|  |  |  |  |
| --- | --- | --- | --- |
| Lithology | Description | Pre-SUPCRT (n=11,480) | Post-SUPCRT (n=10,343) |
| Sandstone | All sand and siltstone lithologies, including those with mention of subsidiary anhydrite and shale. No carbonate can be reported. | 7466 (65.0%) | 6675 (64.5%) |
| Dolomite | Dolomite lithologies including those with mention of subsidiary anhydrite, sandstone, siltstone, shale or chert. No limestone can be reported. | 1310 (11.4%) | 1176 (11.4%) |
| Limestone | Limestone lithologies including those with mention of subsidiary anhydrite, sandstone, siltstone, shale or chert. No dolomite can be reported. | 2045 (17.8%) | 1907 (18.4%) |
| Mixed Carbonate | Dolomite and limestone lithologies including those with mention of subsidiary anhydrite, sandstone, siltstone, shale or chert. Also includes ‘carbonate’, chalk and chert lithologies. | 500 (4.4%) | 439 (4.2%) |
| Shale | Shale lithology. Can mention only 1 other minor lithology e.g. anhydrite, chert | 159 (1.4%) | 146 (1.4%) |

Supplementary Table 4. Classification of samples by lithology. Two datasets are presented; 1) the PWGD dataset (n=11,480) which is simulated using PHREEQC 2) the 90.89% of these samples (n=10,343) with ratios between SUPCRT92-ordered-calcite-dolomite & disordered-dolomite - calcite equilibriums (temperature-dependent) which were used in the principal regression analysis.