SUPPORTING DATA

**Adsorptive potential of *Zea Mays* tassel activated carbon towards the removal of metformin hydrochloride from pharmaceutical effluent**

Menala Kalumphaa,b, Upenyu Guyoa\*, Ngceboyakwethu P. Zinyamaa, Benias C. Nyamundab, Felistus Muhle Vakiraic

aDepartment of Chemical Technology, Midlands State University, Private Bag 9055, Senga, Gweru, Zimbabwe.

bDepartment of Chemical and Processing Engineering, Manicaland State University of Applied Sciences, Private Bag 7001, Off-Vumba Road, Mutare, Zimbabwe.

cPlus Five Pharmaceutical Pvt Ltd, 17181 Nketa Drive, Kelvin West, Bulawayo, Zimbabwe

\*Corresponding author: Email upguyo@gmail.com, phone: +263 542 60464, fax: +263 542 60303

**Figures:**

****

Fig. S1. FTIR spectra of *Zea Mays* tassel activated carbon before adsorption (a) and *Zea Mays* tassel activated carbon after adsorption (b).



Fig. S2. XRD spectrum of *Zea Mays* tassel activated



(a)



(b)



(c)

Fig. S3. Normal probability plot (a) Plot of standard residuals versus the predicted values (b) Plot of predicted versus actual data (c)



(a)



(b)



(c)



(d)

Fig. S4. 3-D surface plot for the combined effect of pH and contact time (a), pH and dosage (b), contact time and dosage (c), and contact time and concentration on Cd(II) adsorption efficiency.

(a)

(b)

Fig. S5. Pseudo-first-order kinetic (a) and pseudo-second-order kinetic (b) plots for the adsorption of Cd(II) (pH 7, dosage concentration 1.05 g, initial concentration 105 mg/L, temperature 20 ºC, time 10 - 160 min).

(a)

(b)

Fig. S6. Langmuir (a), Freundlich (b) adsorption isotherms for MH onto ZMTAC (pH 7, dosage concentration 1.05 g, contact time 125 min, initial concentration 10 - 200 mg/L, temperature 20 ºC).

Fig. S7 Regenerability of ZMTAC through repeated adsorption-desorption studies

**Tables:**

**Table S1**

 Central composite design experimental domain

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Parameter | pH | Contact time | Dosage | Initial concentration |
|   |   | (min) | (g) | (mg/L) |
| Min point | 2 | 10 | 0.1 | 10 |
| Mid point | 7 | 125 | 1.05 | 105 |
| Max point | 12 | 240 | 2.0 | 200 |

**Table S2**

Physicochemical properties of ZMTAC

|  |  |
| --- | --- |
| Parameter | Value |
| pH | 6.7 |
| Loss of mass on ignition (%) | 0.82 |
| Moisture content (%) | 0.42 |
| Bulk density (g/mL) | 0.48 |
| Particle size range (um) | 180 |
| Total ash content (%) | 3.78 |
| Phenolic groups (mmol/g) | 0.837 |
| Carboxylic groups (mmol/g) | 0.562 |
| Phenolic groups (mmol/g) | 0.989 |
| Acidity (mmol/g) | 1.874 |
| Basicity (mmol/g) | 0.911 |
| Total groups (mmol/g) | 2.785 |
| Carbon (%) | 55.24 |
| Hydrogen (%) | 2.46 |
| Nitrogen (%) | 6.87 |
| Oxygen (%) | 28.04 |

Table S3

 Experimental variables and results for MH adsorption using ZMTAC

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Run | Factor 1 | Factor 2 | Factor 3 | Factor 4 | Response |
|  | pH | Contact time | Dosage | Concentration | qe |
|  |  | (min) | (g) | (mg/L) | (mg/g) |
| 1 | 7 | 125 | 1.05 | 105 | 1.4304 |
| 2 | 9.5 | 67.5 | 0.575 | 57.5 | 1.92 |
| 3 | 7 | 125 | 1.05 | 10 | 0.0895 |
| 4 | 9.5 | 182.5 | 0.575 | 57.5 | 1.8469 |
| 5 | 4.5 | 182.5 | 0.575 | 152.5 | 4.1043 |
| 6 | 4.5 | 67.5 | 1.525 | 57.5 | 0.7275 |
| 7 | 4.5 | 67.5 | 0.575 | 152.5 | 4.8838 |
| 8 | 7 | 125 | 1.05 | 105 | 1.1657 |
| 9 | 9.5 | 182.5 | 1.525 | 152.5 | 1.8715 |
| 10 | 4.5 | 182.5 | 1.525 | 152.5 | 1.9554 |
| 11 | 9.5 | 182.5 | 0.575 | 152.5 | 5.1009 |
| 12 | 4.5 | 67.5 | 0.575 | 57.5 | 1.8129 |
| 13 | 7 | 125 | 1.05 | 105 | 1.1836 |
| 14 | 7 | 125 | 0.1 | 105 | 9.984 |
| 15 | 7 | 125 | 1.05 | 105 | 0.9809 |
| 16 | 4.5 | 182.5 | 0.575 | 57.5 | 1.7997 |
| 17 | 12 | 125 | 1.05 | 105 | 0.8891 |
| 18 | 4.5 | 67.5 | 1.525 | 152.5 | 1.9321 |
| 19 | 9.5 | 67.5 | 1.525 | 57.5 | 0.4553 |
| 20 | 2 | 125 | 1.05 | 105 | 1.4242 |
| 21 | 9.5 | 67.5 | 0.575 | 152.5 | 2.704 |
| 22 | 7 | 10 | 1.05 | 105 | 1.6756 |
| 23 | 9.5 | 67.5 | 1.525 | 152.5 | 1.0331 |
| 24 | 4.5 | 182.5 | 1.525 | 57.5 | 0.3142 |
| 25 | 7 | 125 | 2 | 105 | 0.6118 |
| 26 | 7 | 240 | 1.05 | 105 | 0.3659 |
| 27 | 7 | 125 | 1.05 | 200 | 3.268 |
| 28 | 9.5 | 182.5 | 1.525 | 57.5 | 0.15 |
| 29 | 7 | 125 | 1.05 | 105 | 1.3259 |
| 30 | 7 | 125 | 1.05 | 105 | 1.3318 |

**Table S4**

 ANOVA for response surface reduced quadratic model for MH using *MT*AC

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Source** | **Sum of Squares** | **Mean Square** | **F-value** | **p-value** |  |
| **Model** | 33.18 | 3.02 | 59.59 | < 0.0001 | significant |
| A-pH | 0.0046 | 0.0046 | 0.0907 | 0.7678 |  |
| B-Contact time | 1.30 | 1.30 | 25.71 | 0.0002 |  |
| C-Dosage | 11.00 | 11.00 | 217.34 | < 0.0001 |  |
| D-Concentration | 11.15 | 11.15 | 220.15 | < 0.0001 |  |
| AB | 0.3996 | 0.3996 | 7.89 | 0.0139 |  |
| AC | 0.6203 | 0.6203 | 12.25 | 0.0035 |  |
| BC | 1.02 | 1.02 | 20.11 | 0.0005 |  |
| BD | 1.02 | 1.02 | 20.06 | 0.0005 |  |
| B² | 1.15 | 1.15 | 22.78 | 0.0003 |  |
| C² | 1.39 | 1.39 | 27.50 | 0.0001 |  |
| D² | 0.3970 | 0.3970 | 7.84 | 0.0142 |  |
| **Residual** | 0.7088 | 0.0506 |  |  |  |
| Lack of Fit | 0.5810 | 0.0646 | 2.53 | 0.1601 | not significant |
| Pure Error | 0.1278 | 0.0256 |  |  |  |
| Cor Total | 33.89 |  |  |  |  |

**Table S5**

Coefficients in Terms of Coded Factors

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Factor** | **Coefficient Estimate** | **df** | **Standard Error** | **95% CI Low** | **95% CI High** | **VIF** |
| Intercept | 1.22 | 1 | 0.0784 | 1.06 | 1.39 |  |
| A-pH | -0.0150 | 1 | 0.0499 | -0.1220 | 0.0919 | 1.08 |
| B-Contact time | 0.3095 | 1 | 0.0610 | 0.1786 | 0.4404 | 1.31 |
| C-Dosage | -0.9148 | 1 | 0.0621 | -1.05 | -0.7817 | 1.32 |
| D-Concentration | 0.7399 | 1 | 0.0499 | 0.6330 | 0.8469 | 1.08 |
| AB | 0.1764 | 1 | 0.0628 | 0.0417 | 0.3111 | 1.08 |
| AC | -0.2218 | 1 | 0.0634 | -0.3576 | -0.0859 | 1.11 |
| BC | -0.2841 | 1 | 0.0634 | -0.4200 | -0.1482 | 1.11 |
| BD | 0.2813 | 1 | 0.0628 | 0.1466 | 0.4160 | 1.08 |
| B² | 0.2827 | 1 | 0.0592 | 0.1556 | 0.4097 | 1.22 |
| C² | 0.3194 | 1 | 0.0609 | 0.1887 | 0.4500 | 1.28 |
| D² | 0.1212 | 1 | 0.0433 | 0.0284 | 0.2140 | 1.01 |

Table S6

Fit Statistics for the model

|  |  |
| --- | --- |
| Parameter | **Value** |
| Standard deviation | 0.225 |
| Mean | 1.59 |
| C.V. (%) | 14.18 |
| R² | 0.9791 |
| Adjusted R² | 0.9627 |
| Predicted R² | 0.8998 |
| Adeq Precision | 31.949 |

**Table S7**

Kinetic parameters for MH adsorption

|  |  |  |  |
| --- | --- | --- | --- |
| Exp value | Pseudo-first-order kinetic model | Pseudo-second-order kinetic model |   |
| qe (mg/g) | qe (mg/g) | k1 (min-1) | SSE | R2 | qe (mg/g) | k2 (g mg-1 min-1) | R2 | SSE |
|   |   |   |   |   |   |   |   |   |
| 1.03 | 3.023 | 0.0062 | 0.896 | 0.9850 | 0.925 | 0.1537 | 0.9960 | 0.0412 |
|   |   |   |   |   |   |   |   |   |

**Table S8**

Isotherm model parameters for MH adsorption onto ZMTAC

|  |  |  |
| --- | --- | --- |
| Isotherm | Parameter | Value |
| Langmuir | qm (mg/g) | 44.84 |
|   | b (L/mg) | 0.00026 |
|  | SSE | 0.321 |
|   | R2 | 0.9787 |
| Freundlich | KF (mg/g) | 0.156 |
|   | n | 1.041 |
|   | SSE | 2.987 |
|   | R2 | 0.943 |

**Table S9**

Thermodynamic parameters for MH adsorption onto ZMTAC

|  |  |  |  |
| --- | --- | --- | --- |
| Temperature (K) | ΔGo (kJmol-1) | ΔH (kJmol-1) | ΔS (kJmol-1) |
| 298.15 | -5.78887 | +3.096 | +0.0298 |
| 308.15 | -6.08687 |  |  |
| 328.15 | -6.68287 |   |   |