Manual of Diffuser

Diffuser is a software designed to model one-dimensional elemental diffusion in minerals. The code is compiled in MATLAB and can be downloaded from https://github.com/liguangwu/diffuser.git. A web version of Diffuser is also available at http://www.geoapp.cn/. A manual for general use if given below.

Step 1: prepare diffusion profile and diffusion coefficient data

Before starting a diffusion model, a user has to prepare the diffusion profile in an excel file. An example excel is provided within this program (**'example.xlsx'**). The first two columns in this excel sheet should contain the distance and concentration data (Figure 1). If a user assigns the uncertainties of concentration in the third column, Diffuser will read it as well. Otherwise, all concentration data will be treated as equally weighted.

	A	B	C	D	E	F
1	Rubin et al., 2007	Fig. 1, Peak 2	put uncertainty in third column if you have			
2	X(m)	7Li ppb				
3	3.401E-05	0.000				
4	3.470E-05	1.187				
5	3.500E-05	0.591				
6	3.569E-05	1.778				
7	3.598E-05	0.000				
8	3.668E-05	1.179				
9	3.707E-05	3.534				
10	3.737E-05	6.524				
11	3.806E-05	6.553				
12	3.836E-05	16.015				
13	3.905E-05	25.248				
14	3.935E-05	48.689				
15	4.004E-05	75.149				

Figure 1. An excel example containing diffusion profile data.

In addition, a built-in excel file (**'DiffusionCoefficient.xlsx'**) containing diffusion coefficient data collected from literature is provided. The user can add more diffusion coefficient data in this template file (Figure 2).

	A	B	C	D	E
1	**Title**	**Reference**	**D0 (m^2/s)**	**ΔH (kJ/mol)**	**Comment**
2	Quartz Ti	Cherniak et al., 2007, Chem Geol	7.00E-08	273	**D=D0*exp(-ΔH/R/T)**
3	Quartz Ti	Jollands et al., 2020, Geology	5.01E-09	311	**Don't change the sequence of A-D columns**
4	Quartz Al	Tailby et al., 2018, American Mineralogist	2.48E-11	199	**The first two columns will show in the DiffusionModel listbox**
5	Zircon Li	Trail et al., 2016, Contrib Mineral Petrol	9.60E-07	278	
6	Garnet Ca-(Fe,Mg)	Vielzeuf et al., 2007, Contrib Mineral Petrol	6.63E-14	183.5	P=0.6GPa
7	Olivine P	Watson et al., 2015, American Mineralogist	8.71E-11	229	
8	Olivine Li, "slow" diffusion	Dohmen et al., 2010, Geochimica et Cosmochimica Acta	1.20E-06	245.9	
9	Diopside Fe-Mg	Dimanov and Sautter, 2000, Eur. J. Mineral.	9.55E-05	406	
10	Sanidine Ba, normal to 001	Cherniak 2002, Geochimica et Cosmochimica Acta	0.29	455	
11	Sanidine Sr, normal to 001	Cherniak 1996, Geochimica et Cosmochimica Acta	8.4	450	

Figure 2. An excel template containing diffusion coefficient data collected from literature.

Step 2: import data into Diffuser

For running Diffuser directly in MATLAB, the user can run 'Diffuser.mlapp' or type 'Diffuser' in the MATLAB command window. After opening the graphical user interface (GUI) of Diffuser, the user can click 'Select excel' button from the 'Data input' panel (Figure 3) and select a excel file. Diffuser will read this excel and show its sheet names in the listbox. Then, the user can select the sheet and click 'Read data' button to import diffusion profile data and get a quick look at the diffusion profile by a designed plot (e.g., Figure 4).

For the diffusion coefficient data, the program will read it automatically from **'DiffusionCoefficient.xlsx'** and show a list of options on the diffusion coefficient panel (Figure 3) once the program interface is opened. The user can easily select and edit diffusion coefficient parameters on this panel or add more diffusion coefficient data in the template file and read it again ('Read D list' button in Figure 3).

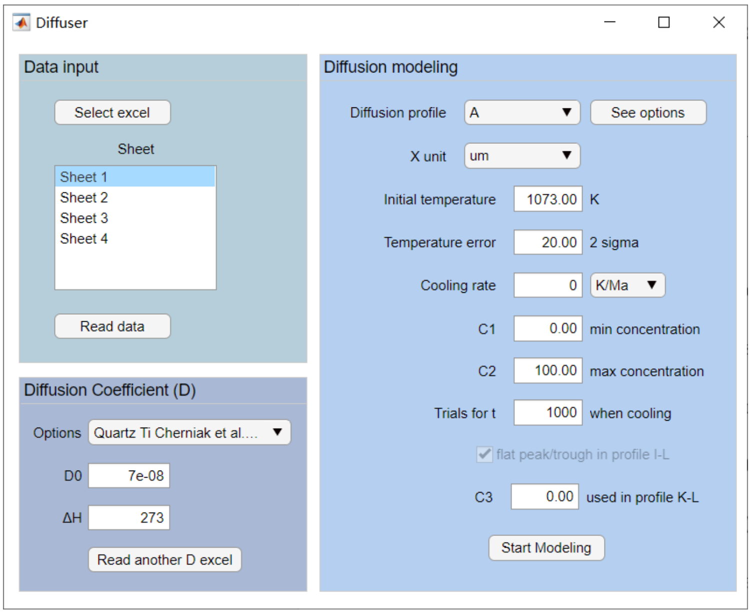


Figure 3. A snapshoot of Diffuser GUI.

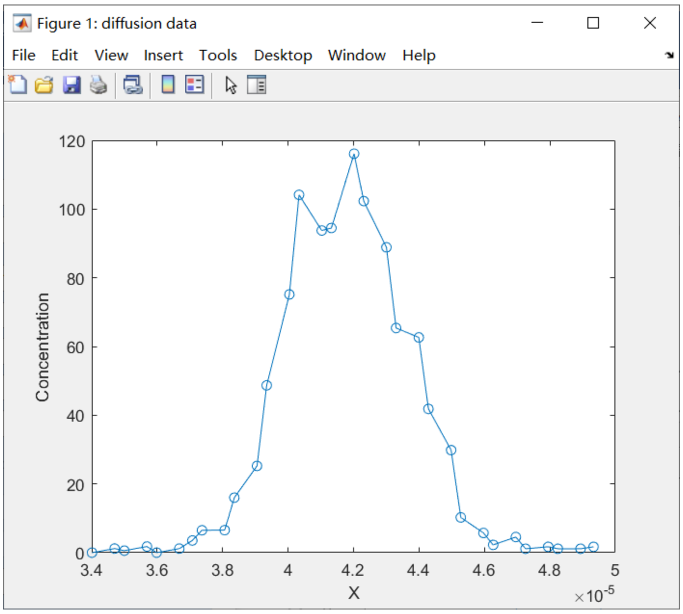


Figure 4. A designed plot for a quick look at the diffusion profile.

Step 3: start a diffusion model

After diffusion data import, the user can choose which diffusion problem is concerned on the diffusion modelling panel ('Diffusion profile' drop-down list; Figure 5) by comparing his own data (Figure 4) with diffusion types presented in a built-in photograph (click 'See options' button to load 'Diffusion profile options.jpg'; Figure 6). The unit of position x, initial temperature with its uncertainties, cooling rate, and initial concentrations (C_1, C_2, and C_3) should be set properly (Figure 3). Also, the user can define how many trials to use for the Monte Carlo method (MC) to determine the average time and its uncertainty when temperature varies with time. One thousand trials of MC are adequate and efficient for most cases. With all parameters set properly, the user can start a diffusion model. Especially, if the user does not define a flat peak or trough for profile I-L (i.e., no tick in the 'flat peak/trough in profile I-L' box in Figure 3), more parameters including minimum and maximum values and a step length (ΔC) of the assumed flat peak or trough (C_0) are required to type in through a new pop-up window after x_0 has been calculated (Figure 7).

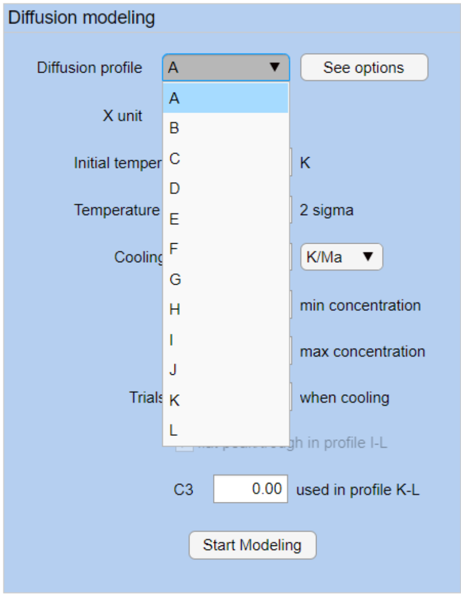


Figure 5. The diffusion profile drop-down list on the diffusion modelling panel.

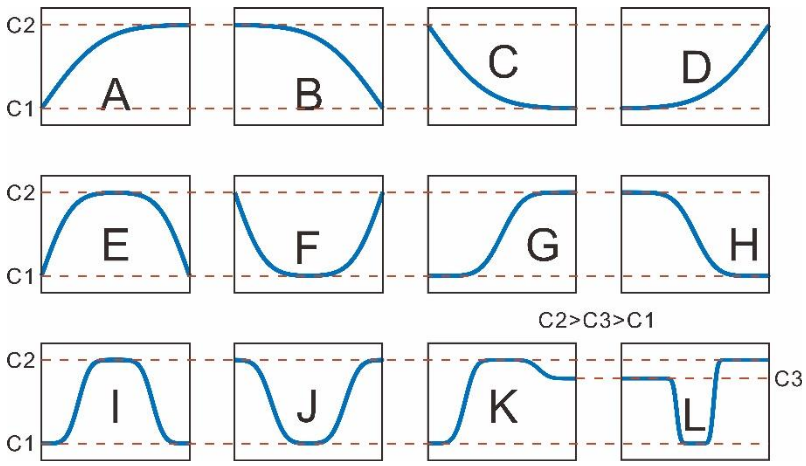
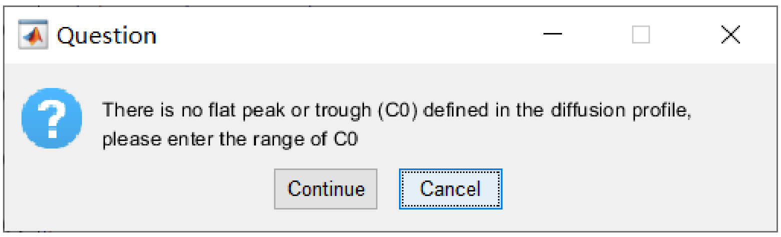


Figure 6. Options of the diffusion profile used in Diffuser.



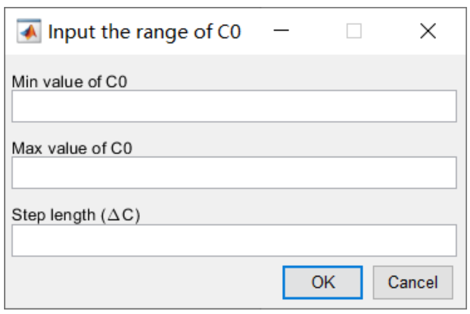


Figure 7. The minimum and maximum values and a step length (ΔC) of the assumed flat peak or trough (C_0) should be entered in a pop-up window if no flat peak or trough for profile I-L is defined.

Step 4: evaluate modelled results from output files

There are two types of output in our program after each modeling process, i.e., a figure showing the curve-fitting result which can be saved as vector graphics (Figure 8) and a text file recording the time calculation result (**'Modeling Result.txt'**, including information of trials, R^2, k, time, and time uncertainty; Figure 9). Especially, during calculation of profile I-L, one more figure showing the x_0 variation with R^2 is provided to check whether x_0 has become stable (Figure 10). If there is no flat peak or trough (C_0) for profile I-L defined by the user, one more figure will also appear showing the process of estimating k with a fixed x_0 value calculated in Figure 10 (Figure 11). In this case, the output text file will include parameters of C_0, x_0, and h (half length of the initially confined region) values for each trial (Figure 12). In addition, if the temperature varies with time (non-isothermal), Monte-Carlo results of calculated time values in each trial are displayed on histograms to show whether they are log-normally distributed based on Lilliefors test and then saved in another text file (**'Monte Carlo result.txt'**; Figure 13). Users can evaluate the calculation process and plot figures easily using these data.

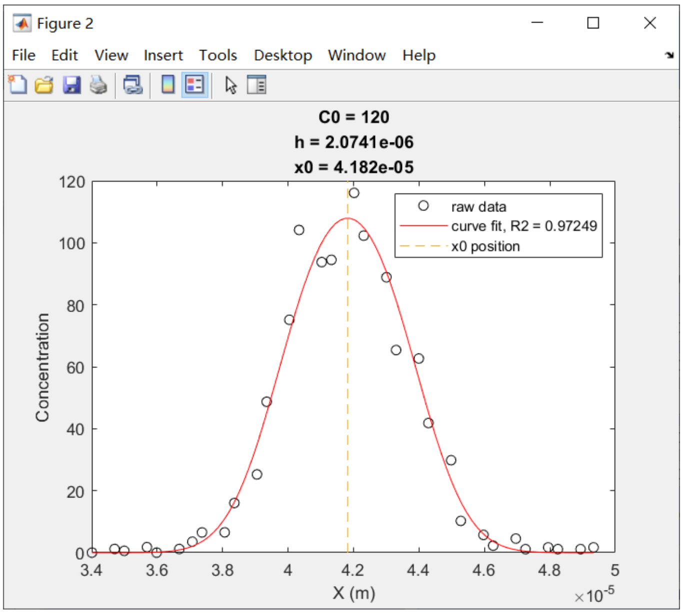


Figure 8. Curve-fitting result of a diffusion profile using Diffuser.

	A	B	C	D	E	F
1	Trials	R2	k	time(Myr)	-2s%	+2s%
2	1	0.99495	0.00029	2.8773	-39.177	39.177

Figure 9. Curve-fitting and calculated time results for profile A-H are stored in 'Modeling Result.txt'.

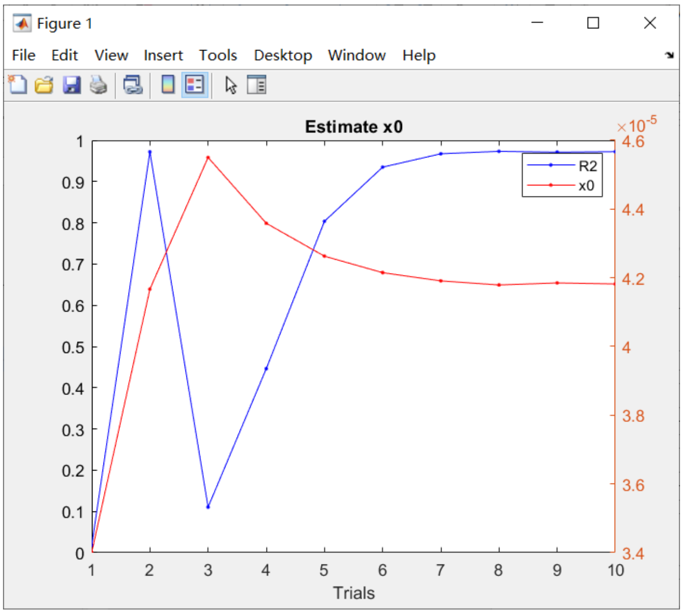


Figure 10. Estimate x_0 for profile I-L.

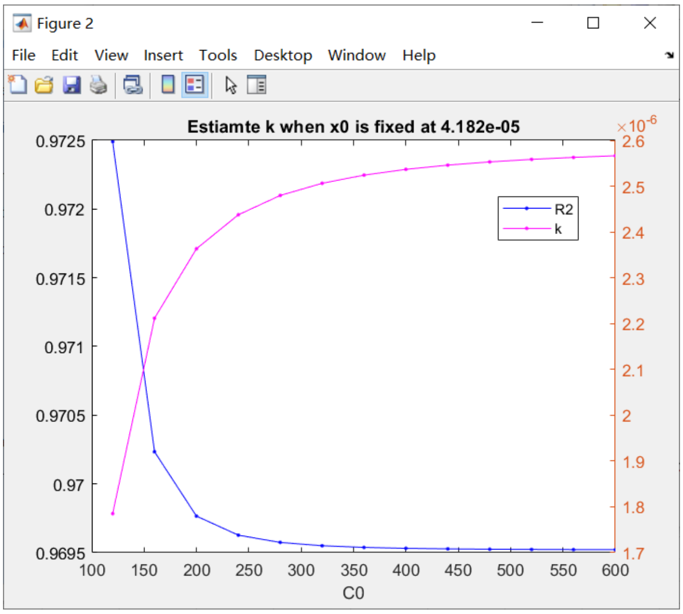
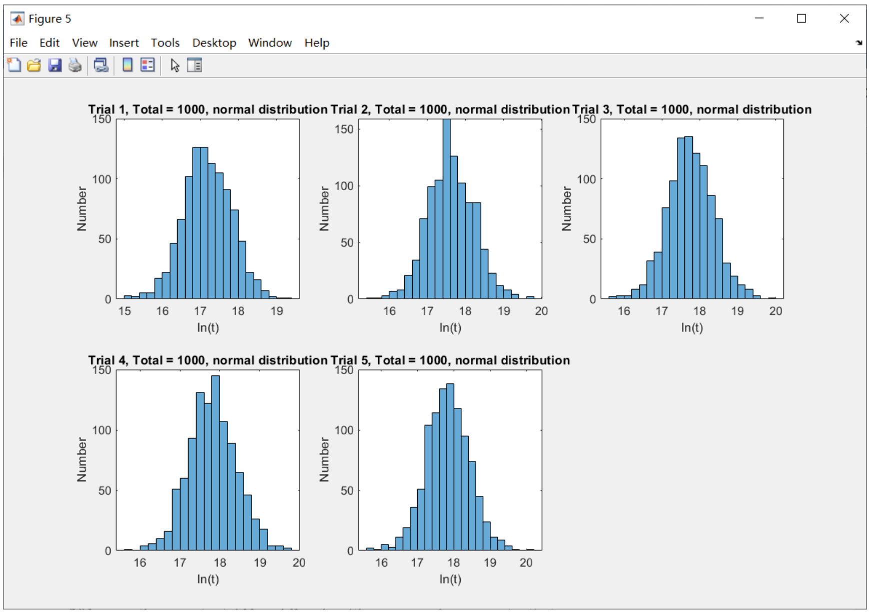


Figure 11. Estimate k with a fixed x_0 value in Figure 10 (4.18×10^{-5}) when no flat peak or trough is defined for profile I-L.

	A	B	C	D	E	F	G	H	I
1	Trials	C0	x0	h	R2	k	time(year)	-2s%	+2s%
2	1	120	4.18E-05	2.07E-06	0.97249	1.79E-06	22.0108	-74.461	74.4612
3	2	160	4.18E-05	1.57E-06	0.97023	2.21E-06	33.7886	-72.696	72.6964
4	3	200	4.18E-05	1.26E-06	0.96977	2.36E-06	38.5776	-72.387	72.387
5	4	240	4.18E-05	1.05E-06	0.96963	2.44E-06	41.0367	-72.269	72.2693
6	5	280	4.18E-05	8.98E-07	0.96957	2.48E-06	42.4689	-72.21	72.2099

Figure 12. Curve-fitting and calculated time results for profile I-L are stored in ‘Modeling Result.txt’. Parameters of C_0, x_0, and h values for each trial are given.



	A	B	C	D	E
1	k=1.7852e-06	k=2.2118e-06	k=2.3633e-06	k=2.4375e-06	k=2.4797e-06
2	t(s)	t(s)	t(s)	t(s)	t(s)
3	8589901.419	18936008.23	18695811.42	21843888.48	17869130.38
4	101301120.8	205087747.4	155900216.9	169981515.1	246469672.8
5	14688003.07	24978704.84	38311917.49	31420525.91	33462156.64
6	26915154.22	35416885.61	37400526.17	39112804.46	41277109.11
7	50958119.61	107253954.9	96596708.29	119371442.7	135164208.8
8	27957903.87	57304850.62	50392710.43	91967838.98	65528535.12
9	26416388.94	43086750.73	40088301.09	37747562.68	55573116.12
10	3647617.236	5490504.82	6968438.898	9961084.557	7075390.072

Figure 13. Monte-Carlo results of diffusion timescales when temperature varies with time (non-isothermal) are displayed on histograms and saved in ‘Monte Carlo result.txt’.