|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | A1 | A2 | A3 | A4 | A5 |
| Model Type (RE) | Linear | Linear | Mixed (2) | Mixed (2) | Mixed (2) |
| Samples | 51 | 51 | 51 | 51 | 51 |
| a (SE) | -2.20×10−1 | -2.01 (1.49×10−1) | -1.59×101 (4.00) | -2.37 (2.44×10−1) | -2.26 (2.38×10−1) |
| t/p | - | -13.44, <2.22× 10−16 | -3.97, 1.04×10−1 | -9.69, 8.64×10−5 | -9.49, 2.00×10−1 |
| b (SE) | 7.21 | 6.80× 10−3 (3.97× 10−4) | 2.56×10−2 (5.36×10−3) | 7.86×10−3  (6.66×10−4) | 7.53×10−3 (6.06×10−4) |
| t/p | - | 17.13, <2.22× 10−16 | 4.77, 6.37×10−2 | 11.80, 2.03×10−5 | 12.42, 1.01×10−4 |
| c (SE) | - | - | 2.56×103 (7.41×102) | - | - |
| t/p | - | - | 3.45, 1.41×10−1 | - | - |
| ^Field I.(G.) | - | - | 0.00 | 3.57×10−2 | 1.93×10−1 (4.63×10−4) |
| ^Formation I.(G.) | - | - | 2.76×10−2 | 5.91×10−2 | 8.64×10−2 (1.23×10−4) |
| Residual | - | - | 7.21×10−2 | 7.77×10−2 | 7.76×10−2 |
| #ICC | - | - | - | 0.441 | - |
| \*R2 m/c & a | 0.94 | 0.86 | 0.87/0.88 | 0.83/0.90 | 0.85/0.89 |
| pKsp°−dol 25°C | -16.92 |  -16.98 | -17.25 | -16.98 | -16.94 |
| †CI 25°C l/u (dif) | - | -16.92/-17.05 (0.13) | -17.48/-17.03 (0.45) | -17.15/-16.76 (0.39) | -17.15/-16.73 (0.42) |
| pKsp°−dol 200°C | -23.32 | -23.31 | -23.69 | -23.45 | -23.40 |
| CI 200°C l/u (dif) | - | -23.23/-23.40 (0.17) | -23.95/-23.43 (0.52) | -23.55/-23.15 (0.39) | -23.60/-23.19 (0.41) |
| AIC | - | -107.1 | -107.4 | -84.4 | -77.1 |

Supplementary Table. 6. For each coefficient estimate (e.g. ‘a’); (SE) represents the standard error associated with the estimate. For each coefficient the ‘t/p’ represents; ‘t’ – the t-test associated with the significance of the coefficient estimate and ‘p’ – the p-value for that t-test. # The intraclass correlation coefficient (ICC) reports the adjusted and conditional ICC. Both ICC values account for all sources of uncertainty but the conditional ICC differs from the adjusted ICC by incorporating the variance associated with the fixed effects; as is common practice we report only the adjusted value. At small sample sizes, using mixed models suffering from singularity in regression analysis, ICC sometimes fails to report. \*Reported R2 values are the marginal (m) and conditional (c) R2 values for mixed models and the adjusted (a) R2 for linear models. †The lower (l) and upper (u) confidence intervals (CI) are accompanied by a calculation of the difference between them (dif).^For each random effect usually only the $log\_{10}(/) $intercept ‘I.’ is reported; these are termed random intercept models and the most common type of model used by this study. For random slope models both the intercept ‘I.’ and also the gradient for the increase in $log\_{10}(/) $with temperature ‘(G.)’ are reported. If a random effect is implemented it is reported; in some cases, e.g. Field for M2, a random effect has zero effect but is still reported as 0.00. For clarity and convenience the total number of random effects ‘(RE)’ implemented is reported in the brackets for the Model Type. Unless otherwise stated models use a 2,3 or 4 term formulation of the Maier-Kelly regression formulae eq (25) with the total number of terms used reflected by the number of coefficients (a, b, c and d) reported. A1. Original Hyeong and Capuano (2001) model for Hyeong and Capuano (2001) dataset. Activities calculated by SOLMNEQ88-Pitzer and fit to eq (28) (note equation is in celsius-see text). A2. Linear model of the Hyeong and Capuano (2001) dataset with activities calculated using PHREEQC-Pitzer. A3. Three term (fixed effect) mixed model of Hyeong and Capuano (2001) dataset. The model incorporates the field and formation attributes as random effects. This three-term model produces a clearly spurious fit (fig. 5a). A4. Two term (fixed effect) mixed model of Hyeong and Capuano (2001) dataset. A5. A random slope (all others are random intercept) mixed model of the Hyeong and Capuano (2001) dataset.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | B1 | C1 | D1 | E1 | F1 |
| Model Type | Linear | Linear | Linear | Linear | Mixed (1) |
| Samples | 35 | 16 | 45 | 6 | 21 |
| a (SE) | -2.75 (3.56×10−1) | -1.03 (2.81×10−1) | -2.28 (1.96×10−1) | -5.06×10−2 (1.81) | -2.11 (1.55) |
| t/p | -7.73, 6.62×10−9 | -3.65, 2.65×10−3 | -11.65, 6.84×10−15 | -2.79×10−2, 9.79×10−1 | -1.36, 0.21 |
| b (SE) | 8.69×10−3 (9.08×10−4) | 3.94×10−3 (8.30×10−4) | 7.51×10−3 (5.13×10−4) | 9.17×10−4 (5.60×10−3) | 7.09×10−3 (4.29×10−3) |
| t/p | 9.57, 4.82×10−11 | 4.75, 3.11×10−4 | 14.65, 2.22×10−16 | 1.64×10−1, 8.78×10−1 | 1.65, 1.37×10−1 |
| Field I.(G.) | - | - | - | - | 8.02×10−2 |
| Formation I.(G.) | - | - | - | - | - |
| Residual | 8.65×10−2 | 4.05×10−2 | 8.01×10−2 | 6.40×10−2 | 3.43×10−1 |
| ICC | - | - | - | - | - |
| R2 m/c & a | 0.74/0.73 | 0.62/0.59 | 0.83/0.83 | 6.66×10−3/-0.24 | 0.13/0.18 |
| pKsp°−dol 25 °C | -16.80 | -17.11 | -16.92 | -17.18 | -16.97 |
| CI 25°C l/u (dif) | -16.63/-16.98 (0.35) | -17.04/17.19 (0.15) | -16.83/17.01 (0.18) | -16.73/-17.59 (0.82) | -16.03/-17.90 (1.87) |
| pKsp°−dol 200 °C | -23.46 | -22.94 | -23.37 | -22.48 | -23.35 |
| CI 200°C l/u (dif) | -23.31/-23.61 (0.31) | -22.70/-23.18 (0.48) | -23.27/-23.47 (0.20) | -20.16/-24.80 (4.64) | -22.12/-24.57 (2.45) |
| AIC | - | - | - | - | - |

B1. Model of the Chocolate/Halls Bayou subset from the Hyeong and Capuano (2001) dataset. C1. Model of the West Columbia subset from the Hyeong and Capuano (2001) dataset. D1. Model of the Frio Fm. subset from the Hyeong and Capuano (2001) dataset. E1. Model of the Miocene Fm. subset from the Hyeong and Capuano (2001) dataset. F1. Model of PWGD samples contained within Test Area A (all samples are from the Frio Fm.).

|  |  |  |  |
| --- | --- | --- | --- |
| Model | G1 | H1 | I1 |
| Model Type | Mixed (2) | Linear | Mixed (2) |
| Samples | 117 | 16 | 204 |
| a (SE) | -8.20×10−1 (1.01) | 4.02×10−2 (9.24×10−1) | -8.09×10−1 (3.04×10−1) |
| t/p | -8.08×10−1, 4.21×10−1 | 4.35×10−2, 9.66×10−1 | -2.66 (9.33×10−3) |
| b (SE) | 4.36×10−3 (2.84×10−3) | 1.75×10−3 (2.49×10−3) | 4.00×10−3 (8.50×10−4) |
| t/p | 1.54, 1.28×10−1 | 7.05×10−1, 4.92×10−1 | 4.71, 9.26×10−6 |
| Field I.(G.) | 2.63×10−1 | - | 1.69×10−1 |
| Formation I.(G.) | -  | - | 1.31×10−1 |
| Residual | 3.77×10−1 | 1.80×10−1 | 1.82×10−1 |
| ICC | 0.328 | - | 0.579 |
| R2 m/c & a | 0.02/0.34 | -0.03 | 0.19/0.66 |
| pKsp°−dol 25 °C | -17.44 | -17.52 | -17.34 |
| CI 25°C l/u (dif) | -16.61/-18.27 (1.67) | -17.92/-17.12 (0.80) | -16.96/-17.73 (0.77) |
| pKsp°−dol 200 °C | -23.34 | -22.97 | -23.18 |
| CI 200°C l/u (dif) | -22.35/-24.33 (1.98) | -22.41/-23.52 (1.11) | -22.76/-23.60 (0.84) |
| AIC | - | - |  - |

G1. Model of all Frio Fm. samples present in PWGD. H1. Model of the Kharaka and others (1987) dataset. I1. Model of all PWGD samples contained within Test Area B.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | J1 | J2 – n=(8201) | J3 – 10m (n=6217)  | J4 – 50m (n=4574) | J5 - 100m (n=3985) |
| Model Type | Linear | Mixed (1) | Mixed (1) | Mixed (1) | Mixed (1) |
| Samples | 10343 | 10343 | 10343 | 10343 | 10343 |
| a (SE) | -3.76 (4.87×10−1) | -3.64 (5.58×10−1) | -3.62 (5.97×10−1) | -3.65 (6.34×10−1) | -3.58 (6.48×10−1) |
| t/p | -7.71, 1.37×10−14 | -6.53, 6.93×10−11 | -6.07, 1.38×10−9 | -5.76, 9.14×10−9 | -5.52, 3.52×10−8 |
| b (SE) | 8.90×10−3 (7.20×10−4) | 8.72×10−3 (8.26×10−4) | 8.61×10−3 (8.85×10−4) | 8.63×10−3 (9.38×10−4) | 8.52×10−3 (9.58×10−4) |
| t/p | 1.24×101, <2.22×10−16 | 1.06×101, <2.22×10−16 | 9.74, <2.22×10−16 | 9.20, <2.22×10−16 | 8.89, <2.22×10−16 |
| c (SE) | 4.13×102 (8.21×101) | 3.93×102 (9.37×101) | 3.99×102 (1.00×102) | 4.07×102, 1.07×102 | 3.96×102 (1.09×102) |
| t/p | 5.03, 4.89×10-7 | 4.19, 2.79×10−5 | 3.98, 7.05×10−5 | 3.82, 1.37×10-4 | 3.63, 2.86×10-4 |
| Depth I.(G.) | - | 1.91×10−1 | 1.71×10−1 | 1.62×10−1 | 1.55×10-1 |
| Residual | 2.25×10-1 | 1.26×10−1 | 1.57×10−1 | 1.70×10−1 | 1.76×10-1 |
| ICC | - | 0.696 | 0.541 | 0.474 | 0.439 |
| R2 m/c & a | 0.30/0.30 | 0.29/0.79 | 0.28/0.67 | 0.27/0.61 | 0.27/0.59 |
| pKsp°−dol 25 °C | -17.24 | -17.24 | -17.24 | -17.25 | -17.25 |
| CI 25°C l/u (dif) | -17.23/-17.25 (0.02) | -16.99/-17.48 (0.50) | -16.94/-17.56 (0.62) | -16.91/-17.59 (0.67) | -16.90/-17.59 (0.68) |
| pKsp°−dol 200 °C | -23.42 | -23.41 | -23.40 | -23.39 | -23.39 |
| CI 200°C l/u (dif) | -23.37/-23.48 (0.11) | -23.16/-23.67 (0.51) | -23.08/-23.71 (0.63) | -23.05/-23.73 (0.68) | -23.03/-23.74 (0.71) |
| AIC | -1455.3 | -2754.0 | -2845.5 | -3034.2 | -3085.8 |

J1. Model of SUPCRT92-Filtered PWGD dataset. J2. Model of SUPCRT92-Filtered PWGD utilizing only the depth random effect. No clustering of samples into defined depth ranges. J3. Model of SUPCRT92-Filtered PWGD utilizing only the depth random effect. Samples are clustered into 10m interval depth groups. J4. Model of SUPCRT92-Filtered PWGD utilizing only the depth random effect. Samples are clustered are clustered into 50m interval depth groups. J5. Model of SUPCRT92-Filtered PWGD utilizing only the depth random effect. Samples are clustered into 100m interval depth groups. J6. Model of SUPCRT92-Filtered PWGD utilizing only the depth random effect. Samples are clustered into 200m interval depth groups.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Model | J6 - 200m (n=3544) | J7 - 300m (n=3296) | J8 - 400m (n=3175) | J9 - 500m (n=3040) |
| Model Type | Mixed (1) | Mixed (1) | Mixed (1) | Mixed (1) |
| Samples | 10343 | 10343 | 10343 | 10343 |
| a (SE) | -3.78 (6.64×10−1) | -3.64 (6.76×10−1) | -3.70 (6.80×10−1) | -3.61 (6.81×10−1) |
| t/p | -5.69, 1.35×10−8 | -5.38, 7.87×10−8 | -5.44, 5.66×10−8 | -5.30, 1.21×10−7 |
| b (SE) | 8.81×10−3 (9.82×10−4) | 8.57×10−3 (1.00×10−3) | 8.66×10−3 (1.00×10−3) | 8.53×10−3 (1.00×10−3) |
| t/p | 8.98, <2.22×10−16 | 8.58, <2.22×10−16 | 8.62, <2.22×10−16 | 8.47, <2.22×10−16 |
| c (SE) | 4.29×102 (1.12×102) | 4.09×102 (1.14×102) | 4.19×102 (1.14×102) | 4.05×102 (1.15×102) |
| t/p | 3.84, 1.23×10-4 | 3.59, 3.34×10-4 | 3.66, 2.51×10-4 | 3.53, 4.22×10-4 |
| Depth I.(G.) | 1.52×10-1 | 1.51×10-1 | 1.49×10-1 | 1.47×10-1 |
| Residual | 1.78×10-1 | 1.80×10-1 | 1.82×10-1 | 1.83×10-1 |
| ICC | 0.418 | 0.411 | 0.400 | 0.393 |
| R2 m/c & a | 0.27/0.57 | 0.26/0.57 | 0.26/0.56 | 0.26/0.55 |
| pKsp°−dol 25 °C | -17.25 | -17.25 | -17.25 | -17.25 |
| CI 25°C l/u (dif) | -16.89/-17.60 (0.70) | -16.90/-17.61 (0.71) | -16.89/-17.61 (0.72) | -16.89/-17.61 (0.72) |
| pKsp°−dol 200 °C | -23.40 | -23.38 | -23.38 | -23.38 |
| CI 200°C l/u (dif) | -23.04/-23.75 (0.72) | -23.02/-23.74 (0.72) | -23.02/-23.74 (0.73) | -23.01/-23.75 (0.74) |
| AIC | -3137.9 | -3196.5 | -3147.0 | -3152.6 |

J7. Model of SUPCRT92-Filtered PWGD dataset. Samples are clustered into 300m interval depth groups. J8. Model of SUPCRT92-Filtered PWGD dataset. Samples are clustered into 400m interval depth groups. J9. Model of SUPCRT92-Filtered PWGD dataset. Samples are clustered into 500m interval depth groups.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | J10 | J11 | J12 | J13 | J14  |
| Model Type | Mixed (1) | Mixed (1) | Mixed (1) | Mixed (1) | Mixed (1) |
| Samples | 10343 | 10343 | 10343 | 10343 | 10343 |
| a (SE) | -2.98 (6.16×10−1) | -2.88 (5.07×10−1) | -1.89 (5.37×10−1) | -3.88 (4.89×10−1) | -3.68 (4.87×10−1) |
| t/p | -4.83, 1.43×10−6 | -5.68, 1.42×10−8 | -3.52, 4.32×10−4 | -7.94, 2.18×10−15 | -7.55, 4.82×10−14 |
| b (SE) | 7.57×10−3 (9.14×10−4) | 7.52×10−3 (7.49×10−4) | 5.71×10−3 (7.95×10−4) | 9.03×10−3 (7.21×10−4) | 8.77×10−3 (7.21×10−4) |
| t/p | 8.29, <2.22×10−16 | 1.00×101, <2.22×10−16 | 7.18, 7.40×10−13 | 1.25×101, <2.22×10−16 | 1.22×101, <2.22×10−16 |
| c (SE) | 2.98×102 (1.04×102) | 2.79×102 (8.54×101) | 1.47×102 (9.04×101) | 4.36×102 (8.23×101) | 4.00×102 (8.21×101) |
| t/p | 2.88, 4.02×10-3 | 3.27, 1.09×10-3 | 1.62, 1.04×10-1 | 5.29, 1.23×10-7 | 4.88, 1.09×10-6 |
| Basin I.(G.) | - | 6.99×10-1 | - | - | - |
| Field I.(G.) | 1.27×10-1 | - | - | - | - |
| Formation I.(G.) | - | - | 1.29×10-1 | - | - |
| Lithology I.(G.) | - | - | - | 3.48×10-2 | - |
| Series I.(G.) | - | - | - | - | - |
| Period I.(G.) | - | - | - | - | 2.25×10-2 |
| Residual | 1.95×10-1 | 2.20×10-1 | 2.03×10-1 | 2.24×10-1 | 2.25×10-1 |
| ICC | 0.297 | 0.091 | 0.288 | 0.024 | 0.010 |
| R2 m/c & a | 0.26/0.48 | 0.27/0.34 | 0.21/0.44 | 0.29/0.31 | 0.30/0.31 |
| pKsp°−dol 25 °C | -17.24 | -17.26 | -17.26 | -17.23 | -17.24 |
| CI 25°C l/u (dif) | -16.86/-17.62 (0.77) | -16.83/-17.69 (0.87) | -16.86/-17.66 (0.80) | -16.79/-17.68 (0.89) | -16.79/-17.68 (0.89) |
| pKsp°−dol 200 °C | -23.34 | -23.37 | -23.22 | -23.41 | -23.41 |
| CI 200°C l/u (dif) | -22.95/-23.72 (0.77) | -22.94/-23.81 (0.87) | -22.82/-23.61 (0.79) | -22.97/-23.86 (0.89) | -22.97/-23.86 (0.89) |
| AIC | -2828.3 | -1815.0 | -2639.5 | -1524.2 | -1481.8 |

J10. Model of SUPCRT92-Filtered PWGD dataset. Only the field random effect is used. J11. Model of SUPCRT92-Filtered PWGD dataset. Only the basin random effect is used. J12. Model of SUPCRT92-Filtered PWGD dataset. Only the formation random effect is used J13. Model of SUPCRT92-Filtered PWGD dataset. Only the lithology random effect is used. J14. Model of SUPCRT92-Filtered PWGD dataset. Only the time-period random effect is used.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | J15 | J16 | J17 | J18 | J19 |
| Model Type | Mixed (1) | Mixed (2) | Mixed (3) | Mixed (4) | Mixed (5) |
| Samples | 10343 | 10343 | 10343 | 10343 | 10343 |
| a (SE) | -3.59 (4.91×10−1) | -3.33 (6.88×10−1) | -2.31 (6.97×10−1) | -1.86 (7.19×10−1) | -1.89 (7.19×10−1) |
| t/p | -7.31, 2.87×10−13 | -4.85, 1.29×10−6 | -3.31, 9.49×10−4 | -2.59, 9.74×10−3 | -2.62, 8.79×10−3 |
| b (SE) | 8.65×10−3 (7.25×10−4) | 8.11×10−3 (1.02×10−3) | 6.42×10−3 (1.03×10−3) | 5.77×10−3 (1.06×10−3) | 5.81×10−3 (1.06×10−3) |
| t/p | 1.92×101, <2.22×10−16 | 7.97, 2.20×10−15 | 6.21, 5.88×10−10 | 5.43, 6.09×10−8 | 5.47, 4.93×10−8 |
| c (SE) | 3.85×102 (8.27×102) | 3.59×102 (1.16×102) | 2.07×102 (1.17×102) | 1.33×102 (1.21×102) | 1.37×102 (1.21×102) |
| t/p | 4.65, 3.29×10-6 | 3.10, 1.94×10-3 | 1.76, 7.78×10-2 | 1.10, 2.73×10-1 | 1.13, 2.57×10-1 |
| Depth I.(G.) | - | 1.21×10-1 | 1.09×10-1 | 1.09×10-1 | 1.09×10-1 |
| Field I.(G.) | - | 8.86×10-2 | 6.90×10-2 | 6.98×10-2 | 6.97×10-2 |
| Formation I.(G.) | - | - | 9.12×10-2 | 7.70×10-2 | 7.68×10-2 |
| Basin I.(G.) | - | - | - | 6.14×10-2 | 6.17×10-2 |
| Lithology I.(G.) | - | - | - | - | 8.53×10-3 |
| Series I.(G.) | 3.39×10-2 | - | - | - | - |
| Period I.(G.) | - | - | - | - | - |
| Residual | 2.24×10-1 | 1.80×10-1 | 1.77×10-1 | 1.77×10-1 | 1.77×10-1 |
| ICC | 0.022 | 0.409 | 0.445 | 0.459 | 0.459 |
| R2 m/c & a | 0.30/0.31 | 0.26/0.56 | 0.23/0.57 | 0.22/0.58 | 0.22/0.58 |
| pKsp°−dol 25 °C | -17.24 | -17.25 | -17.26 | -17.27 | -17.27 |
| CI 25°C l/u (dif) | -16.80/-17.68 (0.87) | -16.89/-17.60 (0.71) | -16.92/-17.60 (0.68) | -16.92/-17.62 (0.69) | -16.92/-17.61 (0.70) |
| pKsp°−dol 200 °C | -23.41 | -23.36 | -23.26 | -23.25 | -23.25 |
| CI 200°C l/u (dif) | -22.97/-23.86 (0.89) | -22.99/23.72 (0.72) | -22.91/-23.63 (0.72) | -22.90/-23.60 (0.71) | -22.89/-23.61 (0.72) |
| AIC | -1501.2 | -3261.5 | -3533.8 | -3590.9 | -3589.7 |

J15. Model of SUPCRT92-Filtered PWGD dataset. Only the time-series random effect is used. J16. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval) and the field random effects are used. J17. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval), field, and formation random effects are used. J18. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval), field, formation, and basin random effects are used. J19. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval), field, formation, basin and lithology random effects are used.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | J20 | J21 | J22 | J23 - pKsp°−dol | J24 - pKsp°−dol |
| Model Type | Mixed (6) | Mixed (7) | Mixed (7) | Mixed (7) | Mixed (7) |
| Samples | 10343 | 10343 | 10343 | 10343 | 10343 |
| a (SE) | -1.94 (7.21×10−1) | -1.90790 (7.21×10−1) | -1.86 (7.21×10−1) | 1.47545×101 (7.22×10−1) | 1.93×101 (5.67×10−2) |
| t/p | -2.70, 7.07×10−3 | -2.65, 8.16×10−3 | -2.58, 9.84×10−3 | 2.04×101, <2.22×10−16 | 339.6, <2.22×10−16 |
| b (SE) | 5.89×10−3 (1.06×10−3) | 5.84297×10−3(1.07×10−3) | 5.85×10−3  (1.07×10−3) | -6.24959×10−2 (1.07×10−4) | -6.919×10−2 (fixed value) |
| t/p | 5.53, 3.42×10−8 | 5.49, 4.44×10−8 | 5.49, 4.32×10−8 | -5.86×101, <2.22×10−16 | - |
| c (SE) | 1.47×102 (1.21×102) | 1.40778×102 (1.21×102) | 1.31×102 (1.21×102) | -3.99350×103 (1.22×102) | -4.75×103 (1.75×101) |
| t/p | 1.21, 2.26×10-1 | 1.16, 2.46×10-1 | 1.08, 2.82×10-1 | -3.29×101, <2.22×10−16 | 270.7, <2.22×10−16 |
| Ionic strength (SE) | - | - | -7.14×10-3 (1.49×10-3) | - | - |
| t/p | - | - | -4.79, 1.68×10-6 | - | - |
| Depth I.(G.) | 1.09×10-1 | 1.09×10-1 | 1.10×10-1 | 1.10×10-1 | 1.12×10-1 |
| Basin I.(G.) | 6.30×10-2 | 6.35×10-2 | 6.40×10-2 | 6.47×10-2 | 6.22×10-2 |
| Field I.(G.) | 6.99×10-2 | 7.01×10-2 | 6.86×10-2 | 6.94×10-2 | 6.90×10-2 |
| Formation I.(G.) | 7.65×10-2 | 7.66×10-2 | 7.67×10-2 | 7.70×10-2 | 7.66×10-2 |
| Lithology I.(G.) | 8.86×10-3 | 8.05×10-3 | 9.80×10-3 | 7.77×10-3 | 9.33×10-3 |
| Series I.(G.) | - | 1.70×10-2 | 1.74×10-2 | 1.70×10-2 | 1.66×10-2 |
| Period I.(G.) | 1.80×10-2 | 1.38×10-2 | 1.44×10-2 | 1.36×10-2 | 1.35×10-2 |
| Residual | 1.77×10-1 | 1.76×10-1 | 1.76×10-1 | 1.76×10-1 | 1.76×10-1 |
| ICC  | 0.464 | 0.466 | 0.469 | 0.469 | 0.467 |
| R2 m/c & a | 0.22/0.58 | 0.22/0.58 | 0.21/0.58 | 0.91/0.95 | 0.96/0.98 |
| pKsp°−dol 25°C | -17.27 | -17.27 | -17.28 | -17.27 | -17.28 |
| CI 25°C l/u (dif) | -16.92/-17.61 (0.69) | -16.92/-17.62 (0.70) | -16.93/-17.62 (0.69) | -16.93/-17.62 (0.69) | (0.69) |
| pKsp°−dol 200°C | -23.25 | -23.25 | -23.28 | -23.26 | -23.50 |
| CI 200°C l/u (dif) | -22.90/-23.61 (0.72) | -22.89/-23.61 (0.72) | -22.92/-23.63 (0.71) | -22.90/-23.61 (0.71) | (0.69) |
| AIC | -3593.6 | -3595.4 | -3599.8 | -3587.1 | -3562.0 |

J20. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval), field, formation, basin, lithology and time-period random effects are used. J21. Model of SUPCRT92-Filtered PWGD dataset. The depth (300m interval), field, formation, basin, lithology, time-period and time-series random effects are used. This is the reference model for the relationship between $log\_{10}(/)$-temperature for the PWGD. J22. Model of SUPCRT92-Filtered PWGD dataset with ionic strength included as a fixed effect. The same 7 random effects used in model J21 used here. J23. Model of pKsp°−dol values calculated for SUPCRT92-Filtered PWGD dataset. Statistical goodness of fit functions (AIC, R2) and t/p values are thought to be somewhat spurious due to the pre-modelling conversion to pKsp°−dol. The same 7 random effects used in model J22 used here. J24. Model of pKsp°−dol values calculated for SUPCRT92-Filtered PWGD dataset where the b term is fixed to -0.06919. The same 7 random effects used in model J22 used here. There appears to be an unresolvable bug in how R calculates confidence intervals for offset models, with the width of the interval which appear to be reliable but not the absolute values (which are significantly incorrect).

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Model | K1 | K2 - pKsp°−dol | L1 | M1 | N1 |
| Model Type | Mixed (6) | Mixed (6) | Linear | Linear | Linear |
| Samples | 11480 | 11480 | 42  | 36 | 28 |
| a (SE) | 8.31×10−1 (9.07×10−1) | 1.19×101 (9.09×10−1) | -1.01 (7.07×10−1) | -1.22 (3.21×10−1) | -1.74×101 (5.25) |
| t/p | 9.17×10−1, 3.59×10−1 | 1.31×101, <2.22×10−16 | -1.42, 1.63×10−1 | -3.79, 5.93×10−4 | 3.33, 2.70×10−3 |
| b (SE) | 1.18×10−3  (1.33×10−3) | -5.76×10−2  (1.33×10−3) | 4.13×10−3 (2.28×10−3) | 4.82×10−3 (1.03×10−3) | -6.88×10−2 (6.36×10−3) |
| t/p | 8.88×10−1, 3.75×10−1 | -4.34×101, <2.22×10−16 | 1.81, 7.73×10−2 | 4.70, 4.23×10−5 | -1.08×101, 6.37×10-11 |
| c (SE) | -2.58×102 (1.54×102) | -3.58×103 (1.54×102) | - | - | -4.22×103 (1.07×103) |
| t/p | -1.68, 9.34×10-2 | -2.32×101, <2.22×10−16 | - | - | -3.95, 5.66×10-4 |
| Depth I.(G.) | 1.38×10-1 | 1.39×10-1 | - | - | - |
| Field I.(G.) | 1.30×10-1 | 1.30×10-1 | - | - | - |
| Formation I.(G.) | 1.00×10-1 | 1.00×10-1 | - | - | - |
| Basin I.(G.) | 8.29×10-2 | 8.54×10-2 | - | - | - |
| Lithology I.(G.) | 2.43×10-2 | 2.39×10-2 | - | - | - |
| Period I.(G.) | 1.30×10-1 | 1.28×10-2 | - | - | - |
| Residual | 2.56×10-1 | 2.56×10-1 | 1.65×10-1 | 5.78×10-2 | 0.29 |
| ICC  | 0.449 | 0.452 | - | - | - |
| R2 m/c & a | 0.08/0.49 | 0.84/0.91 | 0.05 | 0.38 | 0.99 |
| pKsp°−dol 25°C | -17.28 | -17.28 | -17.19 | -17.17 | -17.18 |
| CI 25°C l/u (dif) | -16.77/-17.78 (1.00) | -16.78/-17.79 (1.00) | -17.11/-17.26 (0.15) | -17.14/-17.22 (0.07) | -16.66/-17.71 (0.53) |
| pKsp°−dol 200 °C | -22.94 | -22.94 | -23.05 | -23.16 | -24.00 |
| CI 200°C l/u (dif) | -22.43/-23.47 (1.04) | -22.42/-23.47 (1.05) | -22.30/-23.80 (0.72) | -22.83/-23.50 (-0.67) | -23.85/-24.15 (0.15) |
| AIC | - | - | - | - | - |

K1. Model of PWGD database not filtered using the SUPCRT92-Filter. The model (and K2) are unable to reliably calculate the time series random effect term so it is omitted. K2. Model of pKsp°−dol values for the PWGD database with values not filtered using the SUPCRT92-Filter. L1. Model of Yarmouk gorge samples from Möller and De Lucia (2020) dataset; samples are taken from Siebert and others (2014) and Siebert and others (in prep). The p-value of this model is 7.73×10−2 (identical also to p value on the b-term). We do not report model p-values as they are only output for linear models. The p-values given(reported t/p) are those that describe the significance of model coefficients. M1. Model of Yarmouk gorge samples from Möller and De Lucia (2020) without samples <25°C. The p-value for this model is 4.23×10−5 (again identical to the to p value on the b-term). N1. Reanalysis of the B´en´ezeth and others (2018) dataset using activities calculated by B´en´ezeth and others (2018).