**Supplementary Material**

# A chemometric approach to the interaction of hydrogen peroxide and thermally activated persulfate in the removal of aromatic compounds

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Figure SM1 – Experimental set-up

Table SM1 - Experimental design

| | **Factor 1** | **Factor 2** | **Factor 3** | **Factor 4** | **Response 1** |
|---|---|---|---|---|---|
| **Run** | A:T | B:pH | C:[HP] | D:[PS] | R1 |
| | °C | - | mg/L | mg/L | % |
| **1** | 55 | 7 | 67.5 | 103 | 0 |
| 2 | 70 | 9 | 85 | 85 | 11.4 |
| 3 | 55 | 7 | 67.5 | 67.5 | 2.8 |
| 4 | 40 | 9 | 85 | 50 | 10.8 |
| 5 | 55 | 7 | 67.5 | 32.5 | 8 |
| 6 | 70 | 5 | 85 | 85 | 40.4 |
| 7 | 70 | 5 | 50 | 50 | 94.4 |
| 8 | 40 | 9 | 85 | 85 | 52.8 |
| 9 | 40 | 5 | 85 | 50 | 31.9 |
| 10 | 55 | 3 | 67.5 | 67.5 | 52.4 |
| 11 | 40 | 5 | 50 | 85 | 29.8 |
| 12 | 70 | 9 | 85 | 50 | 23.3 |
| 13 | 85 | 7 | 67.5 | 67.5 | 46.4 |
| 14 | 70 | 5 | 50 | 85 | 48.6 |
| 15 | 70 | 5 | 85 | 50 | 50.1 |
| 16 | 40 | 9 | 50 | 85 | 8.8 |
| 17 | 70 | 9 | 50 | 85 | 11.2 |
| 18 | 55 | 11 | 67.5 | 67.5 | 12.1 |
| 19 | 55 | 7 | 67.5 | 67.5 | 4.12 |
| 20 | 70 | 9 | 50 | 50 | 52.2 |
| 21 | 55 | 7 | 103 | 67.5 | 76.4 |
| 22 | 40 | 5 | 85 | 85 | 71.6 |
| 23 | 40 | 9 | 50 | 50 | 4.48 |
| 24 | 40 | 5 | 50 | 50 | 15.5 |
| 25 | 55 | 7 | 32.5 | 67.5 | 58.8 |

Table SM2 – ANOVA results for quadratic model

| Source | Sum of Squares | df | Mean Square | F-value | P-value | |
|---|---|---|---|---|---|---|
| **Model** | 16665.03 | 14 | 1190.359 | 62.05558 | 8.33E-08 | significant |
| **A-T** | 733.7881 | 1 | 733.7881 | 38.25371 | 0.000103 | |
| **B-pH** | 3453.121 | 1 | 3453.121 | 180.0174 | 1.02E-07 | |
| **C-[HP]** | 163.386 | 1 | 163.386 | 8.51761 | 0.01534 | |
| **D-[PS]** | 24.04002 | 1 | 24.04002 | 1.25325 | 0.289101 | |
| **AB** | 251.381 | 1 | 251.381 | 13.10495 | 0.004689 | |
| **AC** | 2250.079 | 1 | 2250.079 | 117.3007 | 7.62E-07 | |
| **AD** | 2722.231 | 1 | 2722.231 | 141.9148 | 3.13E-07 | |
| **BC** | 15.7609 | 1 | 15.7609 | 0.821644 | 0.38602 | |
| **BD** | 1.6129 | 1 | 1.6129 | 0.084083 | 0.777762 | |
| **CD** | 1029.768 | 1 | 1029.768 | 53.68368 | 2.52E-05 | |
| **$A^2$** | 696.0872 | 1 | 696.0872 | 36.28829 | 0.000128 | |
| **$B^2$** | 907.6082 | 1 | 907.6082 | 47.31527 | 4.31E-05 | |
| **$C^2$** | 4450.503 | 1 | 4450.503 | 232.0128 | 3.02E-08 | |
| **$D^2$** | 0.774107 | 1 | 0.774107 | 0.040356 | 0.844814 | |
| **Residual** | 191.8214 | 10 | 19.18214 | | | |
| **Lack of Fit** | 190.9502 | 9 | 21.21669 | 24.35341 | 0.156075 | not significant |
| **Pure Error** | 0.8712 | 1 | 0.8712 | | | |
| **Cor Total** | 16856.85 | 24 | | | | |

Table SM3 - Fit Statistics

| **Std. Dev.** | **4.379742** |
|---|---|
| Mean | 32.7336 |
| C.V. % | 13.37996 |
| $R^2$ | 0.988621 |
| Adjusted $R^2$ | 0.972689 |
| Predicted $R^2$ | 0.927175 |
| Adeq Precision | 26.00711 |
| $R^2$ | 0.988621 |

Table SM4 - Data for temperature dependence of the rate constant

| **T (K)** | **1/T ($K^{-1}$)** | **$k_1$ ($M^{-1}s^{-1}$)** | **ln k** |
|---|---|---|---|
| 303.15 | $3.30 \times 10^{-3}$ | 0.1562 | -1.857 |
| 313.15 | $3.19 \times 10^{-3}$ | 0.2034 | -1.592 |
| 328.15 | $3.05 \times 10^{-3}$ | 0.2746 | -1.292 |
| 343.15 | $2.91 \times 10^{-3}$ | 0.3451 | -1.064 |