Revisiting the Middle and Upper Palaeolithic archaeology of Gruta do Caldeirão (Tomar, Portugal)

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Procedure
Luminescence dating has been used to provide direct estimates of when the Gruta do Caldeirão infill deposits were last exposed to light prior to burial. In this study, we have focussed on optically stimulated luminescence (OSL) dating of quartz because of the abundance of this mineral type at the site and the expected Late Pleistocene age range of the archaeological deposits (Zilhão et al., 1997). Our luminescence dating study employs single-grain quartz OSL analyses rather than conventional (multi-grain) OSL measurements in order to gain improved insights into any potential methodological complications that could affect dating reliability in this cave setting; particularly the presence of insufficiently bleached grain populations (e.g., Arnold et al., 2007, 2009), contaminant grains associated with syn- or post-depositional mixing (e.g., Arnold et al., 2011, 2013, 2019), or aberrant grains displaying inherently unsuitable luminescence properties (e.g., Demuro et al., 2008, 2013).

Sample collection and preparation
In total, five OSL dating samples were collected from the sedimentary infill sequence exposed in the back chamber (square P11) of Gruta do Caldeirão. The units sampled encompass the Middle Palaeolithic to Upper Palaeolithic transition, as well as the underlying Middle Palaeolithic deposits. One sample was collected from each of the following units: unit K (sample CLD17-1), unit L (sample CLD17-2), unit M (sample CLD17-3), unit N (sample CLD17-4) and unit O (sample CLD17-5). During sampling, care was taken to avoid areas showing sediment heterogeneity and bioturbation, focusing instead on sections of homogeneous, fine grained deposits that were unaffected by post-depositional disturbance. Owing to the consolidated nature of the target sedimentary horizons, OSL samples were carefully hand-collected from cleaned, refreshed profiles under filtered red LED lighting after sealing off the cave chamber from external light contamination. Upon extraction, the hand-collected samples were immediately sealed with black plastic and duct tape to avoid exposure to daylight. Additional bulk sediment was collected from the surrounding 1 cm of each OSL sample position for water content analysis and beta dosimetry evaluation.

Purified coarse-grained quartz fractions were extracted from the luminescence samples under safe light (dim red LED) conditions at the University of Adelaide and prepared for burial dose estimation using standard preparation procedures (Aitken, 1998). The sediment samples were initially sieved to isolate the fine sand fraction (90-300 µm). Organics and carbonates were then eliminated using concentrated (30%) hydrogen peroxide (H₂O₂) and hydrochloric (HCl) acid digestion. Quartz grains were isolated using heavy liquid (LST lithium heteropolytungstate) density ranges of 2.62 g/cm³ to 2.72 g/cm³. The 212-250 µm quartz fractions were then sieved and etched with hydrofluoric (HF) acid to remove the alpha-irradiated external layers (48% HF digestion for 40 min). The etched grains were subsequently washed in 30% hydrochloric acid to remove any precipitated fluorides and re-sieved using a 63 µm sieve to eliminate any disaggregated grains.

Dose rate estimation
Environmental dose rates have been calculated using a combination of low-level beta counting and in situ gamma spectrometry (Table 6). Field gamma spectrometry measurements were made with a Canberra NaI:Tl detector and analysed using the ‘energy windows’ method to determine individual K, U and Th elemental concentrations (Arnold et al., 2012a; Duval and Arnold, 2013). External beta dose rates have been calculated from measurements made on a Risø GM-25-5 beta counter, using homogenised sediment sub-samples collected from the main
luminescence dating sample positions. The conversion factors of Guérin et al. (2011) have been used to derive gamma and beta dose rates from the measured radionuclide concentrations and specific activities. Cosmic-ray dose rates have been calculated as described in Prescott and Hutton (1994) after taking into consideration site altitude, geomagnetic latitude, and density, thickness and geometry of sediment and bedrock overburden. The beta, gamma and cosmic-ray dose rates have been corrected for long-term sediment moisture contents (Aitken, 1985; Readhead, 1987), which are taken to be equivalent to the present-day measured water contents (i.e., 10-12% of dry sediment weight) as the cave environment has remained sufficiently well-protected from major variations in external atmospheric conditions. A relative uncertainty of 20% has been assigned to the long-term water content values to accommodate any minor variations in hydrologic conditions during burial.

High-resolution gamma spectrometry (HRGS) measurements were additionally made on the homogenised bulk sediment samples to assess the presence of secular equilibrium in the $^{238}$U and $^{232}$Th decay series (Table A). Daughter-parent isotopic ratios for $^{238}$U, $^{226}$Ra, $^{210}$Pb, $^{228}$Ra and $^{228}$Th are consistent with unity at either 1σ or 2σ for all samples, confirming that the $^{238}$U and $^{232}$Th decay series are in equilibrium. Table A also includes the corresponding beta dose rates obtained using the HRGS results, which have been calculated after taking into consideration the fractional beta dose rate contributions of different isotopes in the $^{238}$U decay series (Stokes et al., 2003; Guérin et al., 211). For all five samples, the final beta dose rates derived using HRGS are in agreement, at either 1σ or 2σ, with those obtained using beta counting (Table 6).

**Equivalent dose ($D_e$) estimation**

Multi-grain and single-grain OSL measurements have been made using a Risø TL/OSL-DA-20 reader equipped with blue LEDs (470 nm, maximum power 102 mW/cm²), infrared LEDs (peak emission 850 nm, maximum power of 302 mW/cm²), and a 10 mW Nd:YVO₄ (532 nm) single-grain laser attachment (maximum power of c. 50 W/cm²). Ultraviolet OSL signals were detected using Electron Tubes PDM 9107B photomultiplier tubes fitted with 7.5 mm-thick Hoya U-340 filters. Samples were irradiated with a mounted $^{90}$Sr/$^{90}$Y beta source that had been calibrated to administer known doses to multi-grain aliquots and single-grain discs (average single-grain dose rate at the time of measurement = 0.095 Gy/s). Multi-grain OSL measurements (used for dose recovery tests only; see below) were made by mounting monolayers of quartz grains on 9.7 mm stainless steel discs using silicon oil spray (Silkospay). Single-grain $D_e$ measurements were made by manually loading individual 212-250 μm grains onto standard single-grain aluminium discs drilled with a 10 x 10 array of 300 μm diameter holes to ensure true single-grain resolution during $D_e$ evaluation (Arnold et al., 2012b).

Multi-grain dose recovery tests and single-grain $D_e$ measurements were undertaken using modified versions of the single-aliquot regenerative-dose (SAR) protocol described in Murray and Wintle (2000), as shown in Table B. Multi-grain $D_e$ values measured as part of the dose recovery test experiments were calculated by integrating the first 0.4 s of stimulation and subtracting a late-light background from the last 10 s. Single-grain OSL $D_e$ values were calculated by integrating the first 0.09 s of stimulation and subtracting a late-light background from the last 0.25 s. The sensitivity-corrected SAR dose-response curves were fitted with a single saturating exponential function. The uncertainty ranges of each individual $D_e$ value include three sources of error: (i) a random uncertainty term arising from photon counting statistics for each OSL measurement, calculated using Eq. 3 of Galbraith (2002); (ii) an empirically determined instrument reproducibility uncertainty of 1.9% for each single-grain measurement (calculated for the specific Risø reader used in this study according to the...
approach outlined in Jacobs et al., 2006); and (iii) a dose-response curve fitting uncertainty determined using 1000 iterations of the Monte Carlo method described by Duller (2007) and implemented in Analyst.

Single-grain OSL \( D_e \) values were excluded from final age calculations when: (i) the net intensity of the natural test dose signal, \( T_n \), was not \( >3\sigma \) above the late-light background signal; (ii) the low-dose (plus high-dose in the case of single-grain OSL) recycling ratios (i.e., sensitivity-corrected luminescence responses \( L_x/T_x \) for two identical regenerative doses) were not consistent with unity at \( 2\sigma \); (iii) the OSL IR depletion ratio of Duller (2003) was not consistent with unity at \( 2\sigma \) (i.e., the ratio of the \( L_x/T_x \) values obtained for two identical regenerative doses measured with and without prior IR stimulation, designed to detect feldspar contamination or inclusions); (iv) the recuperation ratio, calculated as the ratio of the sensitivity-corrected 0 Gy dose point \( (L_0/T_s) \) to the sensitivity-corrected natural \( (L_n/T_n) \), was \( >5\% \); (v) the net \( T_n \) signal had a relative error of \( >30\% \); (vi) the sensitivity-corrected natural signal \( (L_n/T_n) \) did not intercept the sensitivity-corrected dose-response curve; (vii) the dose-response curve displayed anomalous properties (i.e., zero or negative response with increasing dose) or very scattered \( L_x/T_x \) values that could not be successfully fitted with the Monte Carlo procedure and, hence, did not yield finite \( D_e \) values and uncertainty ranges; (viii) the \( L_x/T_n \) value intercepted the saturated part of the dose-response curve \( (L_x/T_n \) values were equal to the \( I_{\text{max}} \) saturation limit of the dose-response curve at \( 2\sigma \)).

**SAR \( D_e \) validation tests**

Multi-grain dose recovery tests were initially undertaken on 160-grain aliquots of sample CLD17-2 to assess the suitability of the SAR protocol and determine optimal preheat combination for bulk grain fractions of the Caldeirão samples. Five batches of four aliquots were each bleached twice at room temperature for 1000 s using blue LEDs (with an intervening 10,000 s pause to ensure complete decay of any phototransferred charge in the 110 °C TL trap), after which a known laboratory dose of 50 Gy was administered using the calibrated beta source. The surrogate natural dose of each aliquot was then measured using protocol A shown in Table B. A series of different preheat combinations were applied to each batch of four aliquots, as follows: regenerative-dose preheat (PH1) of 200, 220, 240 or 260°C for 10 s in combination with a test-dose preheat (PH2) of 160°C for 10 s; and a PH1 of 220°C for 10 s in combination with a PH2 of 200°C for 10 s. The two preheat combinations that produced multi-grain dose recovery ratios closest to unity (PH1 = 200°C for 10 s and PH2 = 160°C for 10 s; PH1 = 240°C for 10 s and PH2 = 160°C for 10 s) (Fig A, panel A) were further tested via single-grain dose recovery tests. These additional dose recovery tests were performed on 200-300 quartz grains of sample CLD17-2 (Table C) after bleaching their natural signals using the same procedure described above and administering a surrogate natural dose of 75 Gy. The single-grain OSL dose recovery test results indicate that a PH2 of 240 °C for 10 s and PH1 of 160°C for 10 s is optimal for single-grain OSL burial dose estimation. This preheat combination yielded a mean measured-to-given dose ratio of 1.00 ± 0.02 (\( n = 55 \) accepted grains) and an overdispersion value of 10 ± 4% (Fig B, panel A).

**Results**

Between 800 and 1100 grains per sample were measured for single-grain OSL \( D_e \) estimation. Approximately 50% of measured grains produced detectable OSL signals (Table C), with the brightest 1-5% of grains having 150-14,000 net counts / Gy in the first 0.09 s stimulation (Fig C, panel A). The measured OSL signals were bright and fast-decaying, and they were generally
depleted by c. 90% within the first 0.25 s of stimulation. After applying the SAR rejection criteria, 11-16% of the measured grains were considered suitable for De estimation (Table C). An example of a sensitivity-corrected dose-response and OSL decay curve for a moderately bright grain that passed the rejection criteria is shown in Fig C, panel B.

De distributions and the final single-grain OSL ages are presented and discussed in the Main Text (section 2.1.4, Fig 16, and Table 6) and Table D.

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**Fig A. OSL dose recovery test for sample CLD17-2.** Results obtained for 160-grain aliquots using the SAR protocol A in Table C. Showing measured to given dose ratios (A), recycling ratios (B) and recuperation values (C). A known dose of 50 Gy was administered to each aliquot as part of these multi-grain dose recovery tests.
Fig B. Radial plot showing single-grain OSL dose recovery test results obtained sample CLD17-2 using the SAR protocol B in Table B. The grey shaded region is centred on a dose recovery ratio of 1. Individual values that fall within the shaded region are consistent with the administered dose at 2σ. (A) Data obtained using a regenerative-dose preheat (PH1) of 240°C / 10 s and test-dose preheat (PH2) of 160°C / 10 s. (B) Data obtained using a PH1 of 200°C / 10 s and PH2 of 160°C / 10 s.
Fig C. OSL signal brightness and decay curves. (A) OSL signal brightness plot showing absolute net intensities expressed as counts / Gy / 0.09 s. The data shown are for single-grain OSL measurements made using the 212-250 µm quartz fraction for all samples from Gruta do Caldeirão. (B) Examples of OSL decay curves and sensitivity-corrected dose-response curve (inset) for a representative quartz grain of sample CLD17-1. White square denotes the sensitivity-corrected natural OSL signal; filled circles denote the sensitivity-corrected regenerative dose OSL signals; white circles denote the repeated regenerative dose points used to calculate the recycling ratios. The $D_0$ value characterises the rate of signal saturation with respect to administered dose and equates to the dose value for which the saturating exponential dose-response curve slope is $1/e$ (or c. 0.37) of its initial value.
Table A. High-resolution gamma spectrometry (HRGS). Results for OSL samples collected from Gruta do Caldeirão. The beta dose rates shown in the final column have been calculated using the long-term water content corrections, beta attenuation factors and dose rate conversion factors detailed for each sample in Table 6.

| Sample | $^{238}$U | $^{226}$Ra | $^{210}$Pb | $^{228}$Ra | $^{228}$Th | $^{40}$K | Daughter:parent isotopic ratio | Beta dose rate (Gy/ka) |
|--------|-----------|----------|----------|----------|----------|-------|----------------|----------------------|
| CLD17-1 | 35.76 ± 3.40 | 34.24 ± 0.73 | 33.46 ± 3.79 | 44.13 ± 1.53 | 46.76 ± 1.21 | 380 ± 12 | 0.96 ± 0.09 | 0.98 ± 0.11 | 1.06 ± 0.05 | 1.29 ± 0.06 |
| CLD17-2 | 39.21 ± 3.18 | 44.58 ± 0.79 | 45.13 ± 4.01 | 65.52 ± 1.58 | 65.48 ± 1.43 | 494 ± 13 | 1.14 ± 0.09 | 1.01 ± 0.09 | 1.00 ± 0.03 | 1.67 ± 0.07 |
| CLD17-3 | 40.97 ± 2.72 | 44.72 ± 0.78 | 39.95 ± 4.07 | 62.77 ± 1.57 | 64.59 ± 1.39 | 491 ± 13 | 1.09 ± 0.08 | 0.89 ± 0.09 | 1.03 ± 0.03 | 1.64 ± 0.07 |
| CLD17-4 | 43.44 ± 3.74 | 47.42 ± 0.92 | 45.99 ± 4.71 | 74.93 ± 1.97 | 77.76 ± 1.73 | 518 ± 15 | 1.09 ± 0.10 | 0.97 ± 0.10 | 1.04 ± 0.04 | 1.78 ± 0.08 |
| CLD17-5 | 42.62 ± 3.78 | 42.82 ± 0.76 | 36.54 ± 4.55 | 68.15 ± 1.58 | 70.69 ± 1.48 | 434 ± 12 | 1.00 ± 0.09 | 0.85 ± 0.11 | 1.04 ± 0.03 | 1.51 ± 0.07 |

a Measurements made on dried and powdered sediment sub-samples of 0.7 g.
b Mean ± total uncertainty (68% confidence interval), calculated as the quadratic sum of the random and systematic uncertainties.

Table B. SAR protocols used in this study to undertake dose recovery tests on multi-grain aliquots (protocol A) and to obtain single-grain quartz OSL ages (protocol B). $L_n$ and $L_x$ refer to the natural and regenerative-dose OSL signal measurements, respectively. $T_n$ and $T_x$ refer to the test dose OSL signals measured after the $L_n$ and $L_x$ OSL signals, respectively. Each of these SAR measurement cycles was repeated for the natural dose, five different sized regenerative doses and a 0 Gy regenerative-dose (to measure OSL signal recuperation). Both the smallest and largest non-zero regenerative-dose cycles were repeated at the end of the SAR procedure to assess the suitability of the test-dose sensitivity correction. For protocol B, the smallest regenerative-dose cycle was also repeated a second time with the inclusion of step 2 to check for the presence of feldspar contaminants using the OSL IR depletion ratio of Duller (2003).

**A Multi-grain OSL SAR protocol**

| Step | Treatment | Symbol |
|------|-----------|--------|
| 1<sup>a</sup> | Give dose | |
| 2 | Stimulate with infrared diodes at 50ºC for 60 s at 90% power | |
| 3 | Preheat to either 200, 220, 240 or 260ºC for 10 s | |
| 4 | Stimulate with blue LEDs at 125ºC for 60 s | $L_n$ or $L_x$ |
| 5 | Give test dose | |
| 6 | Stimulate with infrared diodes at 50ºC for 60 s at 90% power | |
| 7 | Preheat to 160 or 200ºC for 10 s | |
| 8 | Stimulate with blue LEDs at 125ºC for 60 s | $T_n$ or $T_x$ |
| 9 | Return to 1 | |

<sup>a</sup> Step omitted when measuring the natural signal ($L_n$).

**B Single-grain OSL SAR protocol**

| Step | Treatment | Symbol |
|------|-----------|--------|
| 1<sup>a</sup> | Give dose | |
| 2<sup>b</sup> | Stimulate with infrared diodes at 50ºC for 60 s at 90% power | |
| 3 | Preheat to 240ºC for 10 s | |
| 4 | Stimulate with green laser at 125ºC for 2 s (90% power) | $L_n$ or $L_x$ |
| 5 | Give test dose | |
| 6 | Preheat to 160ºC for 10 s | |
| 7 | Stimulate with green laser at 125ºC for 2 s (90% power) | $T_n$ or $T_x$ |
| 8 | Return to 1 | |

<sup>b</sup> Step added only when measuring the IR depletion ratio described in Duller (2003).
Table C. Single-grain OSL classification statistics for the natural $D_n$ measurements. The proportion of grains that were rejected from final $D_n$ estimation after applying the various SAR quality assurance criteria are shown in columns 3-11. These criteria were applied to each single-grain measurement in the order listed. Also shown are the single-grain OSL classification statistics for the dose recovery tests undertaken using different preheating conditions, where “240/160” equates to a PH1 of 240°C for 10 s and a PH2 of 160°C for 10 s, and “200/160” equates to a PH1 of 200°C for 10 s and a PH2 of 160°C for 10 s. $T_n$ = natural test dose signal response; $L_n/T_n$ = sensitivity-corrected natural signal response. BG = background. DRC = dose response curve.

| CLD sample | 17-1 | 17-2 | 17-3 | 17-4 | 17-5 | 17-2 (dose recovery test 240/160) | 17-2 (dose recovery test 200/160) |
|------------|------|------|------|------|------|-------------------------------|-------------------------------|
| Grains measured (N) | 900  | 1100 | 900  | 800  | 900  | 300                          | 200                          |
| Rejected grains (%) |      |      |      |      |      |                               |                               |
| $T_n$ signal <3xBG | 8    | 6    | 8    | 9    | 11   | 4                            | 7                            |
| Poor low recycling ratio | 4    | 5    | 3    | 5    | 4    | 6                            | 3                            |
| Poor high recycling ratio | 4    | 5    | 4    | 3    | 4    | 3                            | 2                            |
| IR depletion ratio <1 | <1   | <1   | <1   | <1   | 0    | 0                            | 0                            |
| Recuperation >5% | 9    | 8    | 9    | 6    | 9    | 4                            | 4                            |
| Net $T_n$ error >30% | 1    | 2    | 1    | 3    | 3    | <1                           | 0                            |
| $L_n/T_n$ not intercepting DRC | 3    | 5    | 4    | 5    | 6    | 4                            | 6                            |
| Anomalous dose-response curve | 3    | 4    | 4    | 5    | 5    | 4                            | 5                            |
| Saturated | 56   | 49   | 52   | 51   | 44   | 44                           | 56                           |
| Accepted grains (%) | 11   | 16   | 14   | 14   | 14   | 18                           | 22                           |
The preferred age of each sample is highlighted in bold. For these samples, the preferred age has been derived using the statistical age model that yielded the optimum $L_{\text{max}}$ score, following the criterion outlined in footnote $^a$ and Arnold et al. (2009).

Table D. Single-grain OSL $D_e$ summary statistics, dose rates and OSL ages. The preferred age of each sample is highlighted in bold. For these samples, the preferred age has been derived using the statistical age model that yielded the optimum $L_{\text{max}}$ score, following the criterion outlined in footnote $^a$ and Arnold et al. (2009).

| Sample | Sample depth (cm) | Grain size (μm) | Total dose rate (Gy / ka) | Accepted/Measured | Over-dispersion (%) | Weighted skewness | Critical skewness (95% C.I.)$^a$ | Critical skewness (68% C.I.)$^a$ | Age Model$^{b,c}$ | $L_{\text{max}}$ score$^d$ | $D_e$(Gy)$^e$ | Age (ka)$^{e,f}$ |
|--------|------------------|-----------------|---------------------------|-------------------|---------------------|------------------|------------------------|------------------------|----------------|----------------|----------------|----------------|
| CLD17-1 | 393              | 212-250         | 2.23 ± 0.11               | 100/900           | 37 ± 3              | 0.905            | 0.489                  | 0.244                  | CAM           | -55.694        | 98.6 ± 4.1     | 44.2 ± 3.1    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-3        | -47.863        | 84.1 ± 4.2     | 37.7 ± 2.8    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-4        | -47.714        | 85.5 ± 4.2     | 38.4 ± 2.8    |
| CLD17-2 | 459              | 212-250         | 2.99 ± 0.15               | 180/1100          | 24 ± 2              | 0.020            | 0.365                  | 0.183                  | CAM           | -48.832        | 118.4 ± 2.7    | 39.6 ± 2.3    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-3        | -48.635        | 112.2 ± 3.9    | 37.5 ± 2.4    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-4        | -48.510        | 112.4 ± 31.3   | 37.6 ± 10.7   |
| CLD17-3 | 469              | 212-250         | 3.08 ± 0.15               | 127/900           | 27 ± 2              | 0.122            | 0.435                  | 0.217                  | CAM           | -44.512        | 116.6 ± 3.4    | 37.9 ± 2.3    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-3        | -40.409        | 102.8 ± 10.4   | 33.4 ± 3.8    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-4        | -40.212        | 106.0 ± 10.5   | 34.5 ± 3.9    |
| CLD17-4 | 513              | 212-250         | 3.02 ± 0.15               | 108/800           | 23 ± 2              | 0.034            | 0.471                  | 0.236                  | CAM           | -24.530        | 126.8 ± 3.5    | 42.0 ± 2.5    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-3        | -23.339        | 122.2 ± 4.3    | 40.5 ± 2.6    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-4        | -23.189        | 122.1 ± 4.2    | 40.4 ± 2.6    |
| CLD17-5 | 525              | 212-250         | 2.79 ± 0.14               | 129/900           | 35 ± 3              | -0.103           | 0.431                  | 0.216                  | CAM           | -63.595        | 162.9 ± 5.7    | 58.4 ± 3.8    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-3        | -65.695        | 127.9 ± 5.8    | 45.8 ± 3.2    |
|         |                  |                 |                           |                   |                     |                  |                        |                        | MAM-4        | -64.107        | 118.0 ± 10.8   | 42.3 ± 4.5    |

$^a$ Weighted skewness scores have been calculated on log-transformed $D_e$ values using Eq. 7-8 of Arnold and Roberts (2009). Critical skewness scores have been calculated using Eq. 16 of Bailey and Arnold (2006). Critical skewness values are taken to be equivalent to twice the standard error of skewness score (95% C.I.) for single-grain $D_e$ datasets, following the results of sensitivity analyses performed by Bailey and Arnold (2006) and Arnold et al. (2007).

$^b$ CAM = central age model; MAM-3 = 3-parameter minimum age model; MAM-4 = 4-parameter minimum age model (Galbraith et al., 1999).

$^c$ $D_e$ estimates have been calculated after adding, in quadrature, a relative error of 20% to each individual $D_e$ measurement error to approximate the underlying dose overdispersion observed in 'ideal' (well-bleached and unmixed) sedimentary samples from this site (CLD17-2, CLD17-3, CLD17-4), the single-grain dose-recovery tests performed on the Caldeirão samples (CLD17-2) and from global overdispersion datasets (Arnold and Roberts, 2009).

$^d$ Maximum log likelihood score of the CAM, MAM-3 or MAM-4 fit. For a given sample, the $L_{\text{max}}$ score of the MAM-3 is expected to be substantially higher (i.e. at least 1.92 greater) than that of the CAM when the addition of the extra model parameter improves the fit to the data. Likewise, the $L_{\text{max}}$ score of the MAM-4 is expected to be significantly greater than that of the MAM-3 (by at least 1.92 when compared with the 95% C.I. of a $X^2$ distribution) when the addition of the extra model parameter improves the fit to the data. If the extra parameter of the MAM-3 (or MAM-4) is not supported by the data, then its $L_{\text{max}}$ score will be similar to (i.e. within 1.92 of) the CAM (or MAM-3) $L_{\text{max}}$ score, indicating that the simpler age model explains the data equally well (Arnold et al., 2009).

$^e$ Mean ± total uncertainty (68% confidence interval), calculated as the quadratic sum of the random and systematic uncertainties. Total uncertainty includes a systematic component of ±2% associated with laboratory beta-source calibration.

$^f$ The preferred age for each sample is shown in bold. For these samples, the preferred age has been derived using the statistical age model that yielded the optimum $L_{\text{max}}$ score, following the criterion outlined in footnote $^a$ and Arnold et al. (2009).
Pigment analysis procedures and results
Methodology

We employed three techniques to characterise the elemental and mineralogical composition of sediment samples and of residues adhering to three directly dated marine shells from Gruta do Caldeirão: P13sc491 (Fig 12, no. 1; OxA-22299) and P13-402 (Fig 12, no. 2; OxA-22300), from layer Jb (henceforth Shell 1 and Shell 2, respectively); P11sc968 (Fig 12, no. 4; OxA-22301), from layer K (henceforth Shell 3). Raman spectroscopy was applied to residues and uncoated areas of the three shells. A portable X-ray fluorescence (pXRF) analyser was used for sediment samples. Scanning electron microscopy (SEM) coupled with energy dispersive X-ray spectrometry (EDS) was used for the analysis of Shell 3 and sediment samples. The latter were also analysed by means of X-ray micro-diffraction (µXRD).

Raman analyses were conducted with a Raman Senterra (BRUKER) device equipped with a 532 nm laser and using an illumination intensity of 2 mW. Scattered light was collected through a 50× objective.

The SEM-EDS instrument was a PHILIPS XL30 ESEM model with an electron gun LaB6 coupled with Si(Li) EDS. The samples were observed and analysed without any preparation, in controlled pressure mode (pressure of 10⁻⁴ Torr). The acceleration voltage was set to 20 kV.

µXRD analysis were carried out on a dedicated, laboratory-made device using a Rigaku monochromatic source (λ=1.54186 Å) and a 200 μm collimator. The maximum voltage and current were set at 45 kV and a 660 μA, respectively. The incident beam was positioned to form a grazing angle with the surface of the sample. The analysed area was about 1 mm². A 2D Rigaku imaging plate detector (R-AXIS IV++) and a motorized X,Y,Z,φ positioning system with an independent θ axis were coupled to the XRD equipment. Acquisition time was set at 3 minutes. The circular diffractograms were calibrated in 2θ and transformed into linear ones through the software Fit2D v.12.077, developed by Andy Hammersley (European Synchrotron Radiation Facility, Grenoble, France). Data treatment was performed with the EVA© software (Bruker).

pXRF measurements were carried out with a SPECTRO xSORT (AMETEK) instrument, equipped with a silicon drift detector (SDD) and a low power W X-ray tube with an excitation source of 40 kV. Measurements were acquired in the air with a constant working distance by using a lead receptacle to which the spectrometer is fixed. Light elements such as Na, Mg, and Al are not detected with this technique. An area of 8 mm in diameter was analysed. Spectra acquisition times were set to 60 s. The spectrometer is internally calibrated by an automated measure of the contents of a standard metal shutter. Data treatment was realised using standard materials and after two-time calibration of the results.

Results

Observation under a reflected light optical microscope identified remnants of a red coating and whitish residues on Shell 1, and red, orange, and white residues on Shell 2 (Figs D and E). Three superimposed deposits of different colour were detected on the surface of Shell 3 (Figs F-H): the first, adhering to the shell’s test, is bright red in colour and composed of fine, sorted particles; the second is a thicker and coarser orange/reddish layer that, in places, covers the first; the third is an even thicker, whitish layer that covers both and can also be seen in the fill of the shell’s aperture, indicating that it must relate to the sedimentary matrix.

SEM observation confirms the differences in texture between the bright red and orange/reddish layers of Shell 3 (Fig H): most particles composing the inner bright red layer are <1 μm and those in the order of 5 μm are rare, which indicates a clayey texture. However, the elements composing both layers are the same (Si, Al, Ca, K, Fe, P), albeit in different proportions (P is substantially more abundant in the outer orange/reddish layer).
Raman spectroscopy (Table E; Fig D) identified the presence of hematite and calcite in, respectively, the red and the whitish residues coating Shell 1. Hematite was also identified in the red residues found on the surface of Shell 2, whose pale reddish coating was dominated by calcite with traces of hematite; the analysis of the shell’s test reveals diagenetically unmodified aragonite (Fig E). The bright red layer adhering to the surface of Shell 3 is composed of hematite, possibly associated with ferrihydrite, and calcite, while the overlying orange/reddish layer contains either hematite associated with calcite or hematite (and, possibly, magnetite) associated with phosphates. In Shell 3, however, the hematite spectra identified in the bright red and orange/reddish layers differ from reference spectra in the form of line shift, change in relative intensities, and absence of bands beyond 400 cm\(^{-1}\) (Table F). These anomalies can be due to excessive laser power (2 mW, wavelength 532 nm), and are not necessarily related to the crystallinity of the hematite (Faria et al., 1997).

\(\mu\)XRD analysis of the bright red layer of Shell 3 identified quartz, calcite, aragonite, clays of the illites/glauconites family, and kaolinite (Fig G; Table G). Hematite was not detected, but the main peak of this mineral coincides with an aragonite peak, and a secondary peak coincides with a kaolinite one. In light of the Raman results, the failure of \(\mu\)XRD to detect hematite must be due to method limitations. Indeed, \(\mu\)XRD similarly failed when analysing red residues found in the overlying orange/reddish layer. The latter was found to be mainly composed of calcite and aragonite, while the bright red layer also showed traces of illite/glauconite and kaolinite.

The \(p\)XRF analysis of sediments from layers Jb and K identified a notable proportion (4-5%) of iron oxides, as intimated by their reddish colour (Table H). However, iron oxides were not detected by \(\mu\)XRD (Table I), which probably implies that, in the sediment, such oxides are found in poorly crystalline form only. Otherwise, both layers have a similar mineralogical composition: quartz, calcite, feldspar (microcline or other), calcium phosphate (hydroxyapatite family), and illite/muscovite are present in both; kaolinite is the single mineral found in one layer only (layer Jb).

**Synthesis**

The layer of residue adhering to the surface of Shell 3 differs from the overlying orange/reddish layer in colour (bright red), grain size (clayey), and composition (less calcium phosphate). The composition of the orange/reddish layer is intermediate between the underlying bright red layer and the sedimentary matrix of layer K, where the shell was retrieved. The bright red and the orange/reddish layer also feature a higher proportion of clay minerals (illite/muscovite and kaolinite), which is consistent with the clayey grain size of the bright red layer. The layer’s matrix contains a small proportion of iron, but \(\mu\)XRD failed to identify hematite. Iron compounds (oxy-hydroxides or oxides) seem to be present in the sediment in poorly crystalline form, whereas in the residues found on all the shells they appear as hematite (although this difference would need to be confirmed by Raman analysis of the sediment).

Overall, these patterns are consistent with two different interpretations. The first is that the bright red layer seen on Shell 3 represents the remnant of a hematite-rich compound that (a) covered the shell during its use as an ornamental object, and (b) was still present on its surface at the time of loss (or discard) and eventual incorporation in the deposit. The second hypothesis is that said bright red layer (a) corresponds to the finest fraction of the sediment making up archaeological layer K, and (b) represents post-depositional accumulation. Although it cannot formally ruled out, this second hypothesis is unparsimonious and indeed rather unlikely, as it requires us to postulate an unknown mechanism by which, prior to its eventual deposition on the shell’s surface, the fine fraction would have been segregated, with some of the minerals that make it up being eliminated in the process. Provided we interpret the reddish deposits found in Shells 1 and 2 alike the orange/reddish layer of Shell 3, i.e., as remnants of a pigmentatious compound diluted in a calcitic
matrix, we can conclude that, originally, the three shells were coated with a red, hematite-rich colouring mixture.

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**Fig D. Shell 1 (P13sc491; layer Jb)**. Detail of the reddish deposit covering the shell and Raman spectra of that deposit compared to a white spot of the shell’s test itself.
Fig E. Shell 2 (P13-402; layer Jb). Details of the reddish deposit covering the shell and Raman spectra of that deposit compared to a white spot of the shell’s test itself.
Fig F. Shell 3 (P11sc968; layer K). Details of the orange/reddish and bright red deposits covering the shell and Raman spectra of those deposits compared to a white spot of the shell’s test itself.
Fig G. Shell 3 (P11sc968; layer K). Raman spectra and X-ray diffraction pattern of the bright red layer.
Fig H. Shell 3 (P11sc968; layer K). SEM back scattered images and EDS results of the orange/reddish and bright red deposits.
### Table E. Results of the Raman analyses on three marine shells from Caldeirão

| Shell | Layer/Area       | Minerals identified                      | Spectra (N) |
|-------|------------------|-----------------------------------------|-------------|
| 1     | Red layer        | Hematite                                | 1           |
|       | White area       | Calcite                                 | 1           |
| 2     | Red residues     | Hematite                                | 1           |
|       | Orange/reddish layer | Calcite, traces of hematite           | 1           |
|       | White area       | Aragonite                               | 1           |
| 3     | Bright red layer | Hematite (plus magnetite?); calcite    | 10          |
|       | Orange/reddish layer | Hematite, traces of calcite; hematite, phosphates (plus magnetite?) | 3           |

### Table F. Reference Raman bands for the minerals identified on Caldeirão samples

| Minerals     | Reference Raman bands (cm⁻¹)                                                                 | References               |
|--------------|----------------------------------------------------------------------------------------------|--------------------------|
| Hematite     | 225 vs, 240 sh, 290 vs, 410 m, 490 w, 610 w 1320 vs                                             | Faria et al., 1997       |
|              |                                                                                               | Froment et al., 2008     |
| Calcite      | 150 m, 280 m, 710 m, 1085 vs                                                                  | Gillet et al., 1993      |
| Aragonite    | 150, 210, 280, 700 m, 1085 vs                                                                 | Gillet et al., 1993      |
| Phosphates   | 400-490 w, 570-620 w, 970 vs                                                                  | Cuscó et al., 1998       |
| Magnetite    | 300 w, 550 w, 670 vs                                                                          | Faria et al., 1997       |
|              |                                                                                               | Froment et al., 2008     |

### Table G. Results of µXRD analyses conducted on Shell 3 from Caldeirão

| Layer/Area               | Calcite | Aragonite | Quartz | Illite/glauconite | Kaolinite |
|--------------------------|---------|-----------|--------|-------------------|-----------|
| Bright red layer         | -       | +++       | ++     | -                 | -         |
| Red residues in the bright red layer | +++   | +++       | +      | +                 | +         |
| Orange/reddish layer     | +++     | +         | -      | -                 | -         |

### Table H. Results of the X-ray fluorescence analysis of Caldeirão sediments

| Analyses               | SiO₂ (%) | P₂O₅ (%) | SO₄ (%) | K₂O (%) | CaO (%) | TiO₂ (%) | MnO (%) | Fe₂O₃ (%) | (N) |
|------------------------|----------|----------|---------|---------|---------|-----------|---------|-----------|-----|
| Sediment Jb            | Average  | 48       | 10.7    | 1.6     | 1.95    | 33        | 0.45    | 0.168     | 4   |
| sd                     | 1        | 1.7      | –       | 0.08    | 1       | 0.03      | 0.05    | 0.6       | 0   |
| Sediment K             | Average  | 64       | 7.4     | 1.2     | 2.18    | 25.0      | 0.53    | 0.215     | 3   |
| sd                     | 3        | –        | –       | 0.03    | 0.6     | 0.03      | 0.004   | 0.0       | 0   |

*except for phosphorus, element concentration was controlled by the use of standards

### Table I. Results of the X-ray diffraction analysis of Caldeirão sediments

| Layer Jb               | Calcite | Quartz | Illite/glauconite | Kaolinite | Hydroxyapatite | Feldspar |
|------------------------|---------|--------|-------------------|-----------|----------------|----------|
| Layer Jb <200 μm       | ++      | +++    | +                 | +         | +              | +        |
| Layer K                | ++      | +++    | +                 | -         | +              | +        |
Stratigraphic provenance of key finds
O13sc91 (MAMS-38336)
The specimen is a non-plotted horse tooth retrieved in spit E4 of square O13 (see Fig 3 for the location of this grid unit in the Corridor area of the site). The décapage plans illustrating the excavation of that spit, carried out in 1983 between August 26 and August 31, are reproduced in Fig I. The hand-written annotations provide elevations of both the sediment and the upper and lower surfaces of the blocks exposed at the base of each spit. Note the large animal burrows and the linear disturbance features, which denote root paths. The description emphasises the large number of rabbit bones retrieved, especially in and around the larger burrow feature against the cave wall.

O13 was the first grid unit to be opened in order to extend the Back Chamber trench towards the Corridor. At the time, it was assumed that the latter would feature the same stratigraphic succession and, therefore, that the first spits of the reddish-brown deposit below layer ABC-D would correspond to layer Ea. The décapage descriptions reflect that assumption. Only subsequently, with further outward expansion of the excavation trench, was it possible to recognise that layer Ea wedged out at the transition between Back Chamber and Corridor, and that spits E1-E4 belonged in the upper part of layer Eb, not in layer Ea.

O12-84 (OxA-X-2786-13)
The specimen is a human left mandibular fragment. It belonged to an early adolescent: the Caldeirão 2 individual, as described in Trinkaus et al. (2001). The dm2 is preserved in its socket. The fossil was retrieved in a small burrow against the cave wall, during the excavation of spit H1 of grid unit O12 (Fig J). The latter corresponds to a triangular surface created by the site’s gridding against the north wall of the Back Chamber (see Fig 3 for its location on the site plan). Here, layers Fa-Jb were excavated between July 7 and August 5, 1986, i.e., after the surface of layer K in the adjacent P row had already been reached (during the previous field season, in 1985). The idea was to double-check, by careful décapage, the E→W dip of the stratification suggested by observation of the P>O/11-12 profile, and to verify, by comparison with the opposite profile (P>Q/11-13), that the N→S dip was indeed negligible, as the excavation of the P row had suggested.

The hand-written annotations provide elevations of the sediment at the base of each spit. They also contain summary descriptions of matrix and clasts, reflecting how the Fc/H interface was first thought to correspond to the base of spit F8, with continued excavation showing that a few cm remained before the surface of H was truly exposed, which was the case at the base of spit F9. Note that the burrow only appeared as the surface of H was reached. This evidence suggests that the disturbance was a small scale one and that the finds made in the burrow are reworked from layer H itself, not intrusive form layer Fc above.

P13-403 (OxA-5541)
The specimen is a distal metapodial of red deer from spit J6 of square P13, at the base of which the Jb/K interface was reached in most of the square (Fig K). In this part of the cave (squares O-P/13-14), at the 90° angle between Back Chamber and Corridor, controlling for the presence of a double dip (E→W in the former, N→S in the latter) was hindered by the relative homogeneity displayed by the matrix through the succession of layers Fa-L. Even though often aided by such clues as the presence of stone lines, incrustation lenses, or flat-bottomed slabs denoting the actual disposition of past cave floors, the décapage of stratigraphic interfaces in P13 was always rather approximate.

This difficulty may explain the erroneous assignment of P13-403 to “layer K-top” that appeared in previously published reports on the site’s dating (e.g., Zilhão, 1997). As shown by the décapage plans reproduced in Fig K, P13-403 was found at the same elevation and adjacent to the retouched flint knife and directly dated Aporrhais pespelecani shell illustrated in Figs 10 and 12.
When their position is assessed against a virtual surface reconstructed from the elevations found in the more reliable excavation records — the topography of the Jb/K interface in O/13-14, and its elevation along the P>Q/11-13 profile — the three items lay at, or just above the base of layer Jb. Indeed, this exercise shows that, at the base of spit J6 of P13, the surface of layer K had yet to be reached in the square’s SW corner, and (b) conversely, due to the heavy induration of the deposit, which hindered a precise décapage of layer boundaries, it had been somewhat undercut in the square’s SE corner (without consequence, however, as that corner was entirely devoid of finds). Note the root burrow along the wall in O13, which was not detected when, a month before (July 31, 1986), the same surface had been exposed in P13.

**O13-361**

The specimen is a large quartz sidescraper (Fig 11, no. 1) retrieved in square O13 at the surface of layer L. In previous publications (e.g., Zilhão, 1997), it was assigned to layer K, which we correct here. The following reasons explain the original misassignment: (a) the excavation of squares O/13-14 and P13 down to the surface of layer L was carried out at the very end of the project (September 12 and 14, 1988, respectively), and it stopped at the elevation of that boundary; (b) no subsequent field assessment of the stratigraphic accuracy of the assignment of finds then made was therefore possible; (c) through the excavation of the site, all finds made during the last, fine-décapage stage of the exposure of stratigraphic interfaces were by convention recorded as belonging in the unit above the interface. Following this convention dictated that O13-361 be recorded as “K,” even though this was the first artefact found in the excavation of O/13-14 since the quartzite flake O13-346, which lay 30 cm higher-up, at the top of layer Jb. In addition, at the time, layer K was thought to belong in the Middle Palaeolithic. Whether this item came from K or L was therefore not regarded as hugely significant, and whether the convention ought to be ignored in this case was not considered to be an issue of chronostratigraphic importance.

As shown by the décapage plans reproduced in Fig L, the elevation of O13-361 clearly places it at the very top of layer L, not in layer K. The plan also shows that, due to the same “double-dip” problems mentioned in relation to the P13-403 radiocarbon sample, the K/L interface was significantly undercut in the NE part of P13. The same happened in its SE corner, due to induration. Elsewhere along the P>Q13 profile, however, induration had the opposite effect, i.e., the décapage could not proceed to the exact interface and remained a few cm above it.

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Fig I. O13, field records for spits E3-E4. Description and elevation of the surfaces delimiting the thickness of deposit that yielded the O13sc91, non-plotted horse tooth; its radiocarbon age (20,077 ± 100 BP; MAMS-38336) shows that this an upwardly moved find derived from the underlying Solutrean deposit.
Fig J. O12, field records for spits F8-H1. Description and elevation of the surfaces delimiting the thickness of deposit across which the Fc/H interface was exposed and excavated in grid unit O12, and the O12-84 human fossil (whose \([x,y]\) coordinates are indicated by the star) retrieved in the small burrow exposed at that interface and radiocarbon dated to 19,400 ± 150 BP (OxA-X-2786-13).
Fig K. Field records for spit J6 of squares O/13-14 and P13. Description and elevation of the décapage surface approximately corresponding to the interface between layers Jb and K. The arrow indicates the dip of the stratification. The stars mark the [x,y] coordinates of the P13-401, 402 and 403 finds. Their elevations are indicated, and show that all three belong in layer Jb.
Fig L. Field records for spits K1 of O/13-14 and K5 of P13. Description and elevation of the décapage surface approximately corresponding to the interface between layers Jb and K (in O/13-14, excavated as a single spit). The arrow indicates the dip of the stratification. The stars mark the \([x,y]\) coordinates of the O13-361 and P13-483 finds. Their elevations are indicated, showing that both items belong in layer L.
Bayesian age modelling of the succession
Methods

Bayesian modelling was undertaken using OxCal v4.4 (Bronk Ramsey, 2009a), following the general approach outlined in Demuro et al. (2019, 2020). The sedimentary sequence has been modelled using a Sequence depositional model, incorporating stratigraphic units in ordered succession and separated by associated boundaries. The Gruta do Caldeirão Bayesian model focuses on the eleven layers comprising the pre-Magdalenian archaeological sequence excavated in the Back Chamber (layers Fa-O), plus the two Middle Palaeolithic layers from the Entrance Trench (Units 5-6). The dating determinations for individual units are represented as a grouped set of likelihoods (Phase) within the Sequence model. Boundaries have been used to delineate the beginning and end of each stratigraphic unit, and to specify that all likelihoods or events included in these groupings have a uniform prior likelihood of occurrence. Separate rather than shared boundaries have been used to delineate the beginning and end of each stratigraphic unit to ensure the model is able to accommodate potential depositional hiatuses or erosional discontinuities between successive layers.

The single-grain OSL dating likelihoods have been input into the model as calendar ages before year of sample collection, together with their associated 1σ uncertainty ranges, using the date command. The Bayesian model was run using the general outlier function (Bronk Ramsey, 2009b), with prior outlier probabilities of 5% assigned to all dating samples. Likelihood estimates that yielded posterior outlier probabilities >5% were not excluded from the final model but were proportionally down-weighted in the iterative Markov Chain Monte Carlo runs (Bronk Ramsey, 2009b).

To examine the sensitivity of the modelling outcomes to different assumptions about stratigraphic priors and dating likelihoods, we have run five different versions of the Gruta do Caldeirão Bayesian model (Models I to V). The structure of these models, and the main differences in representation of individual stratigraphic layers and dating determinations, are summarised in Table 1. In brief, Model I is set up with separate stratigraphic units defined for each individual layer, with the exception of layers Fa-Fc, which are grouped as a single unit. Model I includes all age determinations depicted in Fig 23, together with the radiocarbon determination obtained on the *Semicassis saburon* ornament from layer K (OxA-22301). The radiocarbon determinations for OxA-1938 and OxA-22301 are assumed to represent maximum age estimates for layers Fa-Fc and K, respectively, and have therefore been input into the model using the After command. The radiocarbon determination for MAMS-41872 is assumed to represent a minimum age estimate for layer L and has thus been input into the model using the Before command. Model II is the same as Model I, except that layers I-Ja and layers L-N are represented as combined stratigraphic units rather than defined as individual units. Model III is the same as Model II, except that the radiocarbon determination for MAMS-33905 is considered as a minimum age estimate for layers L-N and has therefore been input into the model using the Before command. Model IV is equivalent to Model III, but all radiocarbon determinations have been removed from the Middle Palaeolithic units (layers L, M, N) to test the extreme assumption that they all suffer from methodological or stratigraphic reliability issues. Layers L, M and N are also represented as separate stratigraphic units rather than as a single combined grouping in Model IV. Model V is the same as Model III but includes the two radiocarbon determinations from the Entrance Trench (MAMS-41874 and MAMS-41876), and additionally adopts a single stratigraphic grouping for layers L, M, N (Back Chamber), and the Middle Palaeolithic layers from the Entrance Trench (Units 5-6). The CQL codes used to construct Models I to V are provided in the next section.

The results obtained for Models I to V are summarised in Tables K-O and Figs M-O, 24-25. All modelled age ranges have been rounded to the nearest 10 years and are reported as the 68.3 % and 95.4 % highest probability density function (PDF) ranges, as well as the mean and 1σ uncertainty ranges of the modelled posterior distributions. The posterior probabilities of the upper and lower (top and bottom) boundaries have been used to constrain the beginning and end periods for each layer. For comparison, Tables K-O also show the modelled age range of each stratigraphic unit, calculated from the modelled posterior probabilities of the lower and upper unit boundaries using the date command. Tables K-O summarise the convergence
integrals, posterior outlier probabilities and agreement indices for all individual posterior distributions. The agreement indices, including the $A_{\text{model}}$ and $A_{\text{overall}}$ values, are included for completeness but are of limited diagnostic value as all models have been run with the general outlier function.

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The prior age distributions for the dating determinations (likelihoods) are shown as light coloured probability density functions (PDFs): blue = radiocarbon determinations; green = single-grain OSL determinations. The modelled posterior distributions for the dating determinations and stratigraphic unit boundaries are shown as dark coloured and grey PDFs, respectively. Unmodelled and modelled ages are shown on a calendar year timescale, and both are expressed in years before AD1950. The white circles and associated error bars represent the mean ages and 1σ uncertainty ranges of the PDFs. The 68.3% and 95.4% ranges of the highest posterior probabilities are indicated by the horizontal bars underneath the PDFs. The light yellow rectangles highlight the 95.4% interval that the model returns for the end of the Middle Palaeolithic at the site.
Fig N. OxCal plot output for Model II. The prior age distributions for the dating determinations (likelihoods) are shown as light coloured probability density functions (PDFs): blue = radiocarbon determinations; green = single-grain OSL determinations. The modelled posterior distributions for the dating determinations and stratigraphic unit boundaries are shown as dark coloured and grey PDFs, respectively. Unmodelled and modelled ages are shown on a calendar year timescale, and both are expressed in years before AD1950. The white circles and associated error bars represent the mean ages and 1σ uncertainty ranges of the PDFs. The 68.3% and 95.4% ranges of the highest posterior probabilities are indicated by the horizontal bars underneath the PDFs. The light yellow rectangles highlight the 95.4% interval that the model returns for the end of the Middle Palaeolithic at the site.
Fig O. OxCal plot output for Model III.
The prior age distributions for the dating determinations (likelihoods) are shown as light coloured probability density functions (PDFs): blue = radiocarbon determinations; green = single-grain OSL determinations. The modelled posterior distributions for the dating determinations and stratigraphic unit boundaries are shown as dark coloured and grey PDFs, respectively. Unmodelled and modelled ages are shown on a calendar year timescale, and both are expressed in years before AD1950. The white circles and associated error bars represent the mean ages and 1σ uncertainty ranges of the PDFs. The 68.3% and 95.4% ranges of the highest posterior probabilities are indicated by the horizontal bars underneath the PDFs. The light yellow rectangles highlight the 95.4% interval that the model returns for the end of the Middle Palaeolithic at the site.
Table J. Summary of the different priors and likelihoods used to construct Bayesian Models I-V. The individual units, stratigraphic groupings, radiocarbon determinations and OSL determinations included in each model are shown, together with any additional constraints used to account for methodological or stratigraphic complications with individual likelihoods (see main text for further details). The 95.4% calibrated age ranges of the radiocarbon determinations and the ±2σ age ranges of the OSL determinations are shown for reference.

| Model I | Model II | Model III | Model IV | Model V |
|---------|----------|-----------|----------|---------|
| Unit | Sample | age (-2σ) (+2σ) | Unit | Sample | age (-2σ) (+2σ) | Unit | Sample | age (-2σ) (+2σ) | Unit | Sample | age (-2σ) (+2σ) |
| Fa-Fc | OxA-1938 | 23874 25178 | Fa-Fc | OxA-1938 | 23874 25178 | Fa-Fc | OxA-1938 | 23874 25178 | Fa-Fc | OxA-1938 | 23874 25178 |
| OxA-2510 | 22360 23111 | OxA-2510 | 22360 23111 | OxA-2510 | 22360 23111 | OxA-2510 | 22360 23111 | OxA-2510 | 22360 23111 |
| H | OxA-X-2786-13 | 23036 23759 | H | OxA-X-2786-13 | 23036 23759 | H | OxA-X-2786-13 | 23036 23759 | H | OxA-X-2786-13 | 23036 23759 |
| OxA-1939 | 23234 24603 | OxA-1939 | 23234 24603 | OxA-1939 | 23234 24603 | OxA-1939 | 23234 24603 | OxA-1939 | 23234 24603 |
| OxA-2511 | 23922 25331 | OxA-2511 | 23922 25331 | OxA-2511 | 23922 25331 | OxA-2511 | 23922 25331 | OxA-2511 | 23922 25331 |
| I | OxA-1940 | 26379 27789 | I-Ja | OxA-1940 | 26379 27789 | I-Ja | OxA-1940 | 26379 27789 | I-Ja | OxA-1940 | 26379 27789 |
| Ja | MAMS-38337 | 27816 27343 | MAMS-38337 | 27816 27343 | MAMS-38337 | 27816 27343 | MAMS-38337 | 27816 27343 | MAMS-38337 | 27816 27343 |
| Jb | OxA-22299 | 28659 29160 | Jb | OxA-22299 | 28659 29160 | Jb | OxA-22299 | 28659 29160 | Jb | OxA-22299 | 28659 29160 |
| OxA-22300 | 28786 29447 | OxA-22300 | 28786 29447 | OxA-22300 | 28786 29447 | OxA-22300 | 28786 29447 | OxA-22300 | 28786 29447 |
| OxA-5542 | 29696 31038 | OxA-5542 | 29696 31038 | OxA-5542 | 29696 31038 | OxA-5542 | 29696 31038 | OxA-5542 | 29696 31038 |
| K | OxA-22020 | 30346 31272 | K | OxA-22020 | 30346 31272 | K | OxA-22020 | 30346 31272 | K | OxA-22020 | 30346 31272 |
| OxA-1941 | 30446 33311 | OxA-1941 | 30446 33311 | OxA-1941 | 30446 33311 | OxA-1941 | 30446 33311 | OxA-1941 | 30446 33311 |
| CLD-17 | 32100 43300 | CLD-17-1 | 32100 43300 | CLD-17-1 | 32100 43300 | CLD-17-1 | 32100 43300 | CLD-17-1 | 32100 43300 |
| VERA-5454 | 31481 32893 | VERA-5454 | 31481 32893 | VERA-5454 | 31481 32893 | VERA-5454 | 31481 32893 | VERA-5454 | 31481 32893 |
| OxA-22301 | 40916 41682 | OxA-22301 | 40916 41682 | OxA-22301 | 40916 41682 | OxA-22301 | 40916 41682 | OxA-22301 | 40916 41682 |
| L | MAMS-41872 | 31721 32903 | L-N | MAMS-41872 | 31721 32903 | L-N | MAMS-41872 | 31721 32903 | L-N | MAMS-41872 | 31721 32903 |
| CLD-17 | 35000 44200 | CLD-17-2 | 35000 44200 | CLD-17-2 | 35000 44200 | CLD-17-2 | 35000 44200 | CLD-17-2 | 35000 44200 |
| MAMS-41871 | 40868 42028 | MAMS-41871 | 40868 42028 | MAMS-41871 | 40868 42028 | MAMS-41871 | 40868 42028 | MAMS-41871 | 40868 42028 |
| M | MAMS-33905 | 35844 36669 | MAMS-33905 | 35844 36669 | MAMS-33905 | 35844 36669 | MAMS-33905 | 35844 36669 | MAMS-33905 | 35844 36669 |
| CLD-17-3 | 42500 33300 | CLD-17-3 | 42500 33300 | CLD-17-3 | 42500 33300 | CLD-17-3 | 42500 33300 | CLD-17-3 | 42500 33300 |
| N | CLD-17-4 | 47000 37000 | CLD-17-4 | 47000 37000 | CLD-17-4 | 47000 37000 | CLD-17-4 | 47000 37000 | CLD-17-4 | 47000 37000 |
| O | CLD-17-5 | 66000 50800 | CLD-17-5 | 66000 50800 | CLD-17-5 | 66000 50800 | CLD-17-5 | 66000 50800 | CLD-17-5 | 66000 50800 |

minimum age ('Before' command)
maximum age ('After' command)
Table K. Summary of Bayesian modelling results for Model I. The likelihood (unmodelled) and posterior (modelled) age ranges are presented for each of the numerical dating samples. Posterior (modelled) ranges are also shown for the boundaries and age of each stratigraphic layer. Posterior ages are presented as the 68.3% and 95.4% highest probability density ranges. The mean and 1σ uncertainty ranges of the modelled posterior distributions are shown for comparison (assuming a normally distributed probability density function). The unmodelled and modelled age estimates have been rounded to the nearest 10 years.

| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Mean ± 1σ | Modelled age (years) | Mean ± 1σ | Agreement index (A) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|-------------------------|-----------|----------------------|-----------|------------------------|-------------------------------|------------------------|
| Layer Fa-Fc age (a)       |               | 23030 – 22370           | 23390     | 21260                | 22540 ± 540| 99.9                   |                               |                        |
| Boundary Layer Fa-Fc top  |               | 22930 – 22300           | 23110     | 20140                | 22130 ± 780| 99.6                   |                               |                        |
| 14C OxA-1938 (b)          |               | 24940 – 24200           | 25260     | 23830                | 24580 ± 470| 102.6                  | 2.4                           | 99.9                   |
| 14C OxA-2510              |               | 22910 – 22520           | 23080     | 22350                | 22700 ± 230| 105.9                  | 1.3                           | 99.9                   |
| Boundary Layer Fa-Fc bottom|               | 23170 – 22630           | 23510     | 22450                | 22940 ± 290| 99.9                   |                               |                        |
| Layer H age (a)           |               | 24490 – 23460           | 25300     | 23060                | 24090 ± 570| 100                    |                               |                        |
| Boundary Layer H top      |               | 23660 – 23130           | 23790     | 22730                | 23350 ± 290| 100                    |                               |                        |
| 14C OxA-2511              |               | 24240 – 23730           | 24570     | 23360                | 23970 ± 290| 112.6                  | 0.8                           | 100                    |
| Boundary Layer H bottom   |               | 25230 – 24140           | 26190     | 23840                | 24840 ± 600| 99.8                   |                               |                        |
| Layer I age (a)           |               | 27270 – 26360           | 27550     | 25490                | 26650 ± 530| 99.9                   |                               |                        |
| Boundary Layer I top      |               | 27160 – 25880           | 27370     | 24750                | 26250 ± 690| 99.8                   |                               |                        |
| 14C OxA-1939              |               | 27240 – 26440           | 27500     | 26090                | 26820 ± 370| 90.9                   | 2.4                           | 100                    |
| Boundary Layer I bottom   |               | 27440 – 26730           | 27690     | 26380                | 27040 ± 370| 99.9                   |                               |                        |
| Layer Ja age (a)          |               | 278050 – 27350          | 29060     | 27050                | 27850 ± 480| 99.9                   |                               |                        |
| Boundary Layer Ja top     |               | 27710 – 27260           | 27820     | 26270                | 27410 ± 310| 99.9                   |                               |                        |
| 14C MAMS-38337            |               | 27790 – 27530           | 27860     | 27340                | 27650 ± 210| 105.2                  | 2.2                           | 100                    |
| Boundary Layer Ja bottom  |               | 28570 – 27490           | 29640     | 27420                | 28290 ± 630| 99.8                   |                               |                        |
| Layer Jb age (a)          |               | 30140 – 29880           | 30490     | 29550                | 30010 ± 210| 99.9                   |                               |                        |
| Boundary Layer Jb top     |               | 30030 – 29780           | 30090     | 29240                | 29800 ± 260| 99.8                   |                               |                        |
| 14C OxA-22299             |               | 30040 – 29920           | 30100     | 29790                | 29960 ± 80 | 118.3                  | 0.4                           | 99.9                   |
| 14C OxA-5542              |               | 30150 – 29930           | 30440     | 29800                | 30070 ± 150| 102.5                  | 0.7                           | 99.9                   |
| 14C OxA-22300             |               | 30080 – 29960           | 30170     | 29900                | 30030 ± 70 | 113.4                  | 0.2                           | 100                    |
| Boundary Layer Jb bottom  |               | 30270 – 29980           | 30690     | 29930                | 30210 ± 210| 99.7                   |                               |                        |
| Layer K age (a)           |               | 32220 – 30890           | 33570     | 30390                | 31800 ± 860| 99.9                   |                               |                        |
| Boundary Layer K top      |               | 31100 – 30460           | 31480     | 30090                | 30790 ± 350| 100                    |                               |                        |
| 14C OxA-22301 (b)         |               | 42210 – 41980           | 42310     | 41850                | 42090 ± 120| 102.7                  | 2.3                           | 99.9                   |
| Unit / boundary parameter | Dating sample | 68.3% range | Unmodelled age (years) | 95.4% range | Mean ± 1σ | 68.3% range | Modelled age (years) | 95.4% range | Mean ± 1σ | Mean ± 1σ | Agreement index (A_i) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|-------------|------------------------|-------------|----------|-------------|---------------------|-------------|----------|-----------|------------------------|-------------------------------|---------------------|
| Boundary Layer K bottom   | 14C VERA-5454 | 32230 – 31610 | 32910 – 31490 | 32060 ± 370 | 32110 – 31600 | 32790 – 31300 | 31910 ± 340 | 108.2 | 1.6 | 99.9 |                     |                               |                     |
| Boundary Layer L top      | 14C OxA-1941  | 32770 – 31090 | 33600 – 30790 | 31940 ± 720 | 31970 – 31130 | 32920 – 30890 | 31720 ± 520 | 122.2 | 1.1 | 99.9 |                     |                               |                     |
| Boundary Layer N bottom   | SG-OSL CLD17-1 | 40570 – 34790 | 43300 – 32070 | 37680 ± 2810 | 32550 – 30980 | 34070 – 30500 | 32060 ± 960 | 21.8 | 10.3 | 99.9 |                     |                               |                     |
| Boundary Layer M bottom   | 14C OxA-22020 | 31180 – 30800 | 31300 – 30350 | 30930 ± 240 | 31220 – 30860 | 31690 – 30490 | 31110 ± 310 | 103.4 | 4.1 | 100 |                     |                               |                     |
| Boundary Layer L bottom   | 14C MAMS-41871 | 41800 – 41200 | 42040 – 40910 | 41480 ± 290 | 36040 – 33880 | 41870 – 32640 | 35680 ± 2140 | 14 | 90.5 | 84.5 |                     |                               |                     |
| Boundary Layer M top      | 14C MAMS-33905 | 36410 – 36090 | 36690 – 35860 | 36250 ± 190 | 36580 – 36040 | 34330 – 35690 | 37240 ± 2060 | 81.9 | 20.9 | 98 |                     |                               |                     |
| Boundary Layer M bottom   | SG-OSL CLD17-3 | 40180 – 35530 | 42370 – 33340 | 37860 ± 2260 | 37670 – 35680 | 43220 – 35290 | 37500 ± 2030 | 108.5 | 3.4 | 94.4 |                     |                               |                     |
| Boundary Layer N top      | SG-OSL CLD17-4 | 44530 – 39290 | 47000 – 36820 | 41910 ± 2540 | 44630 – 39260 | 46610 – 37020 | 41980 ± 2540 | 100.7 | 3.6 | 93.5 |                     |                               |                     |
| Boundary Layer N bottom   | SG-OSL CLD17-5 | 62160 – 54460 | 65860 – 50760 | 58310 ± 3780 | 55840 – 44280 | 59030 – 38010 | 49170 ± 5340 | 34.4 | 33.2 | 98.1 |                     |                               |                     |

(a) Modelled age ranges of individual layers have been calculated from the posterior probabilities of the upper and lower (top and bottom) boundaries of each stratigraphic layer using the `date` query function in OxCal v4.4.
(b) Modelled as a maximum age estimate using the `After` command in OxCal v4.4.
(c) Modelled as a minimum age estimate using the `Before` command in OxCal v4.4.

\[ A_{\text{model}} = 26.1 \]
\[ A_{\text{overall}} = 35.2 \]
Table L. Summary of Bayesian modelling results for Model II. The likelihood (unmodelled) and posterior (modelled) age ranges are presented for each of the numerical dating samples. Posterior (modelled) ranges are also shown for the boundaries and age of each stratigraphic layer. Posterior ages are presented as the 68.3% and 95.4% highest probability density ranges. The mean and 1σ uncertainty ranges of the modelled posterior distributions are shown for comparison (assuming a normally distributed probability density function). The unmodelled and modelled age estimates have been rounded to the nearest 10 years.

| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index | Posterior outlier probability | Convergence integral |
|---------------------------|---------------|------------------------|----------------------|------------------|-----------------------------|----------------------|
|                           |               | 68.3% range | 95.4% range | Mean ± 1σ | 68.3% range | 95.4% range | Mean ± 1σ | (A) (%) | (%) | (%) | (%) |
| Layer Fa-Fc age (a)       |               | 23060 – 22250 | 22380 – 20870 | 22420 ± 630 | 22290 – 21690 | 22040 – 19660 | 21900 ± 930 | 99.9 | 99.7 | 100 |
| Boundary Layer Fa-Fc top  |               | 24940 – 24200 | 25220 – 23860 | 24570 ± 430 | 24490 – 24200 | 25220 – 23860 | 24570 ± 430 | 100.2 | 4.8 | 99.9 |
| 14C OxA-1938 (b)          |               | 22940 – 22540 | 23140 – 22360 | 22750 ± 210 | 22880 – 22490 | 23060 – 22350 | 22690 ± 220 | 102.5 | 4.5 | 100 |
| Boundary Layer Fa-Fc bottom|             | 23060 – 22490 | 23140 – 22360 | 22750 ± 210 | 22880 – 22490 | 23060 – 22350 | 22690 ± 220 | 102.5 | 4.5 | 100 |
| Layer H age (a)           |               | 24520 – 23460 | 25420 – 23050 | 24130 ± 600 | 24270 – 23440 | 24640 – 23240 | 23960 ± 340 | 99.9 | 100 | 100 |
| Boundary Layer H top      |               | 23180 – 22640 | 23520 – 22460 | 22950 ± 290 | 23060 – 22480 | 22840 – 22350 | 22690 ± 220 | 102.5 | 4.5 | 100 |
| Boundary Layer H bottom   |               | 23180 – 22640 | 23520 – 22460 | 22950 ± 290 | 23060 – 22480 | 22840 – 22350 | 22690 ± 220 | 102.5 | 4.5 | 100 |
| Layer I-Ja age (a)        |               | 24520 – 23460 | 25420 – 23050 | 24130 ± 600 | 24270 – 23440 | 24640 – 23240 | 23960 ± 340 | 99.9 | 100 | 100 |
| Boundary Layer I-Ja top   |               | 27050 – 26350 | 27350 – 25900 | 26700 ± 770 | 27140 – 26490 | 27340 – 26050 | 26700 ± 770 | 104.6 | 4.1 | 100 |
| Boundary Layer I-Ja bottom|             | 27050 – 26350 | 27350 – 25900 | 26700 ± 770 | 27140 – 26490 | 27340 – 26050 | 26700 ± 770 | 104.6 | 4.1 | 100 |
| Layer Jb age (a)          |               | 27980 – 26960 | 28950 – 25840 | 27440 ± 670 | 28360 – 27430 | 29580 – 27370 | 28180 ± 620 | 99.9 | 100 | 100 |
| Boundary Layer Jb top     |               | 27980 – 26960 | 28950 – 25840 | 27440 ± 670 | 28360 – 27430 | 29580 – 27370 | 28180 ± 620 | 99.9 | 100 | 100 |
| Boundary Layer Jb bottom  |               | 27050 – 26350 | 27350 – 25900 | 26700 ± 770 | 27140 – 26490 | 27340 – 26050 | 26700 ± 770 | 104.6 | 4.1 | 100 |
| Layer K age (a)           |               | 27050 – 26350 | 27350 – 25900 | 26700 ± 770 | 27140 – 26490 | 27340 – 26050 | 26700 ± 770 | 104.6 | 4.1 | 100 |
| Boundary Layer K top      |               | 27980 – 26960 | 28950 – 25840 | 27440 ± 670 | 28360 – 27430 | 29580 – 27370 | 28180 ± 620 | 99.9 | 100 | 100 |
| Boundary Layer K bottom   |               | 27980 – 26960 | 28950 – 25840 | 27440 ± 670 | 28360 – 27430 | 29580 – 27370 | 28180 ± 620 | 99.9 | 100 | 100 |
| Unit / boundary parameter | Dating sample | Unmodelled age (years) Mean ± 1σ | Modelled age (years) Mean ± 1σ | Agreement index (A) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|--------------------------|--------------|----------------------------------|---------------------------------|------------------------|----------------------------------|------------------------|
| 14C VERA-5454            | 32230 – 31610 32060 ± 370 | 32120 – 31600 31920 ± 340 | 104.9 4.5 100 |
| 14C OxA-1941             | 32770 – 31090 31940 ± 720 | 31990 – 31130 31730 ± 530 | 117.9 4.2 100 |
| SG-OSL CLD17-1           | 40570 – 34790 37680 ± 2810 | 32670 – 31010 32130 ± 940 | 23 5.9 100 |
| 14C OxA-22020            | 31180 – 30800 30930 ± 240  | 31210 – 30870 31090 ± 260 | 101.5 6 100 |
| Boundary Layer K bottom  | 33360 – 31680 31940 ± 1040  | 31990 – 31130 31730 ± 530 | 100.2 4.8 99.9 |
| Layer L-N age (a)        | 41680 – 36180 31940 ± 1040  | 31990 – 31130 31730 ± 530 | 100.2 4.8 99.9 |
| Boundary Layer L-N top   | 36310 – 34540 36560 ± 1130  | 36560 – 32650 35120 ± 1130 | 100.2 4.8 99.9 |
| 14C MAMS-41871           | 41800 – 41200 41480 ± 290 | 41770 – 41150 41420 ± 390 | 99.1 5.1 99.9 |
| SG-OSL CLD17-2           | 41890 – 37220 40020 ± 2270 | 41480 – 37550 39400 ± 1860 | 108.7 4.7 100 |
| 14C MAMS-41872 (c)       | 32780 – 31790 32240 ± 350  | 32780 – 31790 32240 ± 350 | 100.2 4.8 99.9 |
| 14C MAMS-33905           | 36410 – 36090 36250 ± 190 | 36430 – 36090 36350 ± 580 | 97.8 6.2 99.9 |
| SG-OSL CLD17-3           | 40180 – 35530 37860 ± 2260 | 39860 – 36200 38320 ± 1810 | 109.3 4.7 100 |
| SG-OSL CLD17-4           | 44530 – 39290 47000 – 36820 | 44530 – 36540 40660 ± 1920 | 105.7 4.8 100 |
| Boundary Layer L-N bottom| 44200 – 41320 42850 ± 2100 | 43590 ± 2100 | 99.8 |
| Layer O age (a)          | 57200 – 48370 53110 ± 4450 | 57200 – 48370 53110 ± 4450 | 97.2 |
| Boundary Layer O top     | 54840 – 45780 50660 ± 4290 | 54840 – 45780 50660 ± 4290 | 96.6 |
| SG-OSL CLD17-5           | 62160 – 54460 58310 ± 3780 | 57730 – 49880 53780 ± 3970 | 69.4 6.1 99.9 |
| Boundary Layer O bottom  | 59800 – 50270 65380 ± 4900 | 59800 – 50270 65380 ± 4900 | 92.6 |

(a) Modelled age ranges of individual layers have been calculated from the posterior probabilities of the upper and lower (top and bottom) boundaries of each stratigraphic layer using the date query function in OxCal v4.4.

(b) Modelled as a maximum age estimate using the After command in OxCal v4.4.

(c) Modelled as a minimum age estimate using the Before command in OxCal v4.4.

A<sub>model</sub> = 76.3
A<sub>overall</sub> = 77.8
Table M. Summary of Bayesian modelling results for Model III. The likelihood (unmodelled) and posterior (modelled) age ranges are presented for each of the numerical dating samples. Posterior (modelled) ranges are also shown for the boundaries and age of each stratigraphic layer. Posterior ages are presented as the 68.3% and 95.4% highest probability density ranges. The mean and 1σ uncertainty ranges of the modelled posterior distributions are shown for comparison (assuming a normally distributed probability density function). The unmodelled and modelled age estimates have been rounded to the nearest 10 years.

| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index (Ai) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|------------------------|----------------------|-------------------------|---------------------------------|------------------------|
|                            |               | 68.3% range            | 95.4% range          | Mean ± 1σ               |                                  |                        |
| Layer Fa-Fc age (a)        |               |                        |                      |                         |                                 |                        |
| Boundary Layer Fa-Fc top   | 14C OxA-1938  | 24930 – 24210          | 25200 – 23870        | 24570 ± 350            | 100.3                           | 99.9                   |
|                           | 14C OxA-2510  | 22940 – 22540          | 23140 – 22360        | 22750 ± 210            | 102.3                           | 97.4                   |
| Boundary Layer Fa-Fc bottom|               |                        |                      |                         |                                 |                        |
| Layer H age (a)            |               |                        |                      |                         |                                 |                        |
| Boundary Layer H top       |               |                        |                      |                         |                                 |                        |
|                           | 14C OxA-2511  | 25050 – 24320          | 25520 – 23940        | 24710 ± 360            | 85.6                            | 99.9                   |
|                           | 14C OxA-X-2786-13 | 23720 – 23140           | 23760 – 23040        | 23400 ± 210            | 96.7                            | 100                    |
|                           | 14C OxA-1939  | 24270 – 23440          | 24640 – 23240        | 23960 ± 340            | 102.3                           | 100                    |
| Boundary Layer H bottom    |               |                        |                      |                         |                                 |                        |
| Layer I-Ja age (a)         |               |                        |                      |                         |                                 |                        |
| Boundary Layer I-Ja top    |               |                        |                      |                         |                                 |                        |
|                           | 14C OxA-1940  | 27670 – 26550          | 27820 – 26380        | 27140 ± 400            | 104.6                           | 99.9                   |
|                           | 14C MAMS-38337| 27760 – 27470          | 27820 – 27340        | 27600 ± 130            | 99.5                            | 99.9                   |
| Boundary Layer I-Ja bottom |               |                        |                      |                         |                                 |                        |
| Layer Jb age (a)           |               |                        |                      |                         |                                 |                        |
| Boundary Layer Jb top      |               |                        |                      |                         |                                 |                        |
|                           | 14C OxA-22299 | 30030 – 29840          | 30100 – 29620        | 29880 ± 150            | 114.6                           | 100                    |
|                           | 14C OxA-5542  | 30730 – 30030          | 31050 – 29770        | 30360 ± 330            | 99.3                            | 99.9                   |
|                           | 14C OxA-22300 | 30110 – 29970          | 30230 – 29890        | 30050 ± 80             | 107.9                           | 99.9                   |
| Boundary Layer Jb bottom   |               |                        |                      |                         |                                 |                        |
| Layer K age (a)            |               |                        |                      |                         |                                 |                        |
| Boundary Layer K top       |               |                        |                      |                         |                                 |                        |
|                           | 14C OxA-22301 (b) | 42210 – 41990          | 42310 – 41850        | 42090 ± 120            | 100.1                           | 99.8                   |
| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index (\(A_i\)) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|------------------------|---------------------|-------------------------------|----------------------------------|------------------------|
|                           |               | 68.3% range 95.4% range Mean \(\pm 1\sigma\) | 68.3% range 95.4% range Mean \(\pm 1\sigma\) |                               |                                 |                        |
| 14C VERA-5454             |               | 32230 – 31610 32910 – 31490 32060 ± 370 | 32150 – 31610 32820 – 31350 31960 ± 350 | 104.2                         | 4.5                             | 99.3                   |
| 14C OxA-1941              |               | 32770 – 31090 33600 – 30790 31940 ± 720 | 32060 – 31110 33090 – 30880 31790 ± 580 | 114.1                         | 4.3                             | 98.9                   |
| SG-OSL CLD17-1            |               | 40570 – 34790 43300 – 32070 37680 ± 2810 | 33310 – 30900 36260 – 30470 32680 ± 1570 | 34.9                           | 5.7                             | 99.9                   |
| 14C OxA-22020             |               | 31180 – 30800 31300 – 30350 30930 ± 240 | 31200 – 30870 31640 – 30560 31080 ± 260 | 103.3                         | 5.7                             | 99.6                   |
| Boundary Layer K bottom   |               |                        | 34140 – 31620 38040 – 31350 33690 ± 1920 |                                 |                                 |                        |
| Layer L-N age (a)         |               |                        | 42360 – 39600 44570 – 36280 40880 ± 1870 |                                 |                                 |                        |
| Boundary Layer L-N top    |               |                        | 41580 – 37820 41840 – 34490 38850 ± 2120 |                                 |                                 | 92.8                   |
| 14C MAMS-41871            |               | 41800 – 41200 42040 – 40910 41480 ± 290 | 41750 – 41140 42020 – 40810 41420 ± 340 | 99.4                           | 4.7                             | 98.7                   |
| SG-OSL CLD17-2            |               | 41890 – 37220 44090 – 35020 39550 ± 2270 | 42090 – 39620 43110 – 37280 40600 ± 1400 | 110.2                         | 4.7                             | 99.7                   |
| 14C MAMS-41872 (c)        |               | 32780 – 31790 32910 – 31720 32240 ± 350 | 32780 – 31790 32930 – 31710 32240 ± 390 | 100.2                         | 4.8                             | 99.9                   |
| 14C MAMS-33905 (c)        |               | 36410 – 36090 36690 – 35860 36250 ± 190 | 36410 – 36080 36720 – 35830 36250 ± 250 | 100.2                         | 4.8                             | 99.9                   |
| SG-OSL CLD17-3            |               | 40180 – 35530 42370 – 33340 37860 ± 2260 | 42000 – 39220 42700 – 36580 40210 ± 1550 | 76                             | 5                               | 99.7                   |
| SG-OSL CLD17-4            |               | 44530 – 39290 47000 – 36820 41910 ± 2540 | 42340 – 40000 44070 – 38010 41150 ± 1350 | 122.5                         | 4.7                             | 99.8                   |
| Boundary Layer L-N bottom |               |                        | 43260 – 41170 47050 – 40780 42910 ± 1840 |                                 |                                 | 94.8                   |
| Layer O age (a)           |               |                        | 57200 – 48250 61820 – 44130 53010 ± 4510 |                                 |                                 | 98.4                   |
| Boundary Layer O top      |               |                        | 54800 – 45420 58430 – 42060 50450 ± 4400 |                                 |                                 | 97.8                   |
| SG-OSL CLD17-5            |               | 62160 – 54460 65860 – 50760 58310 ± 3780 | 57730 – 49760 61880 – 45640 53740 ± 3990 | 68.9                           | 6                               | 99.9                   |
| Boundary Layer O bottom   |               |                        | 59800 – 50320 65220 – 46250 55570 ± 4930 |                                 |                                 | 94.1                   |

(a) Modelled age ranges of individual layers have been calculated from the posterior probabilities of the upper and lower (top and bottom) boundaries of each stratigraphic layer using the date query function in OxCal v4.4.
(b) Modelled as a maximum age estimate using the After command in OxCal v4.4.
(c) Modelled as a minimum age estimate using the Before command in OxCal v4.4.
Table N. Summary of Bayesian modelling results for Model IV. The likelihood (unmodelled) and posterior (modelled) age ranges are presented for each of the numerical dating samples. Posterior (modelled) ranges are also shown for the boundaries and age of each stratigraphic layer. Posterior ages are presented as the 68.3% and 95.4% highest probability density ranges. The mean and 1σ uncertainty ranges of the modelled posterior distributions are shown for comparison (assuming a normally distributed probability density function). The unmodelled and modelled age estimates have been rounded to the nearest 10 years.

| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index (A) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|------------------------|----------------------|------------------------|-----------------------------------|------------------------|
|                           |               | 68.3% range | 95.4% range | Mean ± 1σ | 68.3% range | 95.4% range | Mean ± 1σ |                           |                         |                      |
| Layer Fa-Fc age (a)       |               | 23050 – 22300 | 23390 – 21030 | 22470 ± 590 | 23050 – 22300 | 23390 – 21030 | 22470 ± 590 | 99.9                   |                         |                      |
| Boundary Layer Fa-Fc top  |               | 22930 – 21830 | 23060 – 19820 | 21990 ± 870 | 22930 – 21830 | 23060 – 19820 | 21990 ± 870 | 99.7                   |                         |                      |
| 14C OxA-1938 (b)          |               | 24930 – 24210 | 25200 – 23870 | 24570 ± 350 | 24940 – 24210 | 25220 – 23860 | 24570 ± 380 | 100.4                  | 4.6                     | 99.9                  |
| 14C OxA-2510              |               | 22940 – 22540 | 23140 – 22360 | 22750 ± 210 | 22890 – 22500 | 23060 – 22350 | 22700 ± 210 | 102.7                  | 4.3                     | 100                   |
| Boundary Layer Fa-Fc bottom |           | 23180 – 22640 | 23510 – 22460 | 22950 ± 280 | 23180 – 22640 | 23510 – 22460 | 22950 ± 280 | 99.9                   |                         |                      |
| Layer H age (a)           |               | 24530 – 23460 | 25450 – 23050 | 24140 ± 610 | 24530 – 23460 | 25450 – 23050 | 24140 ± 610 | 100                    |                         |                      |
| Boundary Layer H top      |               | 23660 – 23140 | 23780 – 22770 | 23340 ± 270 | 23660 – 23140 | 23780 – 22770 | 23340 ± 270 | 100                    |                         |                      |
| 14C OxA-1939              |               | 24270 – 23440 | 24640 – 23240 | 23960 ± 340 | 24240 – 23740 | 24570 – 23370 | 23970 ± 290 | 109.5                  | 4                      | 100                   |
| Boundary Layer H bottom   |               | 25300 – 24140 | 26460 – 23840 | 24930 ± 680 | 25300 – 24140 | 26460 – 23840 | 24930 ± 680 | 99.9                   |                         |                      |
| Layer I-Ja age (a)        |               | 27920 – 27040 | 28840 – 25980 | 27460 ± 610 | 27920 – 27040 | 28840 – 25980 | 27460 ± 610 | 99.9                   |                         |                      |
| Boundary Layer I-Ja top   |               | 27650 – 26590 | 27740 – 25180 | 26810 ± 720 | 27650 – 26590 | 27740 – 25180 | 26810 ± 720 | 99.9                   |                         |                      |
| 14C OxA-1940              |               | 27670 – 26550 | 27820 – 26380 | 27140 ± 400 | 27710 – 27180 | 27840 – 26540 | 27350 ± 320 | 104.6                  | 4.1                     | 99.9                  |
| 14C MAMS-38337            |               | 27760 – 27470 | 27820 – 27340 | 27600 ± 130 | 27730 – 27440 | 27810 – 27330 | 27570 ± 140 | 99.6                   | 4.1                     | 100                   |
| Boundary Layer I-Ja bottom|               | 28260 – 27430 | 29480 – 27350 | 28100 ± 580 | 28260 – 27430 | 29480 – 27350 | 28100 ± 580 | 99.9                   |                         |                      |
| Layer Jb age (a)          |               | 30140 – 29880 | 30480 – 29540 | 30000 ± 210 | 30140 – 29880 | 30480 – 29540 | 30000 ± 210 | 99.9                   |                         |                      |
| Boundary Layer Jb top     |               | 30030 – 29770 | 30090 – 29230 | 29800 ± 270 | 30030 – 29770 | 30090 – 29230 | 29800 ± 270 | 99.8                   |                         |                      |
| 14C OxA-22299             |               | 30030 – 29840 | 30100 – 29520 | 29880 ± 150 | 30040 – 29920 | 30100 – 29790 | 29960 ± 80 | 114.7                  | 3.6                     | 100                   |
| 14C OxA-5542              |               | 30730 – 30030 | 31050 – 29770 | 30360 ± 330 | 30150 – 29930 | 30440 – 29790 | 30070 ± 150 | 99.1                   | 4                     | 99.9                  |
| 14C OxA-22300             |               | 30110 – 29970 | 30230 – 29890 | 30050 ± 80 | 30080 – 29960 | 30170 – 29900 | 30030 ± 70 | 110.1                  | 3.3                     | 100                   |
| Boundary Layer Jb bottom  |               | 30270 – 29980 | 30680 – 29930 | 30210 ± 210 | 30270 – 29980 | 30680 – 29930 | 30210 ± 210 | 99.8                   |                         |                      |
| Layer K age (a)           |               | 32280 – 30860 | 33940 – 30360 | 31880 ± 940 | 32280 – 30860 | 33940 – 30360 | 31880 ± 940 | 100                    |                         |                      |
| Boundary Layer K top      |               | 31100 – 30460 | 31420 – 30090 | 30780 ± 340 | 31100 – 30460 | 31420 – 30090 | 30780 ± 340 | 100                    |                         |                      |
| 14C OxA-22301 (b)         |               | 42210 – 41190 | 42310 – 41850 | 42090 ± 120 | 42210 – 41190 | 42320 – 41830 | 42090 ± 200 | 100.3                  | 4.6                     | 99.9                  |
| Unit / boundary parameter | Dating sample | Unmodelled age (years) | 68.3% range | 95.4% range | Mean ± 1σ | Modelled age (years) | 68.3% range | 95.4% range | Mean ± 1σ | Agreement index (A) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|-----------------------|-------------|-------------|------------|----------------------|-------------|-------------|------------|--------------------------|-------------------------------|--------------------------|
| 14C VERA-6454             |               | 32230 – 31610         | 32910 – 31490 | 32060 ± 370 | 32120 – 31600 | 32800 – 31310 | 31920 ± 340 | 104.7 | 4.6 | 99.9 |
| 14C OxA-1941              |               | 32770 – 31090         | 33600 – 30790 | 31940 ± 720 | 31990 – 31120 | 32970 – 30890 | 31730 ± 530 | 117.6 | 4.2 | 100 |
| SG-OSL CLD17-1            |               | 40570 – 34790         | 43300 – 32070 | 37680 ± 2810 | 32680 – 31000 | 34700 – 30490 | 32190 ± 1060 | 24.7 | 5.9 | 100 |
| 14C OxA-22020             |               | 31180 – 30800         | 31300 – 30350 | 30930 ± 240 | 31210 – 30870 | 31660 – 30580 | 31090 ± 270 | 101.6 | 5.9 | 99.9 |
| Boundary Layer K bottom   |               |                      |             |             |            |                      |             |             |            |                          |                               |                          |
| Layer L age (a)           |               | 33400 – 31660         | 35610 – 31340 | 32980 ± 1200 | 38490 – 34870 | 39890 – 33320 | 36630 ± 1670 | 99.8 |
| Boundary Layer L top      |               | 37310 – 33600         | 38910 – 32200 | 35590 ± 1770 | 38490 – 35290 | 40010 – 33770 | 36890 ± 1550 | 73.4 | 5.2 | 99.9 |
| Boundary Layer L bottom   |               | 39320 – 35990         | 40930 – 34370 | 37660 ± 1640 | 41260 – 37940 | 43040 – 36330 | 39670 ± 1670 | 99.7 |
| Layer M age (a)           |               | 40490 – 37240         | 42150 – 35620 | 38880 ± 1630 | 41120 – 37910 | 42700 – 36400 | 39540 ± 1560 | 97 | 4.8 | 100 |
| Boundary Layer M top      |               |                      |             |             |            |                      |             |             |            |                          |                               |                          |
| Boundary Layer M bottom   |               | 42140 – 38540         | 44110 – 36930 | 40450 ± 1800 | 46000 – 41360 | 49270 – 39400 | 44100 ± 2490 | 99.8 |
| Layer N age (a)           |               | 44300 – 40310         | 46480 – 38520 | 42430 ± 2000 | 44930 – 39710 | 47530 – 39770 | 43600 ± 1950 | 99.1 | 4.9 | 100 |
| Boundary Layer N top      |               |                      |             |             |            |                      |             |             |            |                          |                               |                          |
| Boundary Layer N bottom   |               | 47880 – 42230         | 52290 – 40180 | 45770 ± 3080 | 54540 – 41500 | 47530 – 39770 | 43600 ± 1950 | 99.3 |
| Layer O age (a)           |               | 55990 – 47950         | 60430 – 44400 | 52250 ± 4020 | 54240 – 46370 | 58200 – 43120 | 50620 ± 3880 | 98.6 |
| Boundary Layer O top      |               |                      |             |             |            |                      |             |             |            |                          |                               |                          |
| Boundary Layer O bottom   |               | 56410 – 48550         | 60490 – 45000 | 52660 ± 3830 | 58090 – 49060 | 62690 – 45660 | 53890 ± 4350 | 94.7 |

(a) Modelled age ranges of individual layers have been calculated from the posterior probabilities of the upper and lower (top and bottom) boundaries of each stratigraphic layer using the date function in OxCal v4.4.
(b) Modelled as a maximum age estimate using the After command in OxCal v4.4.
(c) Modelled as a minimum age estimate using the Before command in OxCal v4.4.

\[ A_{\text{model}} = 63.1 \]
\[ A_{\text{overall}} = 65.7 \]
Table O. Summary of Bayesian modelling results for Model V. The likelihood (unmodelled) and posterior (modelled) age ranges are presented for each of the numerical dating samples. Posterior (modelled) ranges are also shown for the boundaries and age of each stratigraphic layer. Posterior ages are presented as the 68.3% and 95.4% highest probability density ranges. The mean and 1σ uncertainty ranges of the modelled posterior distributions are shown for comparison (assuming a normally distributed probability density function). The unmodelled and modelled age estimates have been rounded to the nearest 10 years.

| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index (Ai) (%) | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|------------------------|----------------------|--------------------------|----------------------------------|-------------------------|
|                           |               | 68.3% range            | 95.4% range          | Mean ± 1σ                |                                  |                         |
| Layer Fa-Fc age a          |               | 23050 – 22280          | 23370 – 20880        | 22440 ± 630              |                                  |                         |
| Boundary Layer Fa-Fc top   |               | 22930 – 21760          | 23030 – 19630        | 21930 ± 930              |                                  |                         |
| 14C OxA-1938 b             |               | 24930 – 24210          | 25200 – 23870        | 24570 ± 350              | 100.3                            | 4.7                     |
| 14C OxA-2510               |               | 22940 – 22540          | 23140 – 22360        | 22750 ± 210              | 102.5                            | 4.4                     |
| Boundary Layer Fa-Fc bottom|               | 23170 – 22630          | 23510 – 22450        | 22950 ± 280              |                                  |                         |
| Layer H age a              |               | 24540 – 23450          | 25470 – 23040        | 24140 ± 620              |                                  |                         |
| Boundary Layer H top       |               | 23660 – 23130          | 23780 – 22760        | 23340 ± 280              |                                  |                         |
| 14C OxA-2511               |               | 25050 – 24320          | 25520 – 23940        | 24710 ± 360              | 86.0                             | 5.5                     |
| 14C OxA-X-2786-13          |               | 23720 – 23140          | 23760 – 23040        | 23400 ± 210              | 97.0                             | 6.4                     |
| 14C OxA-1939               |               | 24270 – 23440          | 24640 – 23240        | 23960 ± 340              | 109.3                            | 4.1                     |
| Boundary Layer H bottom    |               | 25310 – 24140          | 26500 – 23850        | 24940 ± 680              |                                  |                         |
| Layer I-Ja age a           |               | 27920 – 27050          | 28820 – 26010        | 27460 ± 600              |                                  |                         |
| Boundary Layer I-Ja top    |               | 27650 – 26610          | 27740 – 25220        | 26820 ± 710              |                                  |                         |
| 14C OxA-1940               |               | 27670 – 26550          | 27820 – 26380        | 27140 ± 400              | 104.6                            | 4.1                     |
| 14C MAMS-38337             |               | 27760 – 27470          | 27820 – 27340        | 27600 ± 130              | 99.6                             | 4.1                     |
| Boundary Layer I-Ja bottom |               | 28250 – 27430          | 29440 – 27350        | 28090 ± 570              |                                  |                         |
| Layer Jb age a             |               | 30150 – 29880          | 30500 – 29520        | 30000 ± 220              |                                  |                         |
| Boundary Layer Jb top      |               | 30030 – 29760          | 30090 – 29180        | 29790 ± 280              |                                  |                         |
| 14C OxA-22299              |               | 30030 – 29840          | 30100 – 29520        | 29880 ± 150              | 114.6                            | 3.7                     |
| 14C OxA-5542               |               | 30730 – 30030          | 31050 – 29770        | 30360 ± 330              | 99.5                             | 4.9                     |
| 14C OxA-22300              |               | 30110 – 29970          | 30230 – 29890        | 30050 ± 80               | 109.7                            | 3.4                     |
| Boundary Layer Jb bottom   |               | 30280 – 29980          | 30690 – 29930        | 30210 ± 210              |                                  |                         |
| Layer K age a              |               | 32420 – 30820          | 34380 – 30360        | 32000 ± 1050             |                                  |                         |
| Boundary Layer K top       |               | 31090 – 30450          | 31390 – 30080        | 30760 ± 330              |                                  |                         |
| 14C OxA-22301 b            |               | 42210 – 41990          | 42310 – 41850        | 42090 ± 120              | 100.5                            | 4.5                     |
| Unit / boundary parameter | Dating sample | Unmodelled age (years) | Modelled age (years) | Agreement index (Ai) (% | Posterior outlier probability (%) | Convergence integral (%) |
|---------------------------|---------------|------------------------|----------------------|-------------------------|---------------------------------|-------------------------|
|                           |               | 68.3% range 95.4% range | Mean ± 1σ           | 68.3% range 95.4% range | Mean ± 1σ                      |                         |
| 14C VERA-5454             | 32230 – 31610 | 32910 – 31490 32060 ± 370 | 32140 – 31600 32810 – 31330 31950 ± 350 | 104.5 4.5 99.9 |                                |                         |
| 14C OxA-1941              | 32770 – 31090 | 33690 – 30790 31940 ± 720 | 32030 – 31120 33040 – 30880 31770 ± 560 | 115.5 4.2 99.9 |                                |                         |
| SG-OSL CLD17-1            | 40570 – 34790 | 43300 – 32070 37680 ± 2810 | 32970 – 30950 35110 – 30560 32380 ± 1190 | 28.4 5.8 100 |                                |                         |
| 14C OxA-22020             | 31180 – 30800 | 31300 – 30350 30930 ± 240 | 31210 – 30870 31650 – 30560 31090 ± 270 | 102.4 5.9 99.9 |                                |                         |
| Boundary Layer K bottom   |               |                        |                      |                         |                                |                         |
|                           |               | 33750 – 31640 36190 – 31390 33240 ± 1340 | 33240 ± 1340 | 99.5 |                                |                         |
| Layer L-N + Unit 5-6 age * |               | 41590 – 37560 43790 – 35480 39620 ± 2090 | 39620 ± 2090 | 99.9 |                                |                         |
| Boundary Layer L-N + Unit 5-6 top | | 37900 – 35780 38640 – 33880 36520 ± 1190 | 36520 ± 1190 | 99.8 |                                |                         |
| 14C MAMS-41874            | 39350 – 38370 | 39520 – 37670 38730 ± 500 | 39350 – 38390 39540 – 37680 38750 ± 510 | 101.7 4.6 99.9 |                                |                         |
| 14C MAMS-41876            | 37690 – 36880 | 38530 – 36550 37430 ± 480 | 38230 – 36960 38950 – 36760 37680 ± 600 | 86 5.2 99.9 |                                |                         |
| 14C MAMS-41871            | 41800 – 41200 | 42040 – 40910 41480 ± 290 | 41740 – 41110 42060 – 40690 41340 ± 510 | 96 6.6 99.9 |                                |                         |
| SG-OSL CLD17-2            | 41890 – 37220 | 44090 – 35020 39550 ± 2270 | 41250 – 37920 42610 – 36490 39550 ± 1570 | 116.4 4.7 100 |                                |                         |
| 14C MAMS-41872 e          | 32780 – 31790 | 32910 – 31720 32240 ± 350 | 32790 – 31790 32930 – 31710 32240 ± 420 | 100.1 4.8 99.8 |                                |                         |
| 14C MAMS-33905 e          | 36410 – 36090 | 36690 – 35860 36250 ± 190 | 36410 – 36090 36710 – 35830 36250 ± 240 | 100.3 4.6 99.9 |                                |                         |
| SG-OSL CLD17-3            | 40180 – 35530 | 42370 – 33340 37860 ± 2260 | 40200 – 37120 41930 – 35900 38820 ± 1520 | 111.1 4.7 100 |                                |                         |
| SG-OSL CLD17-4            | 44530 – 39290 | 47000 – 36820 41910 ± 2540 | 42030 – 38850 43610 – 37070 40430 ± 1630 | 106.3 4.8 100 |                                |                         |
| Boundary Layer L-N + Unit 5-6 bottom | | 43230 – 41210 46900 – 40680 42730 ± 1600 | 42730 ± 1600 | 99.7 |                                |                         |
| Layer O age *             |               |                        |                      |                         |                                |                         |
| Boundary Layer O top      |               |                        |                      |                         |                                |                         |
| SG-OSL CLD17-5            | 62160 – 54460 | 65860 – 50760 58310 ± 3780 | 57350 – 49570 61810 – 45490 53630 ± 4030 | 67.9 6.2 99.9 |                                |                         |
| Boundary Layer O bottom   |               |                        |                      |                         |                                |                         |

(a) Modelled age ranges of individual layers have been calculated from the posterior probabilities of the upper and lower (top and bottom) boundaries of each stratigraphic layer using the date query function in OxCal v4.4.
(b) Modelled as a maximum age estimate using the After command in OxCal v4.4.
(c) Modelled as a minimum age estimate using the Before command in OxCal v4.4.

\[ A_{\text{model}} = 78.5 \]
\[ A_{\text{overall}} = 80.5 \]
Bayesian model CQL code
Model I

Plot()
{
  Outlier_Model("General",T(5),U(0,4),"t");
  Sequence("Gruta do Caldeirão Sequence")
  {
    Boundary("Boundary Layer O bottom");
    Date("SG-OSL CLD17-5", N(2017-58376,3777))
    {
      Outlier("General", 0.05);
      color="green";
    };
    Boundary("Boundary Layer O top");
    Boundary("Boundary Layer N bottom");
    Date("SG-OSL CLD17-4", N(2017-41978,2544))
    {
      Outlier("General", 0.05);
      color="green";
    };
    Boundary("Boundary Layer N top");
    Boundary("Boundary Layer M bottom");
    Phase("Layer M")
    {
      Date("SG-OSL CLD17-3", N(2017-37921,2258))
      {
        Outlier("General", 0.05);
        color="green";
      };
      R_Date("14C MAMS-33905", 31900, 170)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      };
    };
    Boundary("Boundary Layer M top");
    Boundary("Boundary Layer L bottom");
    Phase("Layer L")
    {
      Before()
      {
        R_Date("14C MAMS-41872", 28150, 160)
        {
          Outlier("General", 0.05);
          color="mediumblue";
        };
      };
      Date("SG-OSL CLD17-2", N(2017-39618,2268))
      {
        Outlier("General", 0.05);
        color="green";
      };
      R_Date("14C MAMS-41871", 36490, 390)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      };
    };
    Boundary("Boundary Layer L top");
    Boundary("Boundary Layer K bottom");}
Boundary("Boundary Layer I bottom");
R_Date("14C OxA-1940", 22900, 380)
{
    Outlier("General", 0.05);
    color="mediumblue";
};
Boundary("Boundary Layer I top");
Boundary("Boundary Layer H bottom");
Phase("Layer H")
{
    R_Date("14C OxA-1939", 19900, 260)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    };
    R_Date("14C OxA-X-2786-13", 19400, 150)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    };
    R_Date("14C OxA-2511", 20530, 270)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    };
};
Boundary("Boundary Layer H top");
Boundary("Boundary Layer Fa-Fc bottom");
Phase("Layer Fa-Fc")
{
    R_Date("14C OxA-2510", 18840, 200)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    }; After()
    {
        R_Date("14C OxA-1938", 20400, 270)
        {
            Outlier("General", 0.05);
            color="mediumblue";
        };
    };
};
Boundary("Boundary Layer Fa-Fc top");
Model II

Plot()
{
  Outlier_Model("General", T(5), U(0,4), "t");
  Sequence("Gruta do Caldeirão Sequence")
  {
    Boundary("Boundary Layer O bottom");
    Date("SG-OSL CLD17-5", N(2017-58376,3777))
    {
      Outlier("General", 0.05);
      color="green";
    }
    Boundary("Boundary Layer O top");
    Boundary("Boundary Layer L-N bottom");
    Phase("Layer L-N")
    {
      Date("SG-OSL CLD17-4", N(2017-41978,2544))
      {
        Outlier("General", 0.05);
        color="green";
      }
      Date("SG-OSL CLD17-3", N(2017-37921,2258))
      {
        Outlier("General", 0.05);
        color="green";
      }
      R_Date("14C MAMS-33905", 31900, 170)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      }
      Before()
      {
        R_Date("14C MAMS-41872", 28150, 160)
        {
          Outlier("General", 0.05);
          color="mediumblue";
        }
      }
      Date("SG-OSL CLD17-2", N(2017-39618,2268))
      {
        Outlier("General", 0.05);
        color="green";
      }
      R_Date("14C MAMS-41871", 36490, 390)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      }
    }
    Boundary("Boundary Layer L-N top");
    Boundary("Boundary Layer K bottom");
    Phase("Layer K")
    {
      R_Date("14C OxA-22020", 26790, 260)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      }
    }
  }
}
Model III

Plot()
{
  Outlier_Model("General",T(5),U(0,4),"t");
  Sequence("Gruta do Caldeirão Sequence")
  {
    Boundary("Boundary Layer O bottom");
    Date("SG-OSL CLD17-5", N(2017-58376,3777))
    {
      Outlier("General", 0.05);
      color="green";
    };
    Boundary("Boundary Layer O top");
    Boundary("Boundary Layer L-N bottom");
    Phase("Layer L-N")
    {
      Date("SG-OSL CLD17-4", N(2017-41978,2544))
      {
        Outlier("General", 0.05);
        color="green";
      };
      Date("SG-OSL CLD17-3", N(2017-37921,2258))
      {
        Outlier("General", 0.05);
        color="green";
      };
      Before()
      {
        R_Date("14C MAMS-33905", 31900, 170)
        {
          Outlier("General", 0.05);
          color="mediumblue";
        };
      };
      Before()
      {
        R_Date("14C MAMS-41872", 28150, 160)
        {
          Outlier("General", 0.05);
          color="mediumblue";
        };
      };
      Date("SG-OSL CLD17-2", N(2017-39618,2268))
      {
        Outlier("General", 0.05);
        color="green";
      };
      R_Date("14C MAMS-41871", 36490, 390)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      };
    };
    Boundary("Boundary Layer L-N top");
    Boundary("Boundary Layer K bottom");
    Phase("Layer K")
    {
      R_Date("14C OxA-22020", 26790, 260)
Boundary("Boundary Layer I-Ja top");
Boundary("Boundary Layer H bottom");
Phase("Layer H")
{
    R_Date("14C OxA-1939", 19900, 260)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    }
    R_Date("14C OxA-X-2786-13", 19400, 150)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    }
    R_Date("14C OxA-2511", 20530, 270)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    }
    Boundary("Boundary Layer H top");
}
Boundary("Boundary Layer Fa-Fc bottom");
Phase("Layer Fa-Fc")
{
    R_Date("14C OxA-2510", 18840, 200)
    {
        Outlier("General", 0.05);
        color="mediumblue";
    }
    After()
    {
        R_Date("14C OxA-1938", 20400, 270)
        {
            Outlier("General", 0.05);
            color="mediumblue";
        }
    }
    Boundary("Boundary Layer Fa-Fc top");
}
Model IV

Plot()
{
    Outlier_Model("General",T(5),U(0,4),"t");
    Sequence("Gruta do Caldeirão Sequence")
    {
        Boundary("Boundary Layer O bottom");
        Date("SG-OSL CLD17-5", N(2017-58376,3777))
        {
            Outlier("General", 0.05);
            color="green";
        }
        Boundary("Boundary Layer O top");
        Boundary("Boundary Layer N bottom");
        Date("SG-OSL CLD17-4", N(2017-41978,2544))
        {
            Outlier("General", 0.05);
            color="green";
        }
        Boundary("Boundary Layer N top");
        Boundary("Boundary Layer M bottom");
        Date("SG-OSL CLD17-3", N(2017-37921,2258))
        {
            Outlier("General", 0.05);
            color="green";
        }
        Boundary("Boundary Layer M top");
        Boundary("Boundary Layer L bottom");
        Date("SG-OSL CLD17-2", N(2017-39618,2268))
        {
            Outlier("General", 0.05);
            color="green";
        }
        Boundary("Boundary Layer L top");
        Boundary("Boundary Layer K bottom");
        Phase("Layer K")
        {
            R_Date("14C OxA-22020", 26790, 260)
            {
                Outlier("General", 0.05);
                color="mediumblue";
            }
            Date("SG-OSL CLD17-1", N(2017-37747,2808))
            {
                Outlier("General", 0.05);
                color="green";
            }
            R_Date("14C OxA-1941", 27600, 600)
            {
                Outlier("General", 0.05);
                color="mediumblue";
            }
            R_Date("14C VERA-5454", 28000, 210)
            {
                Outlier("General", 0.05);
                color="mediumblue";
            }
        }
    }
    After()
Model V

Plot()
{
  Outlier_Model("General",T(5),U(0,4),"t");
Sequence("Gruta do Caldeirão Sequence")
{
  Boundary("Boundary Layer O bottom");
  Date("SG-OSL CLD17-5", N(2017-58376,3777))
  {
    Outlier("General", 0.05);
    color="green";
  }
  Boundary("Boundary Layer O top");
  Boundary("Boundary Layer L-N + Unit 5-6 bottom");
  Phase("Layer L-N + Unit 5-6")
  {
    Date("SG-OSL CLD17-4", N(2017-41978,2544))
    {
      Outlier("General", 0.05);
      color="green";
    }
    Date("SG-OSL CLD17-3", N(2017-37921,2258))
    {
      Outlier("General", 0.05);
      color="green";
    }
    Before()
    {
      R_Date("14C MAMS-33905", 31900, 170)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      }
    }
    Before()
    {
      R_Date("14C MAMS-41872", 28150, 160)
      {
        Outlier("General", 0.05);
        color="mediumblue";
      }
    }
    Date("SG-OSL CLD17-2", N(2017-39618,2268))
    {
      Outlier("General", 0.05);
      color="green";
    }
    R_Date("14C MAMS-41871", 36490, 260)
    {
      Outlier("General", 0.05);
      color="mediumblue";
    }
    R_Date("14C MAMS-41876", 32890, 260)
    {
      Outlier("General", 0.05);
      color="mediumblue";
    }
    R_Date("14C MAMS-41874", 33810, 290)
}
