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| --- | --- | --- | --- |
| Summary of baseline conditions for primary LMC to second LMC recrystallization in phreatic meteoric zone | | | |
| Notation | Definition | Value | Reference and Note |
| *Cf* | Mass of element in fluid (mol/kg) | C = 0.0012 | Ref. (*1*) |
| O = 55.6 | Based on stoichiometry of water |
| *Ms* | Mass of element in primary calcite (ug/g) | C = 1.2e5 | Based on stoichiometry of calcite |
| O = 4.8e5 |
| *δs* | Isotopic value of primary calcite (‰ PDB) | δ13C = 3 | For pre-CIE; Ref. (*2*) |
| δ18O = 0.5 |
| δ13C = -4.5 | For CIE; The upper limited of the lowest carbonate values in primary calcite during the PETM based on model's estimated |
| δ18O = -1 |
| *δf* | Isotopic value of Fluid (‰ PDB) | δ13C = -14 | Ref. (*3, 4*) |
| δ18O = -46 | For pre-CIE; Based on lowest δ18O value in samples at the bottom of Tingri section; |
| δ13C = -14 | Ref. (*3, 4*) |
| δ18O = -47.5 | For CIE, Assume constant difference between primary calcite and meteoric diagenesis in Pre-CIE and the CIE |
| *α* | Isotopic fractionation factor for diagenesis (‰) | α13C = 0.9988 | Ref. (*5*) |
| α18O = 1.031 | Ref. (*6*) |
| *V* | Box volume (m3) | 1 | Ref. (*7*) |
| *ρs* | Density of solid (g/cm3) | 1.8 | Ref. (*7*) |
| *ρf* | Density of fluid (g/cm3) | 1 | Freshwater |
| *n* | Specific box number | 50 | Ref. (*7*) |
| *Kd,u* | Exchange reaction distribution coefficient of U relative to Ca | 0.06 | Ref. (*8*) |
| *Φ* | Porosity | 0.3 | Ref. (*3, 9*) |
| *μ* | Vertical flow rate (m/yr) | 1 | For the top (or first) box; Ref. (*9, 10*) |
| 0.1 | For the bottom (or last) box |
| *R* | Reactive rate (yr-1) | 1.00E-05 | For the top (or first) box; Ref. (*3, 11*) |
| 2.00E-06 | For the bottom (or last) box |

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