**Supplementary Material**

**Hydrothermal carbonisation of mixed agri-food waste: Process optimisation and mechanistic evaluation of hydrochar inorganic chemistry**

**Authors**

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Table S1. Analysis of variance (ANOVA) of the regression model for prediction of hydrochar yield

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 1445.6985 | 9 | 160.633 | 146.4959 | <0.0001 |
| T | 377.43627 | 1 | 377.4363 | 344.2184 | <0.0001 |
| **t** | 12.56785 | 1 | 12.5679 | 11.3706 | 0.0014 |
| SL | 736.16440 | 1 | 736.1644 | 671.3751 | <0.0001 |
| T × t | 51.53870 | 1 | 51.5387 | 47.0028 | <0.0001 |
| T × SL | 34.92094 | 1 | 34.9209 | 31.8476 | <0.0001 |
| t × SL | 11.05684 | 1 | 11.0568 | 10.0837 | 0.0026 |
| T2 | 72.00227 | 1 | 72.0023 | 65.6654 | <0.0001 |
| t2 | 0.61979 | 1 | 0.6198 | 0.5652 | 0.4557 |
| SL2 | 18.17455 | 1 | 18.1745 | 16.5750 | 0.0002 |
| **Residual**  | 54.8251 | 50 | 1.097 |  |  |
| **Lack of Fit** | 23.401228 | 5 | 4.68025 | 6.7023 | <0.0001 |
| **Pure Error** | 31.423894 | 45 | 0.69831 |  |  |
| **Cor Total**  | 1500.5236 | 59 |  |  |  |

Table S2. Analysis of variance (ANOVA) of the regression model for prediction of higher heating value

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 148.45082 | 9 | 16.4945 | 105.3811 | <0.0001 |
| T | 126.25957 | 1 | 126.2596 | 806.6536 | <0.0001 |
| **t** | 16.83003 | 1 | 16.8300 | 107.5246 | <0.0001 |
| SL | 0.15038 | 1 | 0.1504 | 0.9608 | 0.3317 |
| T × t | 0.13157 | 1 | 0.1316 | 0.8406 | 0.3636 |
| T × SL | 0.01274 | 1 | 0.0127 | 0.0814 | 0.7766 |
| t × SL | 1.19662 | 1 | 1.1966 | 7.6450 | 0.0080 |
| T2 | 3.19599 | 1 | 3.1960 | 20.4187 | <0.0001 |
| t2 | 0.11505 | 1 | 0.1151 | 0.7350 | 0.3953 |
| SL2 | 0.10304 | 1 | 0.1030 | 0.6583 | 0.4210 |
| **Residual**  | 7.82613 | 50 | 0.1565 |  |  |
| **Lack of Fit** | 2.0317900 | 5 | 0.406358 | 3.1559 | 0.0159 |
| **Pure Error** | 5.7943431 | 45 | 0.128763 |  |  |
| **Cor Total**  | 156.27695 | 59 |  |  |  |

[[Table S3](https://lunet-my.sharepoint.com/personal/cvfok_lunet_lboro_ac_uk/Documents/PROGRESSION/R3/MANUSCRIPT%201/Supplementary%20data.docx?web=1)](https://lunet-my.sharepoint.com/personal/cvfok_lunet_lboro_ac_uk/Documents/PROGRESSION/TOWARDS%20R1/MANUSCRIPT/JBAB-S-21-00256_word.docx?web=1). Analysis of variance (ANOVA) of the regression model for prediction of ash content

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of squares** | **Degree of freedom** | **Mean square** | **F Value** | **p-value (Prob > F)** |
| **Model** | 75.536712 | 9 | 8.39297 | 27.8725 | <0.0001 |
| T | 0.241203 | 1 | 0.24120 | 0.8010 | 0.3751 |
| **t** | 1.256653 | 1 | 1.25665 | 4.1733 | 0.0464 |
| SL | 59.473920 | 1 | 59.47392 | 197.5092 | <0.0001 |
| T × t | 2.419350 | 1 | 2.41935 | 8.0345 | 0.0066 |
| T × SL | 4.216817 | 1 | 4.21682 | 14.0038 | 0.0005 |
| t × SL | 0.470400 | 1 | 0.47040 | 1.5622 | 0.2172 |
| T2 | 5.282000 | 1 | 5.28200 | 17.5412 | 0.0001 |
| t2 | 2.952027 | 1 | 2.95203 | 9.8035 | 0.0029 |
| SL2 | 1.442727 | 1 | 1.44273 | 4.7912 | 0.0333 |
| **Residual**  | 15.055986 | 50 | 0.30112 |  |  |
| **Lack of Fit** | 9.440875 | 5 | 1.88817 | 15.1320 | <0.0001 |
| **Pure Error** | 5.615111 | 45 | 0.12478 |  |  |
| **Cor Total**  | 90.592698 | 59 |  |  |  |

Table S4. Inorganic elemental composition of the hydrochar at different HTC operating conditions

|  |  |
| --- | --- |
|  | mg/kg (dry basis) |
| Sample\* | Al | Ca | Fe | K | Mg | P | S | Si |
| 190-1-5 | 491 | 2835 | 303 | 898 | 116 | 171 | 627 | 62 |
| 190-5-5 | 397 | 2263 | 229 | 762 | 108 | 136 | 541 | 21 |
| 210-3-5 | 455 | 1223 | 299 | 754 | 117 | 135 | 523 | 30 |
| 230-1-5 | 487 | 589 | 337 | 658 | 160 | 245 | 519 | 30 |
| 230-5-5 | 450 | 1295 | 369 | 900 | 175 | 613 | 631 | 35 |
| 190-3-12.5 | 395 | 2865 | 228 | 2518 | 239 | 325 | 633 | 29 |
| 210-1-12.5 | 512 | 2520 | 327 | 2308 | 233 | 332 | 602 | 39 |
| 210-3-12.5 | 428 | 2208 | 289 | 2278 | 257 | 434 | 651 | 37 |
| 210-5-12.5 | 375 | 1795 | 286 | 2040 | 256 | 611 | 661 | 27 |
| 230-3-12.5 | 468 | 1465 | 394 | 2638 | 314 | 793 | 712 | 36 |
| 190-1-20 | 494 | 3225 | 270 | 4813 | 478 | 708 | 946 | 52 |
| 190-5-20 | 371 | 3115 | 272 | 4730 | 397 | 585 | 773 | 21 |
| 210-3-20 | 424 | 2315 | 294 | 3898 | 405 | 745 | 746 | 32 |
| 230-1-20 | 376 | 2195 | 346 | 5585 | 531 | 893 | 801 | 31 |
| 230-5-20 | 378 | 2375 | 380 | 5613 | 553 | 1101 | 854 | 55 |

\*Samples are denoted as “Temperature (℃)-time (hr)-solid loading (%)” sequence.

(a) 

(b)

Fig. S1. Score plot showing relationship between experimental runs (a) based on principal component 1 and 2 (b) based on principal component 1 and 3.



Fig. S2. Scree plot of eigen values of each principal component for selection of relevant principal component. Principal component with eigen value greater than 1 was the selection criterion [1].



Figure S3 Analysis of the effect of operating parameter on fouling and slagging tendency using main effect plot. A main effect plot shows the mean of the responses across the level of each factor.

# **References**

[1] Abdi H, Williams LJ. Principal component analysis. Wiley Interdiscip Rev Comput Stat 2010;2:433–59. https://doi.org/10.1002/WICS.101.