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Luminescence Dating of Quartz: A MATLAB-Based Program for computation of SAR paleodoses using natural sensitivity correction (NCF)

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Abstract

This study presents a MATLAB based program to implement the natural sensitivity correction (NCF) for the assessment of single aliquot regeneration based paleodoses (Singhvi et al., 2011; Chauhan & Singhvi, 2019). Several software packages /spreadsheets are in use to calculate the SAR paleodoses (D_es) but do not offer the facility for such a correction. The user-friendly program presented here, computes NCF-SAR paleodoses (D_es) and includes the errors in the measured NCF values. Monte-Carlo simulation was used to propagate the uncertainties in the paleodoses from the NCF and uncertainties in curve fitting parameters.

Keywords: NCF-SAR, paleodose, MATLAB, Monte-Carlo simulation

1. Introduction

In luminescence dating, the single aliquot regeneration protocol (SAR) is routinely used to estimate the paleodoses (Murray & Wintle, 2000). An addition to this protocol, the natural sensitivity correction (NCF), was suggested by Singhvi et al. (2011) to account for sensitivity changes that occur during the preheat and readout of natural OSL. When ignored, this sensitivity change leads to systematic offsets in paleodoses (Figure 1) and results in higher dispersion in D_e values, (Singhvi et al., 2011; Chauhan et al., 2015; Chauhan & Singhvi, 2019). Use of NCF also enables handling of samples when the natural OSL intensity is higher than the luminescence intensity at the saturation dose of the regenerated curve for SAR-corrected measurements.

NCF is measured as the ratio of the 110 °C TL peaks before and after the measurement of natural OSL. Tables 1 and 2 provide the measurement schedule for the conventional and the NCF-SAR protocols. Though necessary, available softwares do not include any provision to include the NCF. We present here a user-friendly MATLAB based program for inclusion of NCF in the calculation process. The uncertainties in the paleodoses of NCF are propagated using the Monte Carlo method (MCM) (Figure 2).

This program requires input data on an Excel spreadsheet in a specified format. It then carries out multiple MATLAB functions to calculate the NCF-SAR paleo-doses. It enables analysis of multiple aliquots or samples in a single operation by uploading appropriate files, one for each sample. Appendix A and the supplementary file provide relevant details for the use of the program for computation. The output is provided as an Excel spreadsheet.

Table 1: Generalized single-aliquot regeneration (SAR) protocol by Murray & Wintle (2000)

Steps	Treatment	Remarks
1	Give dose D_i	-
2	Pre-heat (160 – 300 °C,10s)	-
3	OSL (40s, at 125 °C)	L_i
4	Give test Dose	-
5	Preheat (160 – 300 °C)	-
6	OSL (40s, at 125 °C)	T_i
7	Return to step 1	

For the natural sample, i=0, and D_0 = 0 Gy; L_i and T_i are derived from the stimulation curve, typically the first 1 – 10 s of initial OSL signal, minus a background estimated from the last part of the stimulation curve.

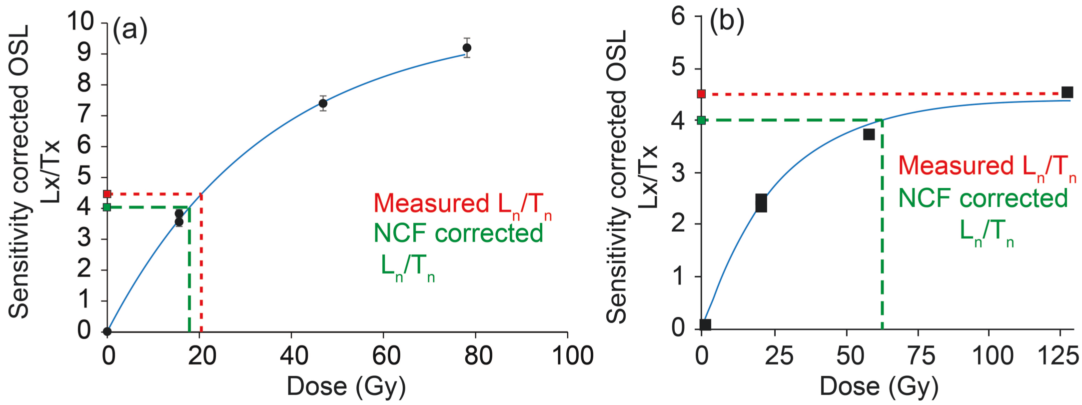

Figure 1: Response curve of sensitivity corrected OSL (L_x/T_x ratio) vs. dose (i.e. growth curve) of quartz samples from desert dunes to show sensitivity change during natural measurement. NCF corrects for these sensitivity changes even in the saturation range. (Data in Figure b from Chauhan et al. 2015).

Steps	Treatment	Remarks
1	Natural Sample	Pure quartz on SS discs
2	Dose for NCF	Small dose added to natural sample
3	*TL to 200 °C at 2 °C/s for 10 s	TL_1
4	Preheat (160 – 300 °C) 10 s	SAR preheat
5	OSL** at 125 °C for 40 s	OSL (L_n)
6	Cut heat (200 °C)	To remove charge from possible phototransfer, if any and photo-transfer
7	Test Dose	Small dose added to sample
8	TL to 220 °C at 2 °C/s for 10 s	TL_2
9	OSL at 125 °C for 40 s	OSL (T_n)
10	Regeneration dose (R_1, R_2, R_3, 0, R_1)	

*TL-integration peak ± 15 °C or peak ± FWHM
** If sample contains feldspar as inclusion, use of IR bleaching at 50 °C for 100 s is recommended before every OSL measurements to subdue the contribution of feldspar.

Table 2: The NCF-SAR method for calculating the natural correction factor (TL_2/TL_1) to correct sensitivity change occurring during natural OSL measurement. The remarks of each step are given for clarity.

2. Calculation Procedure

The following sequence is used to calculate NCF corrected doses (Figure 2).

1. The NCF is computed as

$$NCF = \frac{TL_1(IntegratedCounts)}{TL_2(IntegratedCounts)} \quad (1)$$

TL_1 is integrated TL counts for 110 °C before preheat and natural OSL measurement and TL_2 is integrated photon counts after readout of natural OSL (Table 1, Singhvi et al. 2011). A typical integration range could either be peak ± 15 °C or peak ± FWHM, with measurements at a heating rate of 2 °C/s.

2. These are used to correct individual normalized natural OSL

$$\left(\frac{L_n}{T_n}\right)_{corrected} = \frac{1}{NCF} \times \frac{L_n}{T_n} \quad (2)$$

The error in this is propagated as for a ratio. The NCF corrected (L_n/T_n) ratio and its error are used to generate a Gaussian probability density function (pdf) from which values can be picked randomly.

3. Parameters (*a, b, c*) and their associated errors from the fitting of the typically exponential growth curve

$$Y = a\left(1 - e^{-\frac{x+c}{b}}\right) \quad (3)$$

are then picked up from the instrument software and a Gaussian probability density function for each is generated such that the standard deviation (1-sigma error) represents the width of the distribution. From these, random data points are generated and for each set of such data points, a corresponding D_e is computed. Typically, for each parameter, 10,000 stochastic values are generated using Monte-Carlo simulations. The random numbers are created through the 'rand' function in MATLAB which uses the Ziggurat random normal generator based on Marsaglia (1968).

4. The mean and standard deviation of the resulting distribution give the D_e value and its error for each aliquot respectively whether they are single or multiple grains.

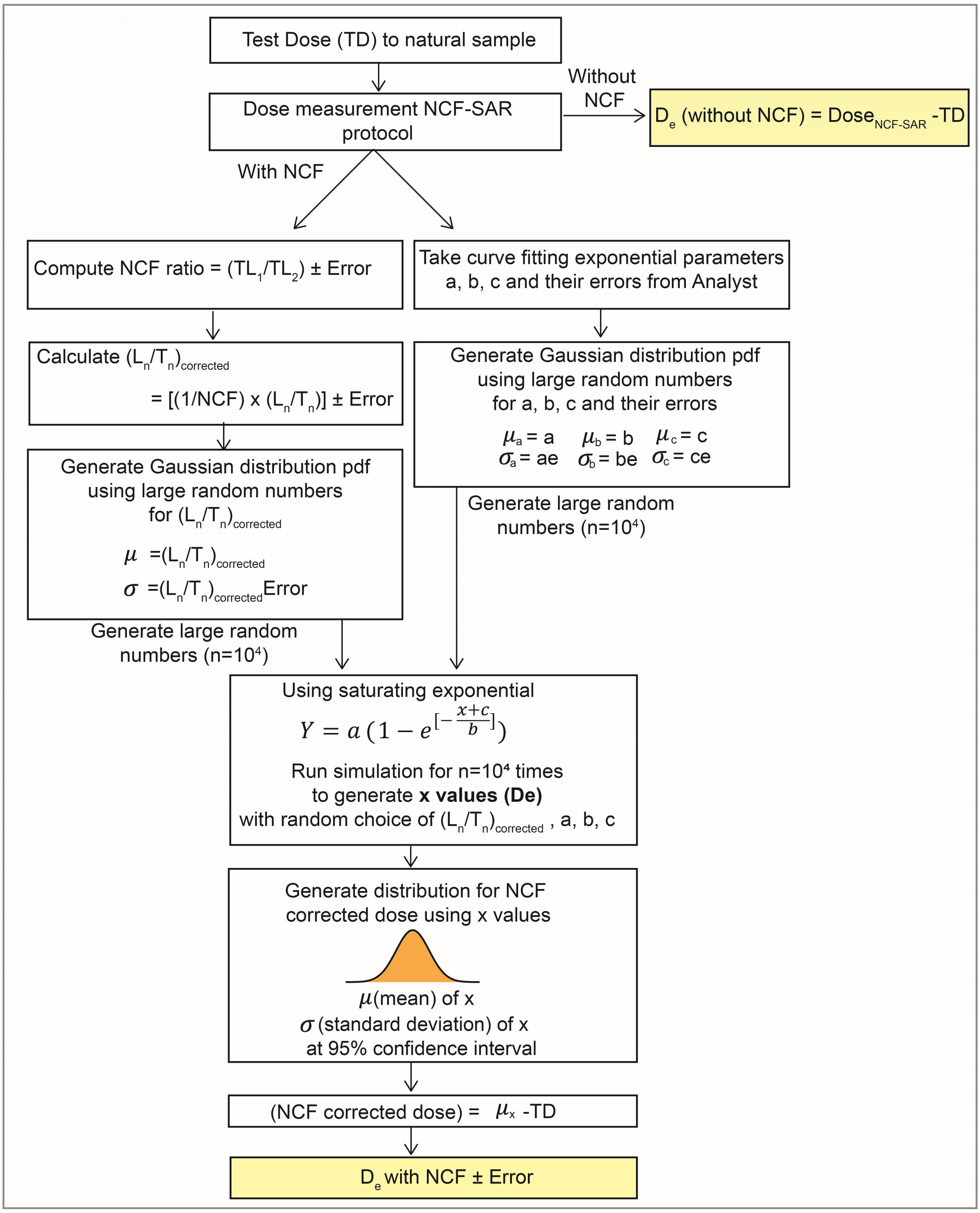

Figure 2: Steps for the calculation of the NCF corrected dose

3. Results and Discussion

Figure 3 shows typical results for the statistical distribution of NCF corrected dose values from the above computations. The histogram shows D_e values for each of 10,000 computations. The number 10,000 was determined based on Figure 4 when D_e and its error stabilized. The mean or central value of the paleodose D_e and its standard deviation (1-sigma uncertainty) was obtained from analysis of the resulting distribution of D_e values of single aliquots (Figure 3). This same procedure was carried out for the remaining aliquots to obtain their mean D_e value along with its error. Finally, data for all of the aliquots with their NCF corrected D_e and their errors were collated to create a histogram (Figure 5). A comparison of NCF-corrected D_e with NCF-uncorrected D_e is given in Table 3 and Figure 5. The NCF ratio for sample TNLW-3 ranges from 0.81 to 1.2 indicating that an aliquot-specific NCF value is needed.

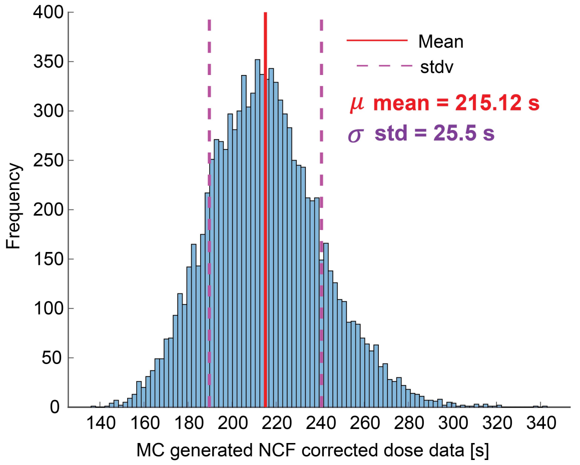

Figure 3: Histogram of Sample TNLW-3 (for disc-5) showing result of the Monte-Carlo simulation to obtain D_e distribution and its standard deviation.

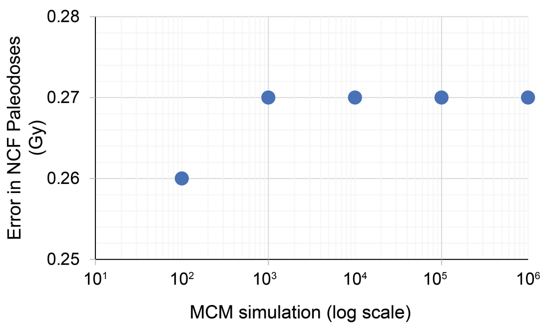

Figure 4: Error in NCF paleodoses stabilises with increasing number of MCM simulations.

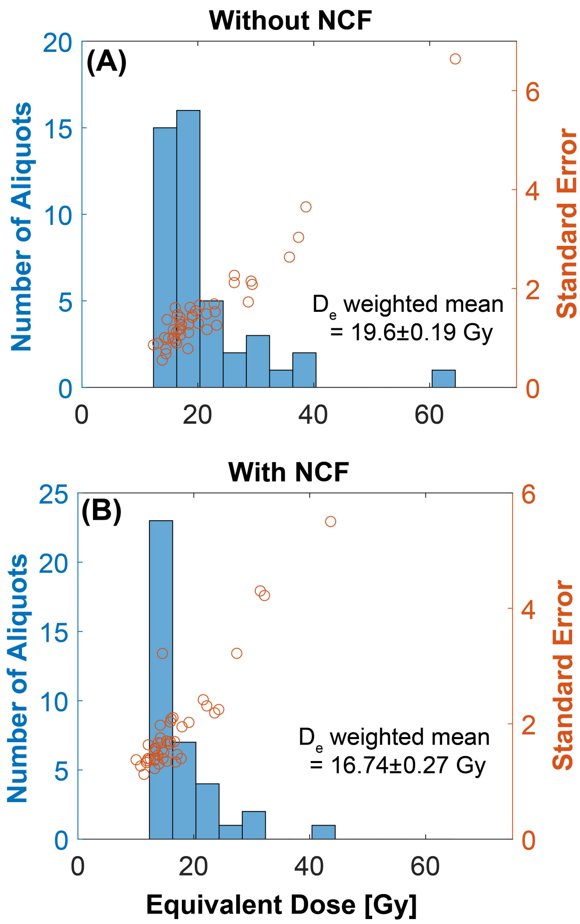

Figure 5: Comparison of dose distributions obtained with and without NCF-SAR correction. Reduced scatter in the MCM-derived standard error of D_e is also noticeable as the NCF correction is applied.

4. Conclusion and Summary

A user-friendly program for applying the NCF-SAR protocol is proposed that uses Monte-Carlo simulations and errors integration in NCF in the final corrected paleodose. On applying an MCM approach for error propagation minor changes in NCF corrected paleo-doses and in their error are seen. The NCF-SAR procedure results in lower dispersion in paleodoses and significantly lower paleodoses.

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Sample	Depth (m)	D_e (Gy)		%-Change in D_e
		Without NCF	With NCF	
TNLW-1	0.5	3.6 ± 0.1	3.0 ± 0.1	16
TNLW-2	1.5	10.1 ± 0.3	8.9 ± 0.3	11
TNLW-3	2.36	19.6 ± 0.2	16.5 ± 0.3	17
TNLW-5	4.26	20.9 ± 0.2	17.2 ± 0.3	17
TNLW-6	5.11	21.3 ± 0.2	19.9 ± 0.2	7

Table 3: Variations in paleodoses (D_e) on applying the NCF correction factor and their percent-change in samples from the Thar Desert.

Appendix: Procedure for input data format and executing NCF-SAR MATLAB program

1. To run these functions, no programming skills or advanced MATLAB capability are needed and the following steps will help computations. Open Relevant Analyst file → Go to top menu bar in Analyst → Records → Unselect All → Every Record

2. Records tab → Select All → Records of type → Select records of OSL → Click on SAR button → A Single Aliquot Analysis: window will open.

3. Choose Integration Limits for Signal and Background → Go to Curve Fitting → Select exponential fit → Set acceptance Criteria: - Recycling ratio limit (%) =10; Max. test dose error (%) = 10; Max. paleodose error (%) = 10; Max. Recuperation (%) = 5; Tick () on Incorporate error on curve fitting.

4. Now Go to Function tab → Analyse All Grains by accounting all acceptance Criteria

5. Go to Summary Data tab → Select all aliquots that have passed criteria and gave D_e values (use Shift + Right arrow on keyboard) → Right click on selected area → Copy data to clipboard with headers → Paste it to any *.txt file or Excel file

6. From this data, select only following columns which will be used for NCF analysis and copy them in an Excel sheet- (1) Filename (2) Disc (3) ED (4) ED_err (5) L_n/T_n (6) L_n/T_n_err (7) Param1 (8) Error1 (9) Param2 (10) Error2 (11) Param3 (12) Error3

7. Close this Single Aliquot Analysis window

8. To extract data for the TL_1 and TL_2 counts- follow step-1 again and make sure Selected column show 'False'.

9. From Display information menu → Click on Integral1 to integrate counts around the peak ± 15 °C region. (For example: lower and upper integration limit was 85 °C and 105 °C respectively for the TNLW-3 sample)

10. Repeat step-9 to obtain TL_2 Integral counts.

11. To export TL_1 and TL_2 integrated counts; Carefully choose Lumin. Type and Run Number as per Table-2 NCF-SAR protocol steps. (For example: Lumin. Type = TL And Run Number = 2 → will select TL_1 integrated counts; Lumin. Type = TL And Run Number = 7 → will select TL_2 integrated counts)

12. Once all necessary data has been extracted, we can arrange the step-6 columns and TL integrated counts in the sequence with headers shown in Table A1

    Note: The fitting parameters (*a, b, and c*) for the saturating exponential are saved as Param1, Param2 and Param3 along with their errors.

    It is to note that the machine dose rate (Gy/min) will be used to calculate the final paleodose (D_e) in Gy by using the actual dose rate calculated at the time of experiment. The irradiation raw data obtained from analyst is in seconds. It is kept in the mentioned units so as to minimize data processing by the user. Date formatting should be as D-M-YYYY.

13. To run ***NCF-SAR*** MATLAB program, MATLAB function files are best kept in the same folder or add them to MATLB path. Then user needs to open a MATLAB command window and recall the function by typing command ***load_NCFSAR_data*** and run the program by clicking on Run button or pressing F5 in MATLAB upper panel. This will open a new menu window and navigate to the current folder where all the sample excel files are placed. User can select any file and follow instructions visible on the MTALB command window (Fig. A1). If any user has multiple files to process, then name them as ***sample name_***. This program takes input file as both .csv or excel file format with a single spread sheet. (The program to run with or without MCM calculation is based on user choice). On execution, the NCF-SAR program provides the sensitivity corrected paleo dose estimates in a separate excel file (***sample name_result_NCF_SAR***) along with a dose distribution plot. These are automatically saved in the ***'result'*** folder. The NCF corrected dose data can be analysed through various platform (e.g., R or DRAC calculator) to calculate final age.

The NCF-SAR MATLAB program, together with steps

1	2	3	4	5	6	7	8	9
File name	date	Disc position	ED	ED_ err	TL_1	TL_2	L_n/T_n	L_n/T_n_err

10	11	12	13	14	15	16	17	18	19
a	a_err	b	b_err	c	c_err	NCF Test dose	Machine Dose Rate (Gy/min)	Machine calibration date (D-M-YYYY)	Experiment date (D-M-YYYY)

Table A1: Arrangement of data (see step 12 of the Appendix)

and the example data presented in this publication as input for the code, can be downloaded from the Ancient TL webpage. It is also available from Github, an open access open-source platform website (`https://github.com/Rahulkaushal009/NCFSAR-tool`).

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Reviewer

Michel Lamothe

Reviewer comment:

A useful and timely manuscript as the NCF correction needs to be easily computable in cases where such quartz OSL sensitivity issues are significant.

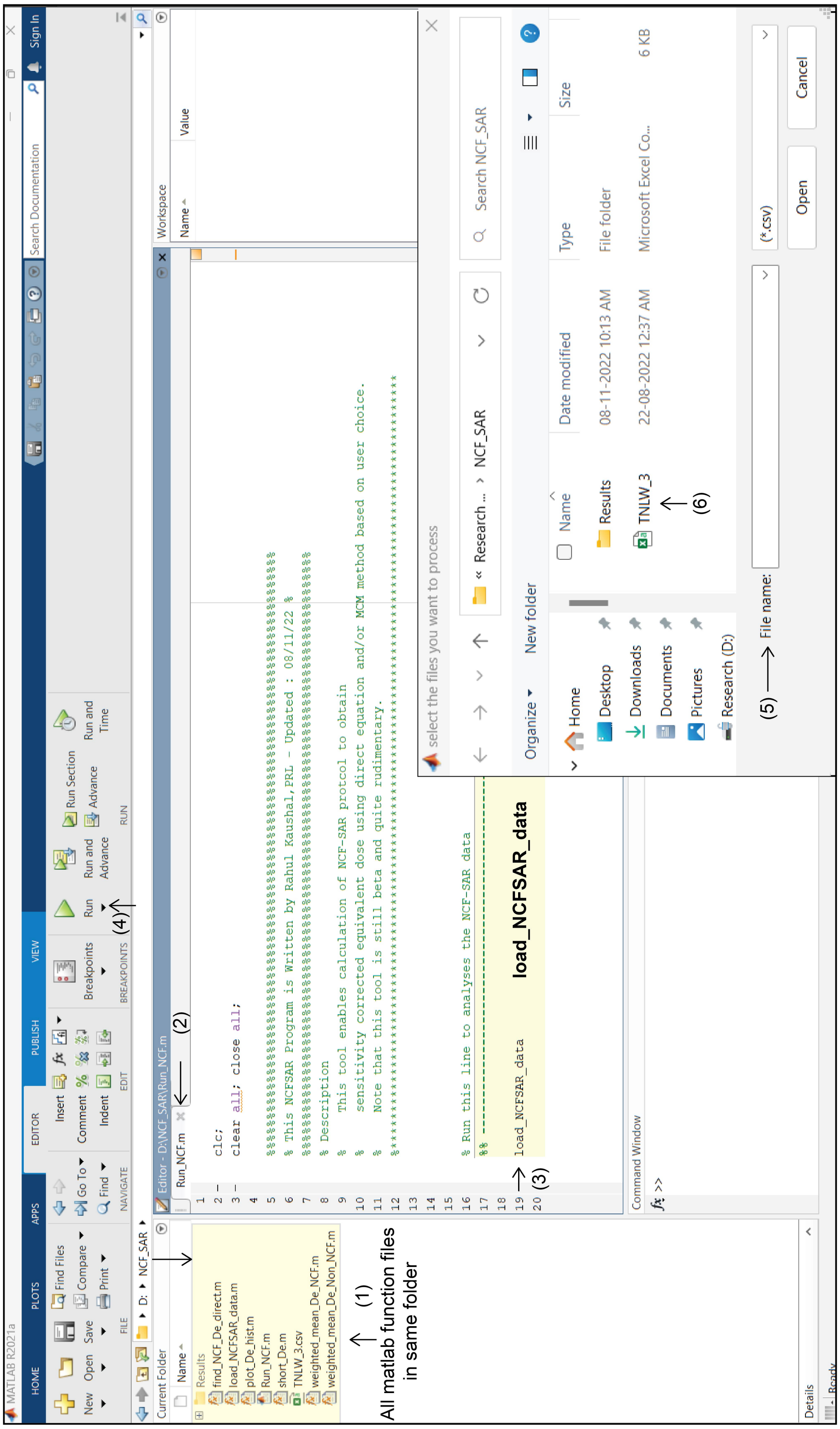

Figure A1: Steps to run the NCFSAR program and select the appropriate file