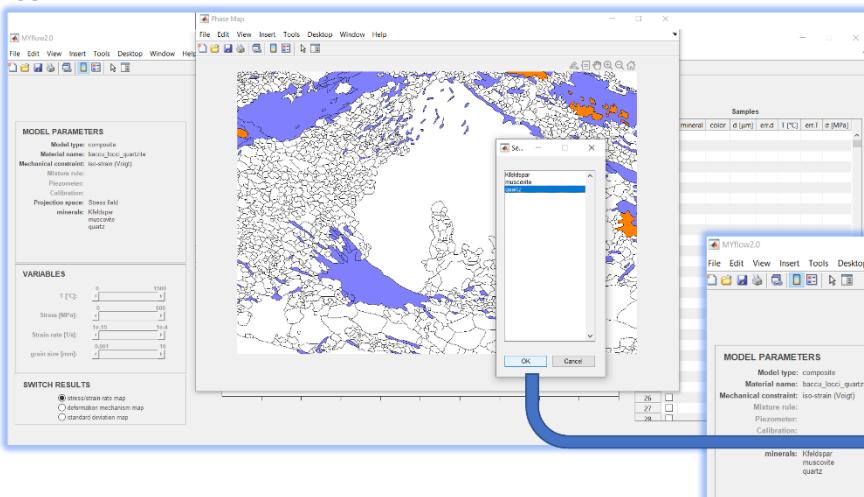
A**B**

Fig. 20. Phase map selection: a) selection of the file that stores the color-coded phase map (from the directory MYflow\SiiEii_map\microstructural_map), b) after selecting the file, MYflow requires setting the dimensions of the phase map by specifying the width of the image [mm].

MYflow automatically access the directory 'MYflow\SiiEii_map\microstructural_map' to load microstructural maps; thus, although it is possible to store the map files everywhere in your system, it is strongly recommended to use this folder to avoid potential search conflicts.

The maps should be provided as color-coded images where each colour (including white) identifies a mineral phase. Phase- and grain-boundaries must be identified using thin black lines. Accepted formats for microstructural maps are .bmp, .png, .jpeg, .tiff, however good results are obtained using .png files. Once the map file has been selected, MYflow opens the color-coded phase map as many times as the number of phases, and request classifying each different phase by selecting the appropriate mineral from the database (Fig. 21). As an example, for a composite mylonite made by quartz + Kfeldspar + muscovite as the one represented below, the image opens three times allowing the user to select a mineral phase by: 1) clicking on the appropriate colour, and 2) selecting the corresponding mineral from the database (Fig. 21a).

A



B

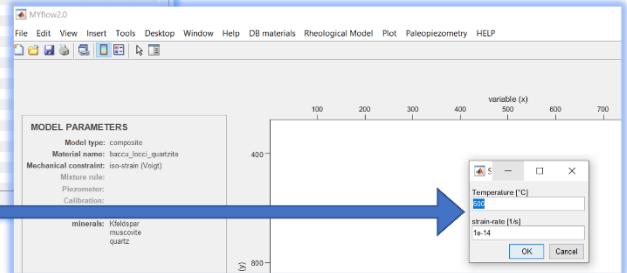


Fig. 21. Phase map classification: a) selection of the mineral phases requires clicking on the color-coded image, and then choosing the corresponding mineral phase from the database. The procedure is repeated as many times as the phases in the composite, b) after all phases (colours) in the image have been classified, MYflow request specifying the independent variables (in this case, temperature and strain-rate as the mechanical constraint is iso-strain-rate).

Multiple selection of the same mineral phase is not allowed and return an error. Once the classification procedure is completed, the software requires setting the temperature of deformation and either the average stress or strain-rate based on the selected mechanical constraint ([Fig. 21b](#)). Finally, the stress/strain-rate xy maps are automatically displayed in the main plot ([Fig. 22a](#)). After the stress/strain-rate maps appear on the screen, the three buttons on the lower left side of the main plot (panel ‘Switch results’, [Fig. 1](#)) activate, allowing to show different information. The first button ‘Stress/strain-rate map’ is selected by default and corresponds to either stress or strain-rate maps. The second button ‘deformation mechanism map’ shows the distribution of effective deformation mechanisms as colour-coded grain-boundary maps ([Fig. 22b](#)).

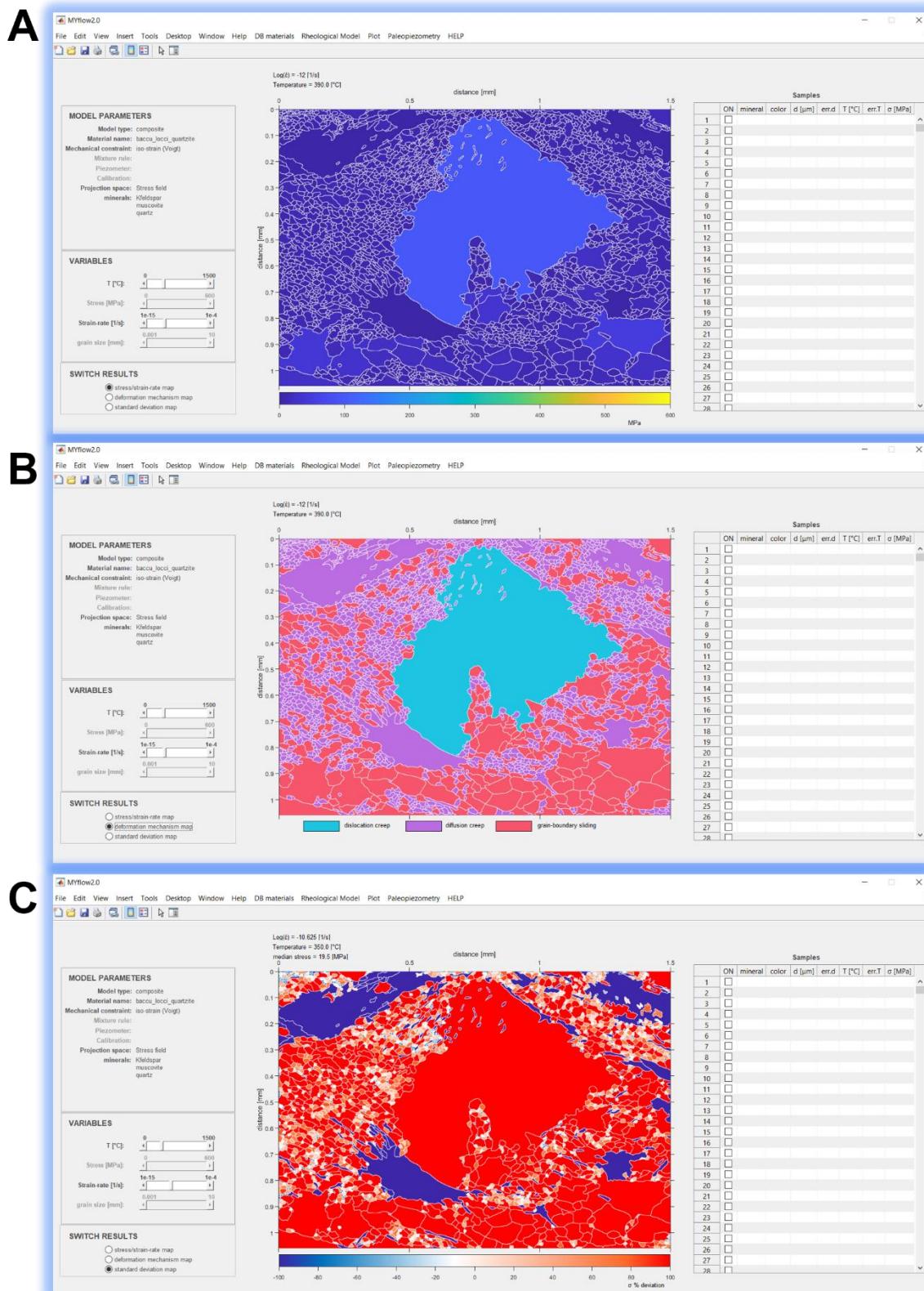


Fig. 22. Stress/strain-rate maps: a) gradient map showing the spatial distribution of stress (or strain rate), b) color-coded image showing the distribution of effective deformation mechanism, c) map of deviations from a mean stress/strain-rate value, which is indicated in the upper-left corner above the main plot.

Stress and strain-rate/xy maps are constructed using a theoretical approach similar to that used for single-phase 0th dimensional models; yet the 2D models account for the variability of both geometrical factors such as grain size and grain boundary topology, and the uneven distribution of mineral phases. 2D models assume that each grain of a mylonite, either monomineralic or composite, deforms independently of the others so that dislocation creep, diffusion creep and grain-boundary sliding compete to accommodate strain at a grain scale. This implies that each grain deforms by just one deformation mechanism under a given range of temperature, stress, strain-rate and grain-size. Also in this case, assuming the principle of least action, we have two stability criteria that indicate the effective deformation mechanism at the grain scale based on the minimization of stress- or maximization of strain-rate criterion ([Eqs. 13,14](#)). However, different deformation mechanisms may act simultaneously on differently sized grains of the same mineral phase, or on grains of similar size but different composition. This cooperative behaviour implies that the bulk strength of mylonite, expressed as the 'mean stress' or 'mean strain-rate' using the [Voigt or Reuss conditions](#), respectively, is computed as:

$$\begin{cases} \sigma_{bulk} = \sum_{i=1}^N \min (\sigma_i) \varphi_{m_i} \\ \dot{\varepsilon}_{bulk} = \sum_{i=1}^N \max (\dot{\varepsilon}_i) \varphi_{m_i} \end{cases} \quad (17)$$

$$\varphi_{m_i} = \frac{A_i V_{m_i}}{\sum_i A_i V_{m_i}} \quad (18)$$

where σ_i and $\dot{\varepsilon}_i$ are the local stress and strain-rate of ith grain, and the term φ_{m_i} ([Eq. 18](#)) is a coefficient used to weight the local stress values based on the molar volume proportion of each grain computed from the grain surface area A_i and the phase molar volume V_{m_i} . The mean stress/strain-rate values are used to calculate standard deviation maps. These maps are accessible by selecting the 'Standard deviation map' option from the 'Switch results' panel ([Fig. 22c](#)) and show, as value ranging from -100% to +100%, the local difference between the mean stress/strain-rate value and the stress/strain-rate value of any grain ([Fig. 22c](#)).

3.3.3. Deformation Mechanism Maps

Both mechanical constraints allow also plotting the results in classical deformation mechanism maps showing the stress dependency on grain size for a given range of strain-rates, for various deformation mechanism. Deformation mechanism maps can be calculated only using the 'single phase model' option as they are actually 0th dimensional plot. The independent variable that should be set by the user is temperature, which is defined through an input dialog box opening automatically after selecting 'Deformation Mechanism Map' as projection space ([Fig. 23a](#)). The stability field of the various deformation mechanism are then shown as colour-coded polygons in a logarithmic plot ([Fig. 23b](#)). The temperature of deformation could be eventually modified by the user through the slider control in the 'VARIABLES' panel to the left of the main plot. Any modification of the slider position adjust dynamically the stability fields of deformation mechanisms.

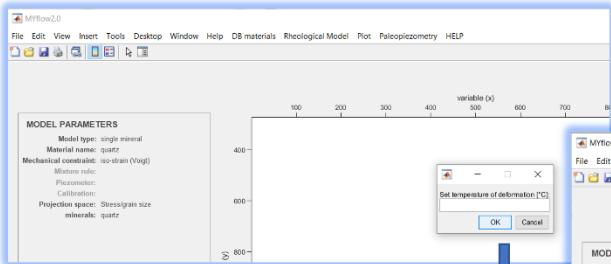
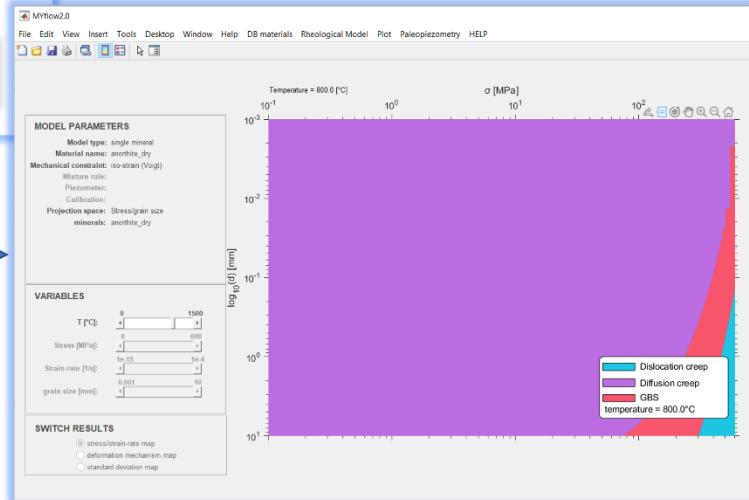
A**B**

Fig. 23. Deformation mechanism map: a) once Deformation Mechanism Map is selected as projection space, MYflow opens an input dialog box to set the temperature that should be used to evaluate the stability of deformation mechanism in stress/grain-size space, b) example of the output; each deformation mechanism is represented as a coloured field in stress/grain-size space

4. Paleopiezometry

MYflow provides an easy-to-use platform to perform paleo-piezometric analysis, which should be eventually compared with the outputs derived from 0th dimensional rheological models (stress/temperature space) as well as a few reference strength envelopes ([Byerlee, 1978](#)). The current version of the software is provided with a database of 17 empirical calibrations developed for five of the main rock-forming minerals such as quartz ([Twiss, 1977; Stipp & Tullis, 2003; Holyoke & Kronenberg 2010, Shimizu 2008](#)), olivine ([Twiss, 1977; Karato et al., 1980; van der Wal et al., 1993](#)), calcite ([Twiss, 1977; Schmid et al., 1980; Rutter et al., 1995](#)), plagioclase ([Twiss, 1977; Post & Tullis 1999; Mehl & Hirth 2008](#)) and pyroxene ([Brujin & Skemer, 2014](#)).

4.1. Import grain-size data

Paleo-piezometric analysis can be done from the ‘Paleopiezometry’ menu (Fig. 24a) using different methods, on minerals already included in the current version of the mineral database (Fig. 24b). The grain-size/T datasets can be imported from external files using the sub-menu ‘Import grain-size’ from the menu ‘Paleopiezometry’ (Fig. 24c). The use of Excel®-derived files (.xlsx) is highly recommended. The data should be organized in four columns with the first for grain size, the second for grain size uncertainty (1σ), the third temperature of deformation, and the last is for temperature uncertainty (1σ). The folder ‘paleopiezometry’ contains a demonstrative template to help formatting data.

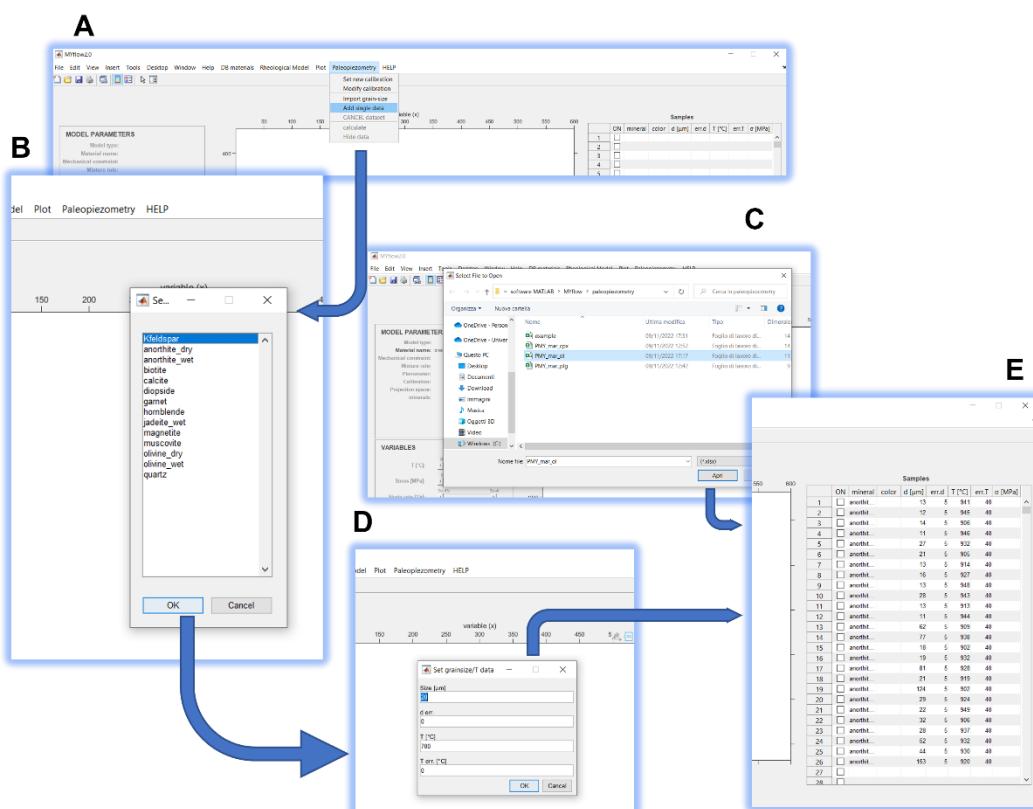


Fig. 24. Import grain-size/T data: a) the Paleopiezometry menu allow to import data from external files (Fig. 24c), or add single data manually from a template that opens after selecting the option ‘Add single data’ (Fig. 24d); regardless of the data import method selected,

MYflow open first an input dialog box that request selecting the mineral composition from one of the available phases in the database (Fig. 24b); e) aspect of the table showing the loaded data.

The columns of uncertainties (2 and 4) are optional and can be left empty. In this latter case, however, the results are plotted as tiny points in stress/temperature space. Additionally, grain-size/temperature data and related uncertainties can be imported manually from the sub-menu ‘Add single data’ from the menu ‘Paleopiezometry’ (Fig. 24d). The data selected are added to the currently active dataset shown in the table right to the main plot.

4.2. Select calibration

After a dataset, just one grain-size/T pair at the very least, has been imported, the ‘Calculate’ sub-menu allow selecting one of the available calibrations from the calibration database, and perform the calculus just after selecting the required piezometer. MYflow is programmed to keep in memory the composition of the last grains, or group of grains, added to the dataset. Therefore, the software allows selecting the calibration from a list of calibrations available for that mineral composition without showing the calibrations developed for different mineral phases (Fig. 25). However, it is possible to display at the same time stress/T data for different mineral phases, provided that the proper piezometric calibration and subsequent paleo-stress calculation are done before adding new phases to the dataset.

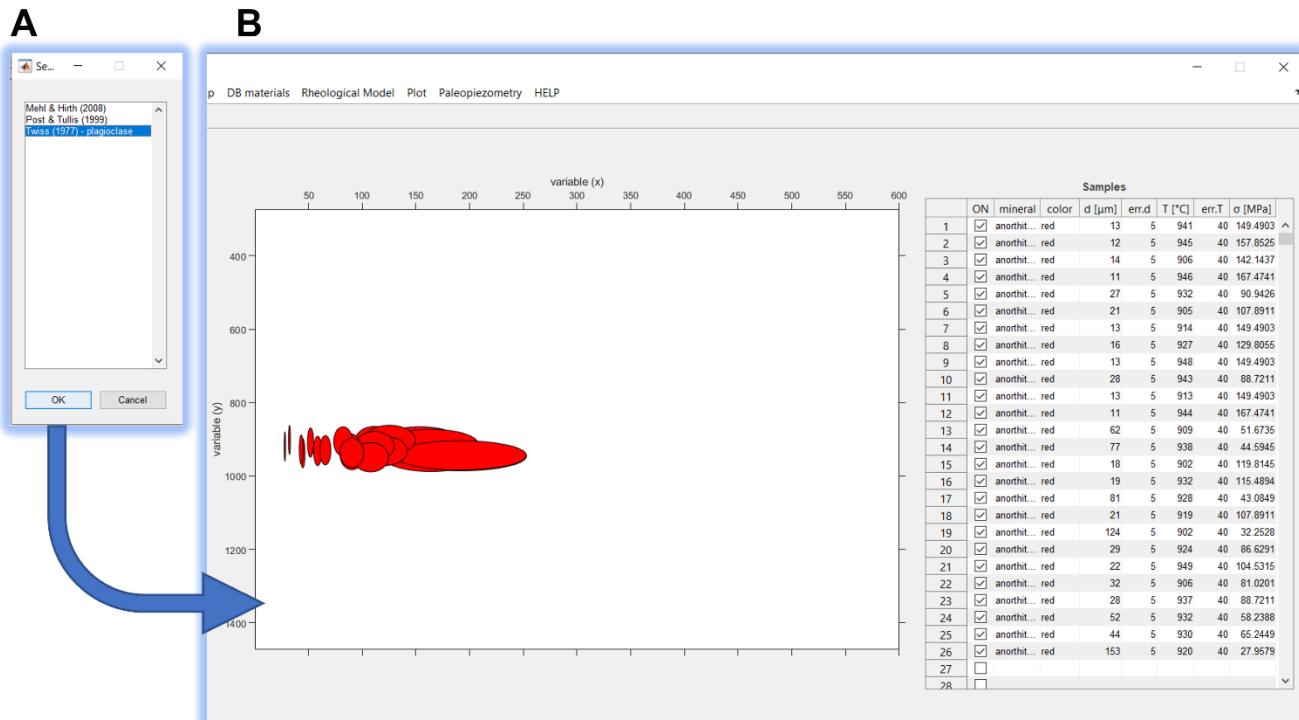


Fig. 25. Select calibration: a) list of available piezometric calibrations for mineral phase ‘anorthite_dry’; b) plot of the results after selecting the calibration of [Twiss \(1977\)](#). Note that the last column of the table now shows the calculated grain stress values.

4.3. Calculate paleostress

Calculation of paleo-stress values from grain-size/T pairs of data is automatic on selection of the sub-menu 'Calculate' from the menu 'Paleopiezometry' (Fig. 24a). Mixing datasets composed of different mineral phases is allowed, provided that the proper calibration is selected after each change of mineral composition. This implies that the user must click on the sub-menu 'Calculate' (and then select a piezometric calibration that will be used to perform calculation of paleo-stress) every one time the composition of the next data will be different from the last added to the dataset. Although not mandatory, it is recommended to change the colour of the various datasets to track the stress/grain-size differences recorded by different mineral phases (Fig. 26).

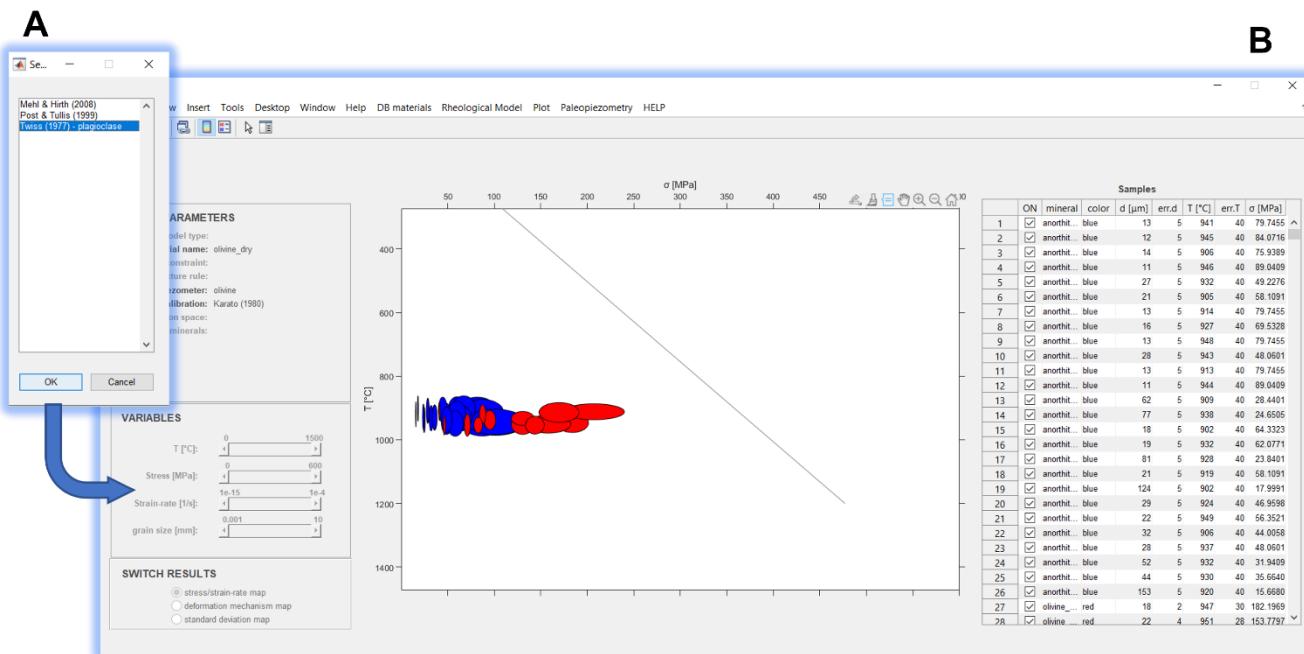


Fig. 26. Calculate and plot paleostress data: a) Select one of the available calibrations for the current mineral phase, b) appearance of a plot showing paleostress data for two different mineral phases as blue ellipses (plagioclase) and red ellipses (olivine). Note that the data zone to the left of the main plot (Model parameters panel) retain only information (i.e., mineral composition, type of piezometric calibration) of the last calculated subset of data, in this case olivine. The oblique black line is the reference strength envelope for normal faults (Byerlee, 1978), optionally shown as a reference curve (see par. 5.1).

5. Plotting functions

MYflow incorporates several functions designed to help data visualization, interpretation, and re-use of the outputs resulting from rheological modelling. These functions all go into the ‘Plot’ menu and allow to add reference curves, hide stress/T data calculated from paleopiezometric analysis, export the main plot as high-resolution figure, or reset current plot.

5.1. Add reference curves in 0th dimensional plots

Several reference strength envelopes can be optionally displayed in stress/temperature space along with paleo-stress data computed from r grain-size/temperature databases, or stress/T curves obtained for either single-phase or composite rocks. The reference curves include three frictional envelopes calculated for normal, strike-slip and reverse faults according to the empirical relation of [Byerlee \(1978\)](#), as well as two groups of curves describing the viscous strength of quartzite (calculated after [Stipp & Tullis, 2003](#)) and the viscous strength of dry olivine ([van der Wal et al., 1993](#)). The viscous envelopes are calculated for strain-rates ranging from 1×10^{-8} to $1 \times 10^{-16} \text{ s}^{-1}$ to cover the full spectrum of long-term viscous or brittle-viscous flow processes (Fig. 27).

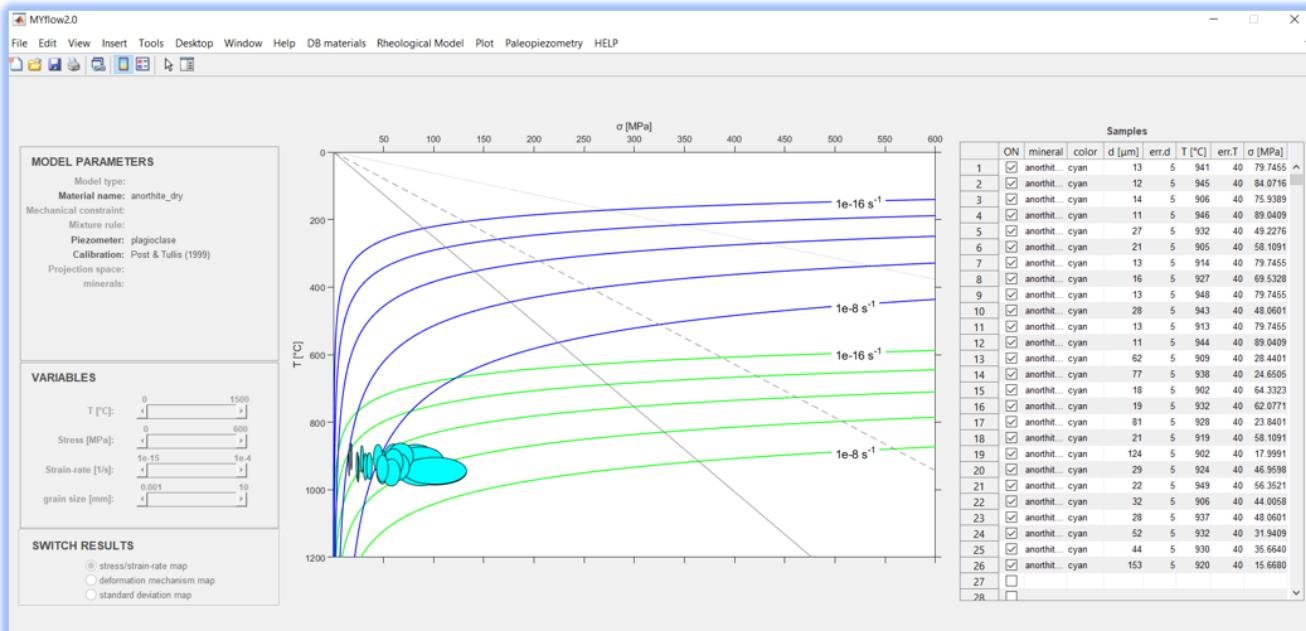


Fig. 27. Add reference curves to stress/T projection spaces: the blue curves indicate the reference stress/T curves for viscous creep of quartzite ([Stipp & Tullis, 2003](#)) for strain-rates between 1×10^{-8} to $1 \times 10^{-16} \text{ s}^{-1}$, the green curves indicate the reference stress/T curves for viscous creep of dry olivine ([van der Wal et al., 1993](#)). The straight grey lines mark the Byerlee’s frictional envelope for normal faulting (solid line), strike-slip faulting (dashed line) and reverse faulting (pointy line).

5.2. Cancel plot

The sub-menu ‘Reset plot’ restore the main plot to its initial configuration, however this action has no effect on the uploaded paleopiezometric dataset(s) and on the rheological model; thus, the command

'cancel plot' does not change the projection space, the type of mechanical constraint or the eventually selected mixing rule.

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