Geochemical Arc Moho Estimator (GAME)

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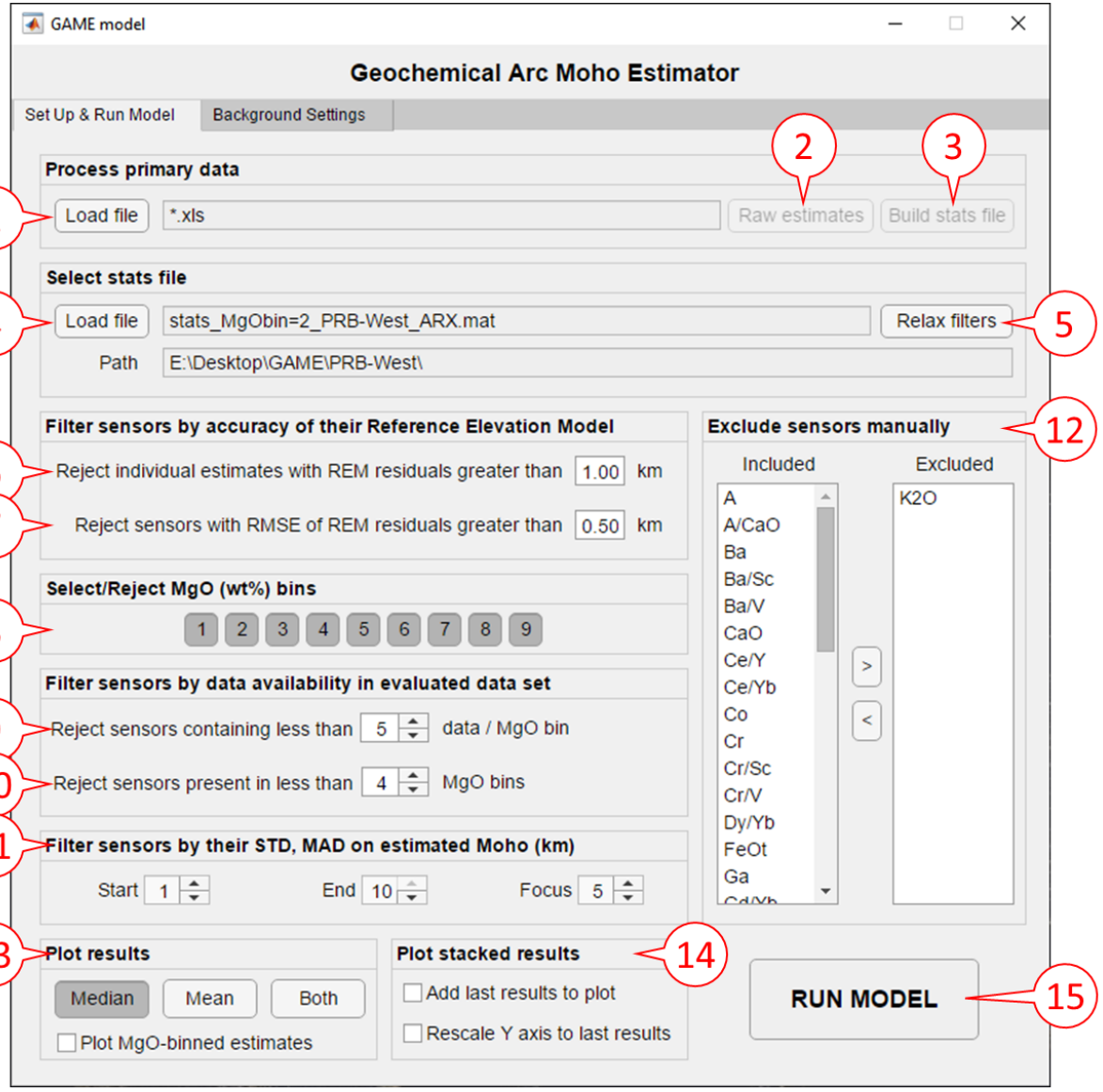
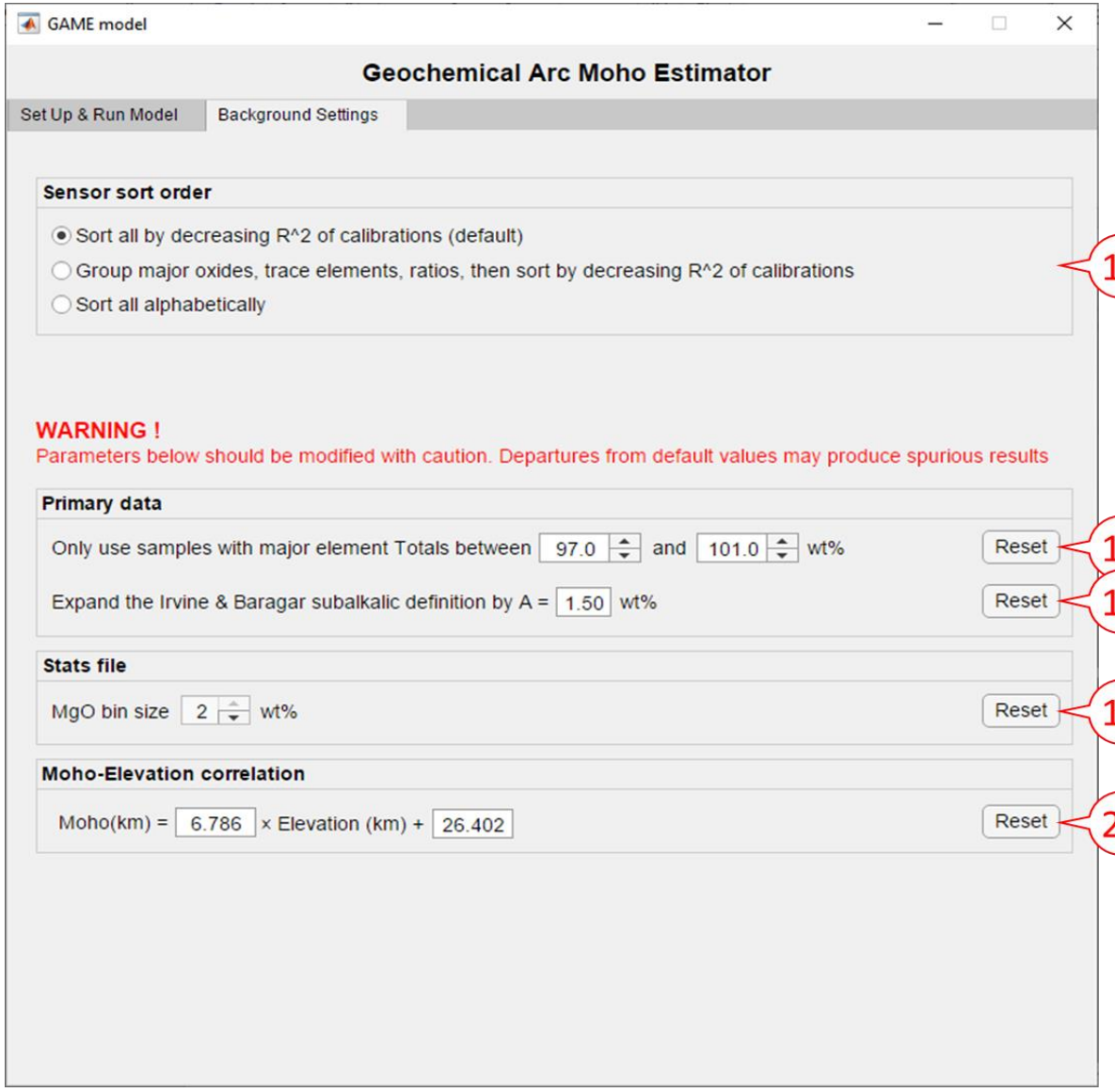
Peter Luffi (peter.luffi@gmail.com) and Mihai N. Ducea (ducea@arizona.edu)

GAME interface





GAME interface

Set Up & Run Model

Process primary data

1. Load file. Import primary data file (e.g., *EXAMPLE.xls*) and set its location as working folder. See provided example primary data file for data structure. Primary data file should have *xls* extension. Skip to point 3 if data file is already imported or no raw estimates (point 2) are desired.
2. Raw estimates (optional). Calculate elevations and Moho depths for all individual samples included in primary data file. Output file is named automatically (e.g., *GAMEresults_RAW_EXAMPLE_ARX.xlsx*; see description below) and written to working folder. Primary data are filtered by ε_{max} set in point 6.

3. Build stats file. Generate statistical file from MgO-binned primary data. Output file is named automatically (e.g., *stats_MgObin=2_EXAMPLE_ARX.mat*) and written to working folder. String '*MgObin=2*' in file name indicates MgO bin size (wt%) [see '**Stats file**' option in '**Background settings**' tab]

Select stats file

4. Load file. Load stats file created in point 3. Last model settings will be loaded in the case of previously used stats files.
5. Relax filters (optional). Relax al filters (points 6–12) to min/max tolerated values in order to evaluate all applicable sensors.

Filter sensors by accuracy of their Reference Elevation Model

6. *Reject individual estimates with REM residuals greater than ε_{max} km. Eliminate sensors falling outside or in poorly modeled domains of the calibration range; decreasing this value should reduce STD, MAD. Default value: ε_{max} = 1 km.
7. *Reject sensors with RMSE of REM residuals greater than $rmse_{max}$ km. Filter sensors based on their overall performance; decreasing this value should reduce STD, MAD. Default value: $rmse_{max}$ = 0.5 km.

Select/Reject MgO (wt%) bins

8. *Reject undesired MgO (wt%) bins from the modeling process (evaluate panel **G** in main plot); unpopulated bins are deactivated by default. At least two bins need to remain selected.

Filter sensors by data availability in evaluated data set

9. *Reject sensors containing less than *nr* data/MgO bin. Exclude statistically unsubstantiated sensors; the higher the value the better (strive for ≥5). Default value: *nr* = 5.
10. *Reject sensors present in less than *j* MgO bins. Exclude sensors present in too few MgO bins. Higher values should produce more robust results. Default value: *j* = 2.

Exclude sensors manually

11. *Reject sensors based on personal judgment, e.g., obvious outliers affecting the quality of results (evaluate panels **G-H** in main plot); useful after at least one model run.

Filter sensors by their STD, MAD on estimated Moho (km)

12. *Retain sensors based on their precision in the evaluated case. Set *Start* and *End* to filter the results shown in panels **J-K** based on STD (standard deviation) and/or MAD (median absolute deviation) of employed sensors. *Focus*: set std_{max} and mad_{max} values (i.e., maximum STD and MAD, evaluate panels **E-F**) to limit sensors used in panels **G-I** in main plot. Default values: *Start* = 1 km; *Focus* = 5 km; *End* = 10 km.

Plot results

13. Choose to plot Moho depths as medians and/or means of individual estimates (panels **G-K**). Check Plot MgO-binned estimates to show individual estimates in panels **G-H**. Default option: 'Median'.

Plot stacked results

14. (optional) Create a copy of panel **K** in which results from different runs can be added for comparison (e.g., compare different arc segments or different filter settings). Plot must be saved manually.

RUN MODEL

15. Run calculations, generate on-screen plot(s) and output files in the working folder. The following output files are created automatically:
    - *figure_stats_MgObin=2_EXAMPLE_ARX.pdf* (copy of on-screen main plot)
    - *GAMEresults_stats_MgObin=2_EXAMPLE_ARX.xlsx* (detailed results; string '*MgObin=2*' in file name indicates MgO bin size (wt%); see '**Stats file**' option in '**Background settings**' tab and description below)
    - *model_stats_MgObin=2_ EXAMPLE_ARX.mat* (model settings)
    - *results_log_stats_MgObin=2_ EXAMPLE_ARX.xlsx* (log of model settings and results; see description below

WARNING! All resulting .xlsx and .pdf files must be closed before re-running the model!

Background Settings

Sensor sort order

16. Select the order in which sensors are listed in plot and detailed results files

Primary data

17. Only use samples with major element Totals between Σ_{min} and Σ_{max} wt%. Decreasing Σ_{min} and increasing Σ_{max} allows for including poorer analyses; helpful in the case of small datasets, but may affect the quality of results. Default values: Σ_{min} = 97 wt%; Σ_{max} = 101 wt%.
18. Expand the Irvine & Baragar subalkalic definition by A = dA wt%. Increasing dA allows for including more alkaline samples (A = Na_2O+K_2O); helpful in the case of small datasets, but may imply undesired model extrapolations. Default value: dA = 1.5 wt%.

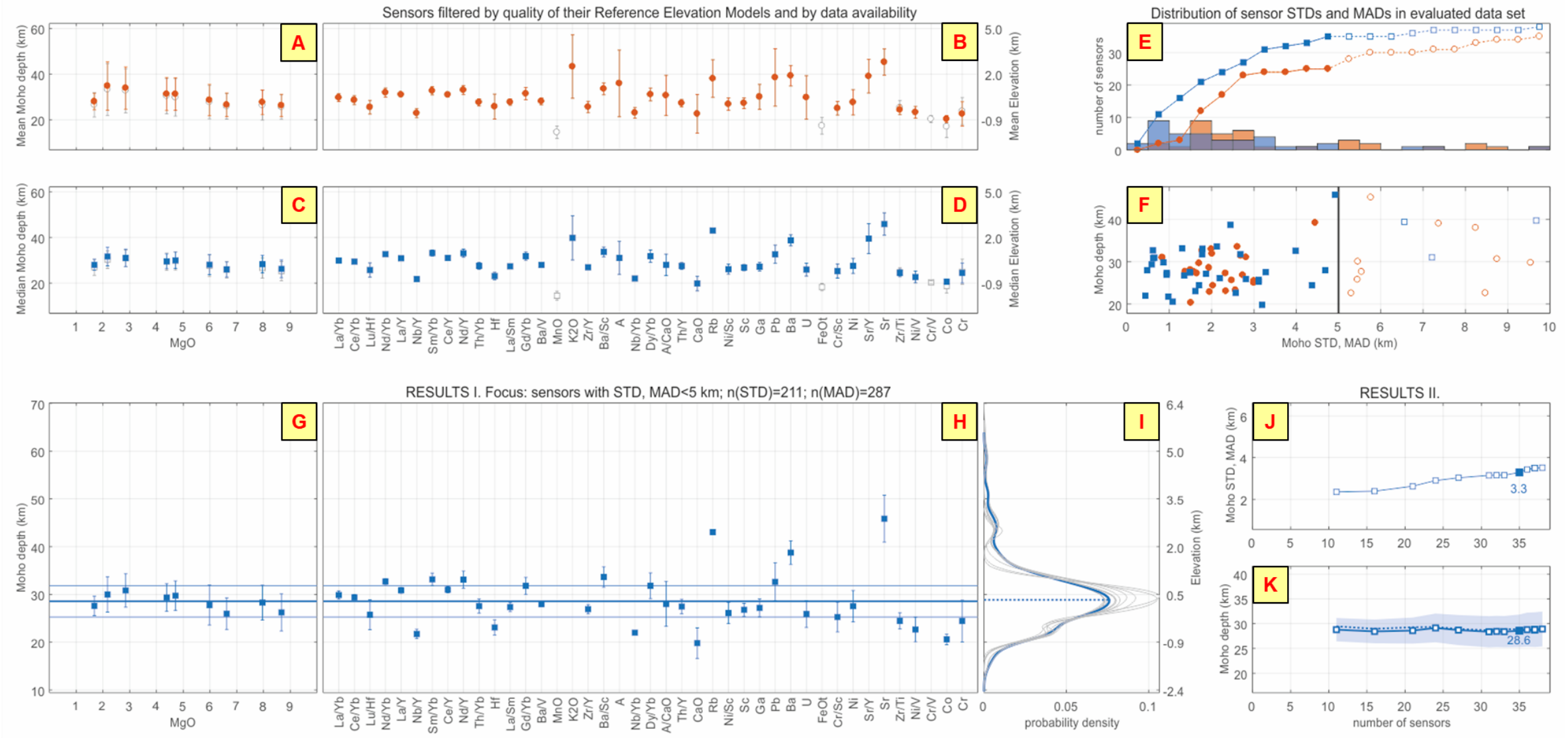
Stats file

19. MgO bin size $dMgO$ wt%. Two options are available: $dMgO$ = 2 wt% (default value used in model calibration; partially overlapping MgO intervals: 0–2, 1–3, 2–4, …,8–10 wt%) and $dMgO$ = 1 wt% (non-overlapping MgO intervals: 0.5–1.5, 1.5–2.5, 2.5–3.5, …,8.5–9.5 wt%)

Moho-Elevation correlation

20. Moho (km) = α × Elevation (km) + β. Should not be modified unless there are good reasons to do so. Default values: α = 6.79, β = 26.40.

Main plot


Sensors filtered by quality of their Reference Elevation Models and by data availability
A
B
C
D
Mean Moho depth (km)
Median Moho depth (km)
Mean Elevation (km)
Median Elevation (km)
MgO
Distribution of sensor STDs and MADs in evaluated data set
E
F
number of sensors
Moho depth (km)
Moho STD, MAD (km)
RESULTS I. Focus: sensors with STD, MAD<5 km; n(STD)=211; n(MAD)=287
G
H
I
probability density
Elevation (km)
RESULTS II.
J
K
Moho STD, MAD (km)
3.3
28.6
number of sensors

Main plot (e.g., *figure_stats_MgObin=2_EXAMPLE_ARX.pdf*)

Panels **A-D**: **Median**±MAD and **Mean**±STD Moho results obtained with sensors applicable to the dataset after applying first-order quality filters (points **6-11**). Grey empty symbols in the background show primary (unfiltered) results for reference. Elevation scale shown on the right corresponds to the isostatic equilibrium from which Moho is calculated (see '**Moho-Elevation correlation**' in '**Background Settings**' tab).

Panel **E**: Histograms and cumulative curves of sensors sorted by **MAD** and **STD** associated with the estimated Moho depths (km) in the **Start-End** interval set in point **12**.

Panel **F**: Estimated Moho depths (km) sorted by their **MAD** and **STD** limited to the **Start-End** interval. Solid black line: cut-off value (mad_{max} and std_{max} set in point **12**, **Focus**) used in panels G-I.

Panels **G-H**: Similar to **A-D**, but restricted to MAD < mad_{max}, STD < std_{max} (i.e., filled symbols in panel **F**). **Median**±MAD and/or **Mean**±STD Moho results obtained with sensors applicable to the dataset after applying all filters, and the resulting overall **Median**±MAD and/or **Mean**±STD (shown as horizontal lines) as selected in point **13**. **n(MAD)** and **n(STD)** in title of panel **H** indicate the number of MgO-binned median datapoints used to calculate **Median**±MAD and **Mean**±STD.

Panel **I**: Kernel probability density distribution of individual estimates used in **G** and **H**; **blue** and/or **red** curves correspond to **MAD** = mad_{max} and/or **STD** = std_{max}**,** grey curves correspond to MAD and/or STD values in 0.5 km steps between **Start** and **End**.

Panel **J**: Variation of overall **MAD** and/or **STD** depending on the number of employed sensors falling in the **Start-End** interval. Highlighted value(s) correspond(s) to **Focus**.

Panel **K**: Variation of overall **Median**±MAD and/or **Mean**±STD depending on the number of employed sensors falling in the **Start-End** interval. Highlighted value(s) correspond(s) to **Focus**. Dashed line(s): trace of probability curve peaks in panel **I**.

Output data files

GAMEresults_RAW_EXAMPLE_ARX.xlsx

Sheet: *ELEVref*. Values of MgO (first column) and reference elevations (km) calculated using the 0.14º×0.14º GMRT model for samples for which geographic coordinates are provided in the primary data file.

Sheet: *CHEM*. Values of MgO (first column) and other chemical parameters calculated for all imported samples.

Sheet: *ELEVmodel*. Values of MgO (first column) and elevations computed for all imported samples using the applicable mohometers.

Sheet: *MOHOmodel*. Values of MgO (first column) and Moho depths computed for all imported samples using the applicable mohometers.

Sheet: *refMODELresid*. Values of MgO (first column) and Reference Elevation Model residuals (km) calculated for *CHEM–MgO* datapoints. Residuals of datapoints falling outside the applicability envelope of the models are set to 10 km.

Sheet: *ELEVmodel REMresid*<ε_{max}*km*. Values of MgO (first column) and results from *ELEVmodel* sheet filtered by ε_{max} set in point 6. Repeating 'Raw estimates' (point 2) using a different ε_{max} value results in a new '*ELEVmodel REMresid*<ε_{max}*km*' sheet appended to the file.

Sheet: *MOHOmodel REMresid*<ε_{max}*km*. Values of MgO (first column) and results from *MOHOmodel* sheet filtered by ε_{max} set in point 6. Repeating 'Raw estimates' (point 2) using a different ε_{max} value results in a new '*MOHOmodel REMresid*<ε_{max}*km*' sheet appended to the file.

GAMEresults_stats_MgObin=2_EXAMPLE_ARX.xlsx

Sheet: *ELEVref*. Midpoint of MgO bin (1–9 wt%) and reference elevations (km) calculated using the 0.14º×0.14º GMRT model for MgO-binned samples for which geographic coordinates are provided in the primary data file.

Sheet: *MgO*. Midpoint of MgO bin (1–9 wt%) and median MgO values calculated for each bin.

Sheet: *CHEM*. Midpoint of MgO bin (1–9 wt%) and median values of chemical parameters calculated for each bin.

Sheet: *NR*. Midpoint of MgO bin (1–9 wt%) and number of data in each bin.

Sheet: *ELEVmodel*. Midpoint of MgO bin (1–9 wt%) and elevations computed for *CHEM–MgO* datapoints passing the filters in points 6–11.

Sheet: *MOHOmodel*. Midpoint of MgO bin (1–9 wt%) and Moho depths computed for *CHEM–MgO* datapoints passing the filters in points 6–11.

Sheet: *refMODELresid*. Midpoint of MgO bin (1–9 wt%) and Reference Elevation Model residuals (km) calculated for *CHEM–MgO* datapoints. Residuals of datapoints falling outside the applicability envelope of the models are set to 10 km.

Sheet: *STDlimitedMOHOmodel*. Midpoint of MgO bin (1–9 wt%) and results from *MOHOmodel* sheet filtered by std_{max} = *Focus*.

Sheet: *MADlimitedMOHOmodel*. Midpoint of MgO bin (1–9 wt%) and results from *MOHOmodel* sheet filtered by mad_{max} = *Focus*.

results_log_stats_MgObin=2_ EXAMPLE_ARX.xlsx

After each run, 20 lines are appended to the file, each line corresponding to results obtained for a *Focus* increment of 0.5 km between 0.5 and 10 km.

Column: *Focus*.

Column: *Mean_sensor_ct*. Number of mohometers constrained by std_{max} = *Focus*.

Column: *Mean_Moho_Peak*. Moho depth at the maximum point of the kernel probability density distribution curve obtained for std_{max} = *Focus*.

Column: *Mean_Moho*. Mean Moho depth obtained for std_{max} = *Focus*.

Column: *Mean_Moho_STD*. Standard deviation associated with *Mean_Moho* obtained for std_{max} = *Focus*.

Column: *Median_sensor_ct*. Number of mohometers constrained by mad_{max} = *Focus*.

Column: *Median_Moho_Peak*. Moho depth at the maximum point of the kernel probability density distribution curve obtained for mad_{max} = *Focus*.

Column: *Median_Moho*. Median Moho depth obtained for mad_{max} = *Focus*.

Column: *Median_Moho_MAD*. Median absolute deviation associated with *Median_Moho* obtained for mad_{max} = *Focus*.

Column: *maxREMresid*. Value set in point 6 (=ε_{max}).

Column: *rmseMAX*. Value set in point 7 (=$rmse_{max}$).

Column: *MgO_bins*. MgO bins selected/deselected in point 8.

Column: *minDataBin*. Minimum number of data in MgO bins set in point 9 (=*nr*).

Column: *minNoBin*. Minimum number of MgO bins set in point 10 (=*j*).

Column: *Rejected_sensors*. List of sensors excluded manually in point 12.

Column: *alpha*. Value set in point 20.

Column: *beta*. Value set in point 20.

Column: *Timestamp*. CPU timestamp of run.