

Welcome to EMBER's first release.

Abstract

Magma decompression rate is one of the most important parameter in controlling eruption dynamic. One way to determine decompression rate is by modelling volatile diffusion in crystal-hosted embayments. Previous such studies have used a variety of distinct diffusion models, limiting the possibility for inter-study comparison. Here, we introduce EMBER (EMBayment-Estimated Rates), a standalone versatile tool that models diffusion processes of volatile elements along melt embayments. Our model relies on the *pdepe* function of MATLAB to calculate diffusion profiles of H₂O, CO₂ and S through finite difference method. EMBER uses a grid search seeking out the best fits for decompression rates, initial concentration of each studied volatile and pre-existing volatile content, while fixing three parameters: temperature along the ascent and pressure at the beginning and end of the ascent. Our model allows computations for basaltic, intermediate, and rhyolitic compositions. We apply EMBER to previous literature studies to evaluate our model and obtain results that are directly comparable between studied eruptions. Compiling the re-calculated data available to date, we compare magma decompression rates to eruption magnitude and find no statistically significant correlation. We hope our model will increase the number and inter-comparability of future petrological studies aiming at constraining magma decompression and ascent rates.

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Requirements: MATLAB runtime environment 2019

Versions: 1.0

Tutorial

1. Preparation:

Before using EMBER, you have to make sure that every file is set in the same directory, you can name it however you want.

There are 8 files needed for each analysis (figure1).

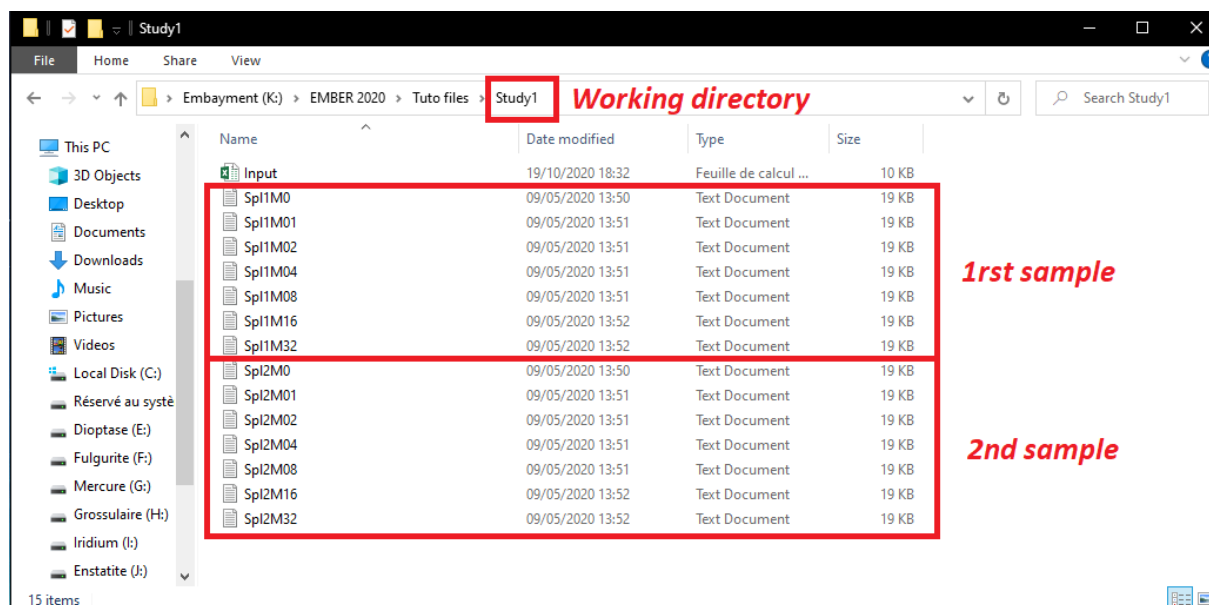


Figure 1: An example of a readable working directory. The input file contains data at least for samples 1 and 2. Each studied sample must be accompanied by 7 .txt files corresponding to degassing paths calculated for different pre existing volatile content ($M_0 = 0.1 \ 0.2 \ 0.4 \ 0.8 \ 1.6 \text{ and } 3.2\text{wt}\%$)

2. Making an Input file

The “Input.xlsx” (**case sensitive**) records all the sample data. First row is dedicated to the names of the columns. Starting from the second row data must be put in order from the mouth to the end of the embayment. Columns are organized from left to right “Analysis Name”, “Short name of the sample”, “CO₂”, “H₂O”, “S”, “F”, “Cl” and “Distance from the start/mouth of the embayment”. First point of each set of analysis must start with the values at the mouth (with a distance of 0). You might need to extrapolate data for the point $x = 0\mu\text{m}$. You should obtain a result similar to Figure 2. Please note that each names used along this tutorial are **case sensitive**.

	A	B	C	D	E	F	G	H
1	Analysis Name	Short name of the sample	CO2 (ppm)	H2O (wt%)	S (ppm)	F (ppm)	Cl (ppm)	Embayment distance from start (μm)
2	Extrapolation	Spl1						
3	Analysis#1	Spl1						
4	Analysis#2	Spl1						
5	Analysis#3	Spl1						
6	Analysis#4	Spl1						
7	Extrapolation	Spl2						
8	Analysis#1	Spl2						
9	Analysis#2	Spl2						

Figure 2: Example of a correct input file, the blue cells are the ones which will be read by EMBER. If any value is missing you may need to interpolate it. If that missing value is not on a blue cell, fill it with a '0'. To be read correctly, the "analysis name" cell must be in position A1 of the spreadsheet

3. Making the degassing path files

Seven .txt files containing the degassing path for each pre_existing volatile content value are also needed. For now, degassing paths are calculated for values of M_0 equal to 0, 0.1, 0.2, 0.4, 0.8, 1.6 and 3.2 wt%. Each of the .txt file must be named "[Short name of the embayment]M[0 to 32].txt". The first part to fill will be either "Spl1" or "Spl2". For example, for the previous case, the file related to the degassing path for $M_0=0.4\text{wt}\%$ will be named "Spl1M04.txt". There is currently two styles of degassing path file accepted by EMBER.

3.1. Using SolEx

If the program used is SolEx, the resulting text file can directly be read by EMBER. If H_2O values are not reached for the lowest pressure, you may extrapolate the volatile content for 1 bar and add a row under the 5 bar row for each file of the same embayment.

Generate different degassing paths files using SolEx

To do so, you mainly have to consider that you want to put back a certain quantity of volatile content back into your melt. To do so, you need to consider the proportion of each volatile into the gas phase and which melt compositions need to have these volatiles added.

-Define your "anchor" point. Which composition and at which pressure will you be adding the volatiles. This will help you find the proportion of volatiles you want to add.

Run a regular SolEx computation with major element analysis and your estimated initial concentration (Figure 3).

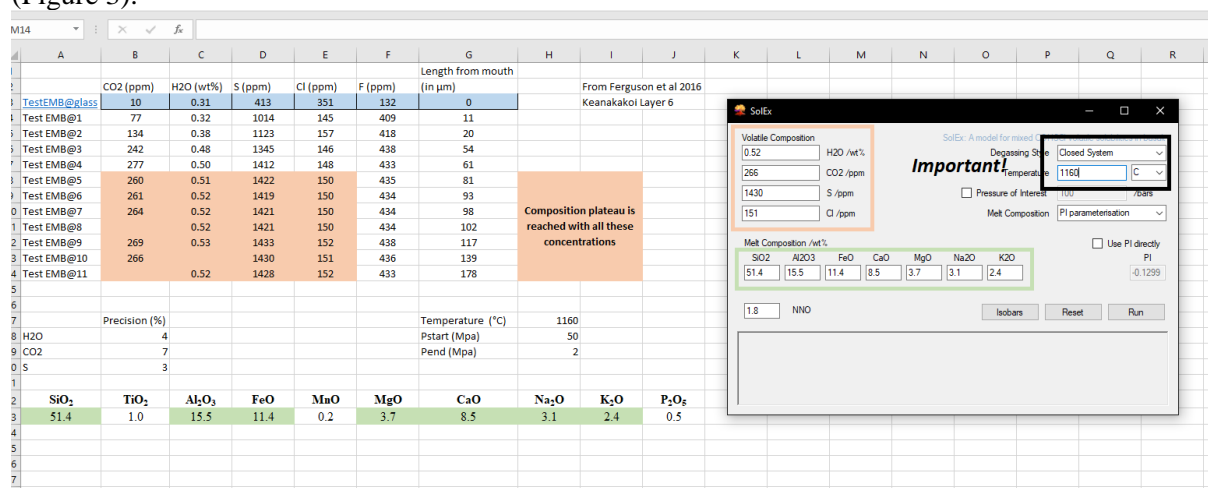


Figure 3: Setup of your first SolEx run. Do not forget to consider a closed system and to input the temperature, volatile concentrations and major concentration before clicking on "run".

Once you have your first "Solex_Output.txt" file, open it and check the pressure values (in bar) (figure4). Those txt files can get a bit tricky to read because columns can become very unclear sometimes. The way to find your "anchor point" is by looking for a change in behaviour from the volatile (usually the CO2). For example on this case, for P between 1000 and 600 bar, CO2 is stable around 264ppm. Then, for P=550bar, CO2 start decreasing noticeably to 245ppm. That marks you "anchor point", I usually take the values for higher pressure just before this change of behaviour. It sometimes coincide with the pressure you can find with solubility models but not always. Once you have the right line, extract values from columns 6 to 10.

Copy the extracted values in a spreadsheet so you can do the next calculations more easily.

WTH200	PPMC020	PPMS0	PPMC10									
0.52	266	1430	151									
P	Melt: WTH20	PPMC02	PPMS	PPMC1	Fluid: by mass			by mols				
					Exsol. vol%	XVH20	XVC02	XVS	XVC1	XVH20	XVC02	XVS
1000	0.519998		264.762	1429.99	150.993	0.00127176	0.0188004		0.967593		0.00808554	
950	0.519998		264.762	1429.99	150.992	0.00132637	0.0186545		0.966136		0.00901234	
900	0.519998		264.761	1429.99	150.991	0.00138708	0.0185016		0.964307		0.0101558	
850	0.519998		264.761	1429.99	150.99	0.00145497	0.0183403		0.962023		0.011563	
800	0.519998		264.76	1429.98	150.988	0.00153139	0.018169		0.959186		0.0132884	
750	0.519998		264.76	1429.98	150.986	0.00161805	0.0179856		0.955683		0.015398	
700	0.519998		264.76	1429.98	150.983	0.00171715	0.0177875		0.95135	0.0179896		0.0128
650	0.519998		264.759	1429.97	150.98	0.00183156	0.0175695		0.945891		0.0212466	
600	0.519998		264.759	1429.97	150.976	0.00196512	0.0173214		0.938731		0.0255385	
550	0.51996	245.651	1429.24	150.703	0.0348996	0.0184989	0.932991		0.0348759		0.0136	
500	0.519904		221.977	1427.7	150.588	0.0025443	0.0200949		0.923047		0.0482271	
450	0.519836		198.341	1424.99	150.606	0.140215	0.0218975		0.90575	0.0670784		0.0052
400	0.519752		174.855	1420	150.675	0.211642	0.0238595		0.876831		0.0961842	
350	0.519643		151.393	1409.81	150.752	0.303464	0.0257782		0.826771		0.145666	
345	0.51963	149.046	1408.26	150.76	0.314138	0.0259466	0.819926		0.152443		0.0016	
340	0.519617		146.708	1406.56	150.767	0.325111	0.026105		0.81264	0.159667		0.0015
335	0.519603		144.378	1404.71	150.774	0.336394	0.0262511		0.804875		0.167376	
330	0.519589		142.001	1402.66	150.78	0.348171	0.0263942		0.796581		0.175614	
325	0.519575		139.69	1400.43	150.787	0.360122	0.0265108		0.787736		0.184423	
320	0.51956	137.333	1397.95	150.793	0.372602	0.0266201	0.778269		0.193859		0.0012	

Figure 4 : Extraction of volatile proportion and gas proportion for your « anchor point » from the first SolEx file.

Extracted proportions correspond to the upper part of both tables from Figure 5 and constitute half of the input. The second half is the compositions that you put inside SolEx at first to make the calculation (Figure 5).

Now, since “Exsol. Vol%” which is the equivalent of M_0 , is different from 0, we have to calculate a $M_0=0\text{wt}\%$ back by removing a proportion of volatile for each volatile (STEP 1, Figure 5). Repeat the calculation with respective proportion for each volatile.

Now that the $M_0=0$ column is filled, you can add the proportion of each volatile by adding $M_0 \times X_{\text{Vola}}$ for each $M_0=0\text{wt}\%$ volatile composition and each M_0 value.

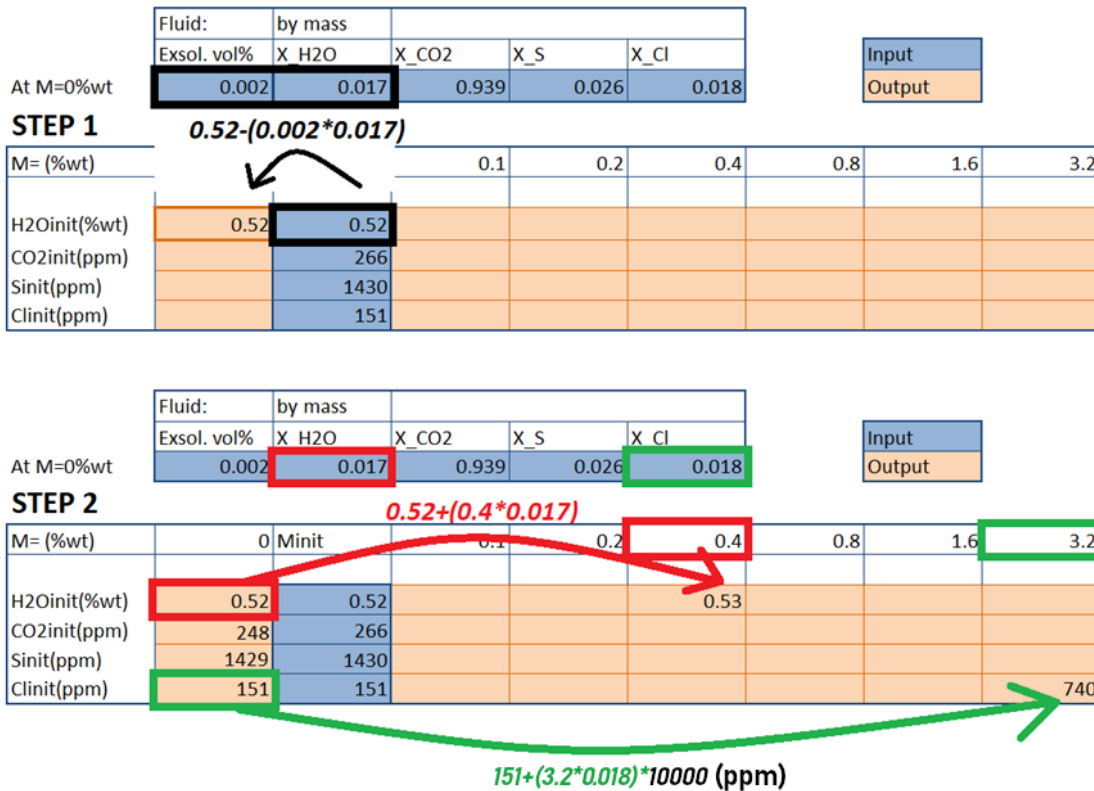


Figure 5: An example of calculations of SolEx volatiles input for different M_0 values. The STEP1 calculation is repeated for each line (with related proportion value). X_{H_2O} , X_{CO_2} , X_S and X_{Cl} stand respectively for the gas proportion of H_2O , CO_2 , S and Cl . M_{init} stands for $M_0 = \text{Exsol. vol\%}$ which is the pre-existing volatile content calculated by SolEx for the concentrations in blue and for $P = P_{start}$, the pressure at the beginning of the ascent. I usually make an automated excel file to calculate those different M_0 compositions. Do not forget to convert wt% to ppm for CO_2 , S and Cl

Now you can run SolEx 7 times with the same major element but different volatile compositions to emulate different M_0 values. Do not forget to put the right name for each file.

Hang thigh, we are almost done, there is still one more step remaining.

Among all the SolEx calculations that you will do, some calculation error can happen for very low pressure and usually for high M_0 values. I advise you to check every .txt files and mostly the high M_0 ones (Figure 6). When those errors appear, you may extrapolate the data for columns 2, 3 and 4. They usually are very low and close to 0. The other values can be replaced by "0".

25	0.175431	10.3683	5.78093e-007	601.643	92.8648	0.110214	0.824804	0.0612134	0.
20	0.143154	8.45196	9.08698e-008	584.761	94.3102	0.11791	0.817251	0.060649	0.00419008
15	0.0977547	6.55786	8.2312e-009	561.633	95.7773	0.128502	0.80687	0.0598749	0.00475287
10	1.#QNAN	1.#QNAN	2247	740	1.#QNAN	0	0	0	0
5	1.#QNAN	1.#QNAN	2247	740	1.#QNAN	0	0	0	0

Figure 6: Example of a calculation problem with SolEx files. I usually consider a point for 1bar with associated concentrations of H_2O at 0.01wt% and CO_2 and S at 0ppm and interpolate missing and error values from those "1.#QNAN" lines. I do that only for the columns 2, 3 and 4 (respectively for H_2O , CO_2 and S). The rest can be replaced by 0.

SolEx calculations are done, you have done the biggest (and sometimes the longest) part of the whole process!

3.2. Using VolatileCalc

VolatileCalc is easier and faster to use than SolEx but does not compute S.

Follow the regular utilization of VolatileCalc, just remember to choose “closed system” so you can input different M values. You have to choose the same number of step each time. Copy every column of the output to a new Excel spreadsheet.

Add an extra column right of the “CO2vmol%” column for the S degassing path (Figure 7). Usually, it is not calculated directly by VolatileCalc but this column exists in case you are using your own model to estimate S degassing, like Newcombe et al, (2020). If you are not interested in S, add the S column nonetheless and fill it with “0”. You should obtain a result similar to the one displayed in Figure 7. Once done, you can save this spreadsheet as a tabulation-separated .txt file. VolatileCalc based data is automatically extrapolated by EMBER to cover even the lowest pressure compositions (such as 1 or 5 bar).

	A	B	C	D	E	F	G	H	I
1	Wt%H2O	PPMCO2	WtH2Om	WtOHm	Temp (iC)	P (bars)	H2Ov mol%	CO2vmol%	PPMS
2									0
3									0
4									0
5									0
6									0
7									0
8									0
9									0

Figure 7: Example of a correct degassing path file, following the VolatileCalc model. The blue cells are the ones which will be read by EMBER. If any value is missing you may need to interpolate it. If that missing value is not on a blue cell, fill it with a 0, unless it's S and you don't want to study it. If you can model S, fill in the "PPMS" column with your modeled values. To be read correctly, the "Wt%H2O" cell must be placed in position A1 and the file saved as a tabulation separated .txt

3.3. Using another program (like D-compress or rhyolite Melts)

To make other programs being readable by EMBER, just use the format of VolatileCalc outputs. Copy the columns related to Pressure, H₂O, CO₂ and S concentrations the same way you would fill a VolatileCalc excel result file. Fill the rest with 0 and save the file as a tabulation-separated txt file. Do not forget to choose the **VolatileCalc** model on EMBER.

4. Required installation

Once this is done, make sure that MATLAB Runtime Environment 2019 is installed and just launch EMBER.exe (or EMBER.app on MAC). EMBER runs on the fly and does not need to be installed.

MATLAB runtime enables the use of intrinsic MATLAB functions, like *pdepe*, and its logical setting. It will also enable you to reopen calculated figures for data treatment, if needed. It remains a convenient tool to observe and move around generated 3D plot.

5. Procedure:

The left part of the GUI display is dedicated to inputs. Fill in the grid search, additional parameters and uncertainty parameters accordingly to your case (Figure 8).

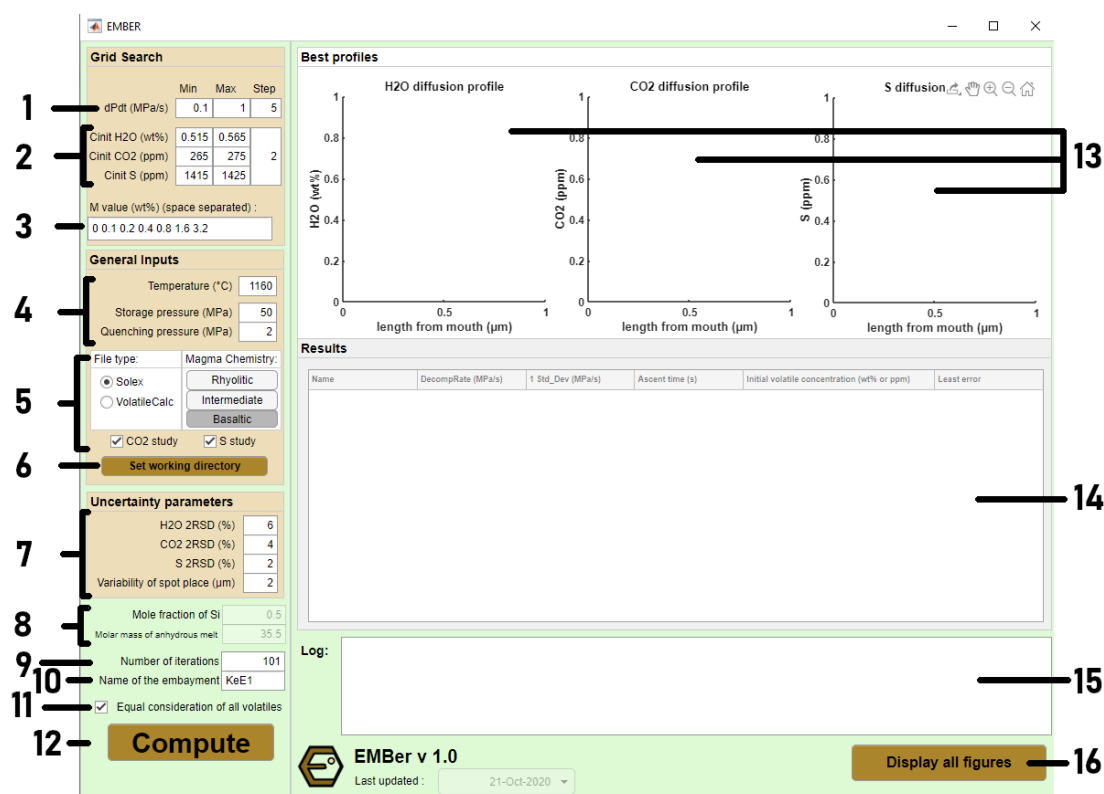
Without any a priori to decompression rate, I advise you to try out values of dPdt between 0.001 and 0.1 with a step of 5. If your resulting profile is noticeably lower than the measured points, try within 0.1 to 10 with a step of 5. If resulting profile is higher than the measured profile, try out between 0.00001 and 0.001 with a step of 5. During this phase of research, I advise to put a small step for Ci research (like 2) and put two to three M value at best (I usually do 0, 1 and 3.2) so that calculations do not last too long.

Do not forget to select the right working directory and to put the right short name of the embayment on the GUI (second column of the “Input.xlsx” file). You need to put at least two values of M_0 . Otherwise, an error will appear halfway of the calculation. Check the right decompression model architecture (VolatileCalc or SolEx) and the right diffusion model between Rhyolitic, Intermediate or Basaltic. Also, tick the desired elements (CO₂ or/and S) you want to study.

Please note that you can have access to “Mole fraction of Si” and “Molar mass of anhydrous melt” only if you are studying intermediate compositions as those parameters are only required when estimating diffusion coefficient following Ni and Zhang (2018) method.

The number of iterations is 101 by default because it is our best compromise between calculation stability for a wide range of cases and calculation duration.

Once everything is done, press “Compute”.



1 Decompression rate

2 Initial concentration

3 Pre existing volatile content

4 Temperature and pressure

5 Model and volatile choice

6 Folder path selection

7 Uncertainty input

8 Additional parameters (for Intermediate compositions)

9 Iterations (101 by default)

10 Name of the embayment (case sensitive)

11 Consideration of each volatile

12 Starting button

13 Plot displays

14 Results window

15 Log window

16 Display all computed plots

Figure 8 : Quick look at each parts of the GUI. Each part can be taken chronologically. Parts 13-16 become important after a full run of calculation. 1, 2, 4 and 10 are usually the parts that change the most between two embayments of the same eruption. They usually require extra care from the user.

Please note that, in general, when using 30 step for the decompression rate, 4 step for C_i , 7 values of M_0 and all three volatile species, the calculation usually last an hour to an hour and a half. I have added a

timer on the log that estimates the remaining time of calculation. This timer is updated after each loop of calculation (each time the M_0 value changes).

6. Overview of calculation flow:

EMBER will start by reading all the files. Upon reading the "Input.xlsx" file, a pop up window will open where you will have to follow what the log windows instructs you to do:

-click on "Next"

-click on "Finish".

The calculation will automatically start with H₂O then CO₂ then S and repeat itself for each M_0 . For each part of the calculation, profiles will be generated for each values of decompression rate and initial volatile concentration, and then compared to the measured profile to extract the best solution. You will see up to 3 figures appear with those diffusion profiles. It can help you track how the calculation is going or if you need to stop the calculation early on.

Please note that the **STOP button isn't instantaneous**. To be effective, this kind of interruption requires a built-in pause so the program can check if the button has been pressed or not. Since most of the calculations are often repeated loops, adding a pause would add too much unused time. Hence, those checks are made twice for each volatile specie and for each M_0 value. If you have clicked pause and you see messages like "Computing for $M = X$ wt% for H₂O/CO₂/S" or "Finding H₂O/CO₂/S best fit", it means that the stop order have not correctly been issued.

Once calculation is done for all cases, every result for each volatile specie studied will be scaled (or not, depending on the option you chose) and added to find the best fit with all the constraints. All results and figures are then saved and the results are displayed on the GUI. A progression bar and comments on the "log" windows will help you track the ongoing calculation.

EMBER's calculation will be done once the progress bar window is closed, the log displays "Calculation fully terminated" and there is a bright green "Calculation done" panel under the "Compute" button. Then you should be able to see diffusion profiles and result values on the right part of the GUI.

Only then, if you need to see every resulting figures, click on "Display all figures"

7. Reading the output files

Most of the output files are pretty straightforward to read (Figure 9). "[...]_M= X wt%_EMBER_Profiles.xls" provides profiles for each dPdt value tested, with the best C_i and M_0 . EMBER_input.xls files provides the inputs you entered in the GUI, EMBER_BestProfiles.xls provides the list of the best profiles for each M_0 value for species taken separately and altogether. EMBER_output.xls files provide decompression rates, associated error, time of ascension and C_i for each best case and for volatiles species taken separately and altogether. The "Least error" column with the lowest value for each volatile species corresponds to the best case for species taken separately. Cumulative error results are shown at the bottom of the file. This file corresponds exactly to what is displayed on the "Results" windows in the GUI. Finally, the _EMBER_fig.fig file is directly opened through EMBER. Launch the software, select the directory with the file you want to open, input the name of the embayment and directly click on "Display all figures".

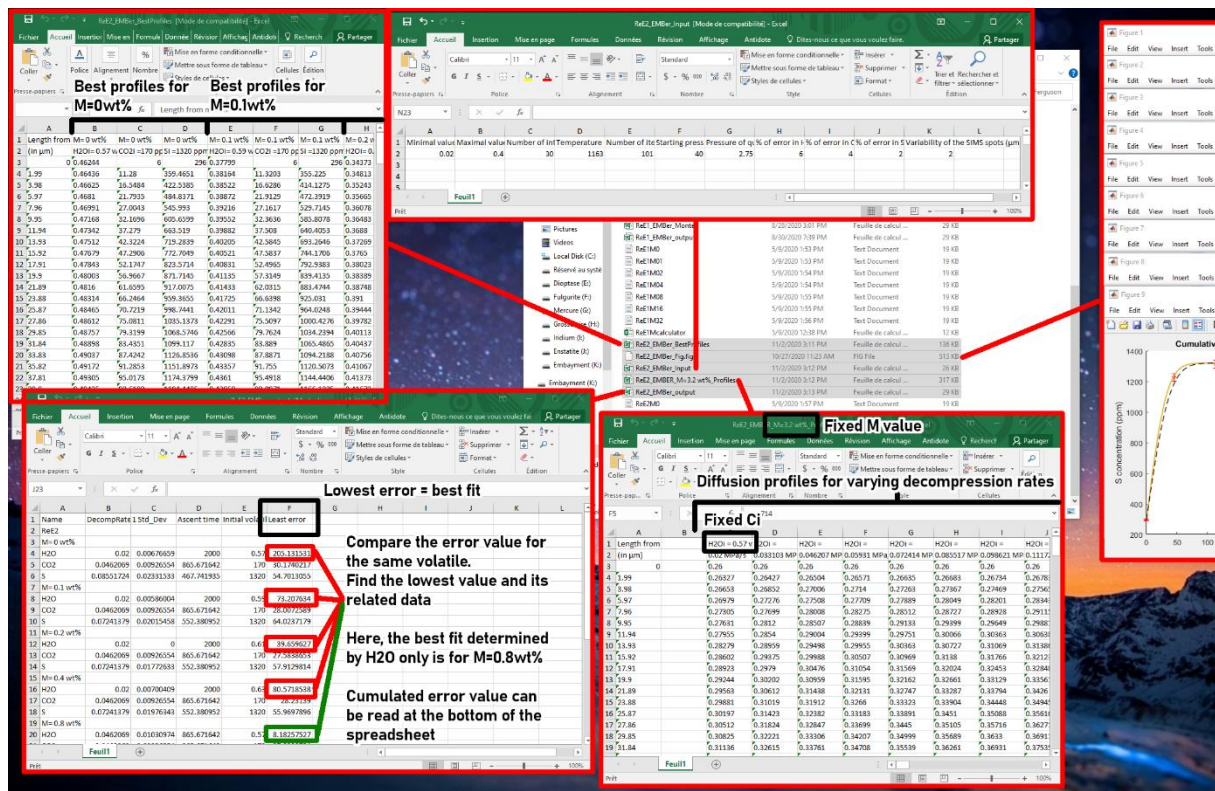


Figure 9: Overview of the resulting files from EMBER calculation. The `_EMBER_input` file provides a list of the inputs, the `_EMBER_fig` file 6 2d plots and 3 3D plots which can only be opened with EMBER, the `_EMBER_BestProfiles` file provides the best fit profiles for each volatile and each M_0 value. The `_EMBER_M=X wt%_Profiles` file provides diffusion profiles for the panel of tested decompression rate for each volatiles, with fixed M_0 and C_i values corresponding to the ones for the cumulative best fit. Lastly, the `_EMBER_output` file provides the parameters of the best fit for each M_0 value and volatile specie. The lowest error associated with each volatile provides results (decompression rate and its uncertainty, C_i and M_0 value) for each single specie best fit. Results for the cumulative error best fit are shown at the bottom of the file. This file correspond to what can be seen in the “Results tab (Figure 8, n°14)

8. Troubleshooting:

If the windows with the progression bar turns white, it means that a problem has occurred and has stopped the calculation

EMBER was developed and written so that it displays any error related to inputs on the log part. It mostly concern the two occasionally occurring errors: not entering/badly writing the name of the embayment and not selecting the correct working directory.

If a problem occur:

-Check that you are in the right directory and that the name of the embayment is the correct one.

-Check the name of all degassing path file, make sure they are correctly written.

-If SolEx generated, check that there are no errors for low pressure (bottom of the .txt). If any, you might need to manually extrapolate and write those error values. Each column is separated by one tabulation.

257 -Check the species you want to study (CO₂ and S) and that columns exists without blank values for
258 those on input.xlsx and, if using VolatileCalc, that you have added the S column.

259 -Check that the number of iterations is an odd number. For some reasons, the code sometimes struggles
260 with even number of iterations (which is why default number is 101 and not 100 tries).

261 -If the calculation stops close to the end of the calculation, please check that there are at least 2 values
262 of M_0 and that the number of steps for dPdt and Ci is higher than 2, in the input part.