**Green synthesis of carbon nanospheres from *Vachellia nilotica* for pendimethalin removal**

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**Supplementary Material**

**Table S1. Physico-chemical properties of PND.**

|  |  |
| --- | --- |
| Property  | Value  |
| Molecular formula | C₁₃H₁₉N₃O₄ |
| IUPAC Name | N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine |
| Molecular weight | 281.31 g/mol |
| CAS number | 40487-42-1 |
| Sructure  | A green hexagon with letters and numbers  AI-generated content may be incorrect. |
| Appearance | Yellow-orange crystals/powder |
| Melting point | Yellow-orange crystals/powder |
| Boiling point | 54 to 60 °C |
| Solubility in water (25 at °C) | 0.3 to 0.54 mg/L(insoluble) |
| Solubility in organic solvents | Very soluble (acetone, methanol, xylene, etc.) |
| pKa (25 at °C) | 2.8 |
| log Kow | 5.2 |
| Half-life in soil | ~90 days  |
| Vapor Pressure | 3.3 × 10⁻⁵ mmHg at 25 °C (low volatility) |

**Table S2. Liner and non-liner expression of adsorption kinetics and isotherm models.**

|  |  |  |  |
| --- | --- | --- | --- |
| Model | Linear form | Non-linear form | Parameters / Notes |
| Pseudo-first order (PFO) |  |  | adsorption capacity *qe* (mg g-1) and *qt* (mg g-1) and *K1* is rate constant. |
| Pseudo-second order (PSO) |  |  | k2 is pseudo second-order rate constant (g/mg·min) |
| Intraparticle diffusion (IPD) |  | same as linear form | kid is intraparticle diffusion rate constant (mg/g·min^0.5) and C is the intercept related to boundary level thickness. |
| Langmuir isotherm |  |  | qm = maximum amount of adsorbent,Ce = model constant,KL= adsorption equilibrium constant. |
| Freundlich isotherm |  |  | Kf = adsorption capacityn= adsorption intensity |
| Temkin isotherm |  |  | B = Temkin constant,RT/BT= heat of adsorption,R= gas constantT= temperature (K) |

**Table S3 Cost analysis for preparation of CNSs.**

|  |  |  |  |
| --- | --- | --- | --- |
| Description of item required for  | Unit cost (INR) | No. of Units | Price(INR) |
| 1 | Biomass | 0 | 0 | 0 |
| 2 | Electricity |  |  | 39.6978 |
|  | 1. Microwave irradiation

(800 W for 3 min) | 5.2 per KWh | 0.04 KWh | 0.21 |
|  | 1. Muffle furnace

(3000 W for 2.5 hours) | 5.2 per KWh | 7.5 kWh | 39 |
|  | 1. Ultrasonication

(170 W for 30 minute) | 5.2 per KWh | 0.085 kWh | 0.442 |
|  | 1. Vortex

(55 W for 10 min) | 5.2 per KWh | 0.0092 kWh | 0.048 |
| 3 | Chemicals |  |  |  |
|  | 1. ferrocene
 | 550 per 25 gm  | 0.150 g (150 mg) | 3.30 |
|  | 1. ethanol
 | 140 per 500 mL  | 100 mL (assumed) | 28 |
| 4 | Distilled Water | 20 Rs per L | 1 L  | 20 |
| Total (per batch) | 90.998 |

Approximate 91 (INR) was required to synthesize 200 mg of CNSs. Therefore, the cost of CNSs per gram will be 455 INR (~$5.45/g).

**Figure S1. pHZPC of CNSs using pH drift method.**

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**Figure S2. Comparative PND removal efficiency at 50 mg L-1 concentration, 7 pH, 100 ml volume and 100 mg CNS and VNBC dose.**



**Figure S3. FEG-SEM image of VNBC at 25000x magnification.**