SUPPLEMENTARY MATERIAL

TABLE SI. ANN structure and performance used for prediction of the decolourisation process for textile dyes RO 16, RB 19 and DR 28

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Dye | | RO 16 | | RB 19 | DR 28 | |
| Inputs | | t (min), Q (dm3/min), % O2 | | | | |
| Number of neurons | Input | 3 | 3 | | | 3 |
| Pattern | 40 | 34 | | | 77 |
| Summation | 2 | 2 | | | 2 |
| Output | 1 | 1 | | | 1 |
| Outputs | | Decolourisation efficiency (A/A0) | | | | |
| Performance metrics | |  | | | | |
| RMSEa | | 0.045 | 0.091 | | | 0.055 |
| MAEb | | 0.027 | 0.077 | | | 0.037 |
| Dataset | | Data points | | | | |
| Training | | 40 | 34 | | | 77 |
| Validation | | 12 | 10 | | | 21 |
| Test | | 9 | 6 | | | 10 |

a Root Mean Square Error 40, b Mean Absolute Error 40

TABLE SII a. Descriptive statistics of the model for entire dataset and created subsets for RO 16

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Input/  Output | Training | | | | | Validation | | | | | Test | | | | |
| Ma | S. Eb | | Min | Max | Ma | S. Eb | | Min | Max | Ma | S. Eb | | Min | Max |
| t (min) | 24.9 | | 3.5 | 0 | 90 | 18.9 | | 4.7 | 2 | 60 | 18.4 | | 6.4 | 0 | 45 |
| Q (dm3/min) | 4.1 | | 0.3 | 1.0 | 8.0 | 4.2 | | 0.6 | 1.0 | 8.0 | 4.6 | | 0.7 | 1.0 | 8.0 |
| % O2 | 0.01 | | 0.00 | 0.00 | 0.05 | 0.02 | | 0.01 | 0 | 0.05 | 0.01 | | 0.00 | 0.00 | 0.02 |
| A/A0 | 0.38 | | 0.05 | 0.00 | 1.00 | 0.41 | | 0.08 | 0.00 | 0.87 | 0.50 | | 0.14 | 0.02 | 1.00 |

TABLE SII b. Descriptive statistics of the model for entire dataset and created subsets for RB 19

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Input/  Output | Training | | | | Validation | | | | | | Test | | | | |
| Ma | S. Eb | Min | Max | Ma | S. Eb | | Min | | Max | Ma | S. Eb | | Min | Max |
| t (min) | 18.5 | 3.4 | 0 | 90 | 37.9 | | 12.7 | | 2 | 120 | 17.0 | | 8.9 | 2 | 60 |
| Q (dm3/min) | 4.2 | 0.4 | 1.0 | 8.0 | 4.0 | | 1.0 | | 1.0 | 8.0 | 4.2 | | 0.9 | 1.0 | 8.0 |
| % O2 | 0.01 | 0.00 | 0 | 0.05 | 0.00 | | 0.00 | | 0.00 | 0.02 | 0.02 | | 0.01 | 0.00 | 0.05 |
| A/A0 | 0.41 | 0.06 | 0.00 | 1.00 | 0.33 | | 0.10 | | 0.00 | 0.89 | 0.30 | | 0.14 | 0.00 | 0.84 |

TABLE SII c. Descriptive statistics of the model for entire dataset and created subsets for DR 28

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Input/  Output | Training | | | | | Validation | | | | | Test | | | | |
| Ma | S. Eb | | Min | Max | Ma | S. Eb | | Min | Max | Ma | S. Eb | | Min | Max |
| t (min) | 68.4 | | 79.6 | 0 | 330 | 64.3 | | 13.0 | 0 | 180 | 108 | | 29.2 | 5 | 240 |
| Q (dm3/min) | 4.0 | | 2.0 | 1.0 | 8.0 | 4.1 | | 0.4 | 1.0 | 8.0 | 3.4 | | 0.4 | 1.0 | 4.0 |
| % O2 | 0.03 | | 0.04 | 0.00 | 0.10 | 0.02 | | 0.01 | 0.00 | 0.10 | 0.01 | | 0.01 | 0.00 | 0.05 |
| A/A0 | 0.39 | | 0.30 | 0.02 | 1.00 | 0.37 | | 0.06 | 0.04 | 1.00 | 0.28 | | 0.08 | 0.06 | 0.81 |

a Mean Value; b Standard Error