Table . Performance of the oxidation model across the temperature spectrum.

|  |  |  |  |
| --- | --- | --- | --- |
| Temperature Range →  ↓Hydroperoxide | **Chilled and ambient Temperatures**  **(7-40°C)** | **Intermediate Temperatures**  **(45-80°C)** | **High Temperatures  (140-200°C)** |
| **L1OOH**  *a*CCC range  *b*PICP range (%)  *c*RD range  Outliers‡:  *a*CCC range  *b*PICP range (%)  *c*RD range | *references†: E,F,G*   * 0.92 – 0.96 * 44.0 – 72.7 * 0.66 – 1.28   *references†: N/A* | *references†: C*   * 0.79 – 0.92 * 30.0 – 42.9 * 0.76 – 1.56   *references†: D (70°C)*   * 0.43 * 23.3 – 83.25 * 1 - 7.82 | *references†: B*   * 0.81 – 0.88 * 33.3 – 60.0 * 0.53 – 0.79   *references†: A (200°C)*   * 0.11 * 2.52 – 55.61 * 0.029 – 0.39 |
| **L2OOH**  *a*CCC range  *b*PICP range (%)  *c*RD range  Outliers‡:  *a*CCC range  *b*PICP range (%)  *c*RD range | *references†: D,F,I,J,K*   * 0.79 – 0 .99 * 45.2 – 76.9 * 0.69 – 1.2   *references†: N/A* | *references†: B,D*   * 0.86 – 0.97 * 45.5 – 63.3 * 0.49 – 1   *references†: N/A* | *references†: B*   * 0.78 – 0.90 * 60.0 – 77.8 * 0.82 – 1.0   *references†: A (200°C)*   * 0.02 * 2.52 – 55.61 * 0.027 – 0.19 |
| **L3OOH**  *a*CCC range  *b*PICP range (%)  *c*RD range  Outliers‡:  *a*CCC range  *b*PICP range (%)  *c*RD range | *references†: F,G*   * 0.96 * 33.5 – 79.7 * 0.98 – 1.7   *references†: N/A* | *references†: F*   * 0.92 * 14.3 – 82.7 * 0.54 – 1.11   *references†: L (70°C)*   * 0.45 * 5.3 – 85.3 * 0.01 – 1 | *references†: B*   * 0.91 – 0.92 * 37.5 – 96.3 * 0.81 – 1.12   *references†: N/A* |

†References used in Figure 4.

‡ Datasets were considered outliers when their CCC was lower than 0.5.

*a* Concordance Correlation Coefficient defined in Eq. (S5) of the Supplementary Material: Measures the agreement between predicted and experimental values, accounting for both precision and bias. Values range from −1 (perfect disagreement) to 1 (perfect agreement).

*b* Prediction Interval Coverage Probability defined in Eq. (S8) of the Supplementary Material: Estimates the fraction of experimental data points within the model's prediction intervals, reflecting the reliability of uncertainty quantification. For multiple datasets, the range of values represents the minimum and maximum of the likeliest PICP value observed across the datasets. For a single dataset, the 95% confidence interval is provided, as calculated in Eqs. (S9)-(S10) of the Supplementary Material.

*c* Relative Deviation characterizes the systematic under- or over-estimation of predictions relative to experimental values. For multiple datasets, the range of values represents the minimum and maximum of the likeliest deviation ratio. For a single dataset, the 95% confidence interval is provided instead.