Electronic Supplementary Material (ESI) for RSC Advances.

Supporting material

Aqueous Carbofuran Removal Using Slow Pyrolysis Sugarcane Bagasse Biochar-Equilibrium and Fixed-bed Studies

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1. Kinetic models:

Pseudo-first order[1] (eqn. SM1) and Pseudo-second order[2] (eqn. SM2) kinetic equations applied on the sorption data to assess the effect of both initial concentration and adsorbent dose. The equations were present below:

$$q_t = q_e\left(1 - e^{-k_1 t}\right) \quad \text{(SM1)}$$

Where k_1 (min^{-1}) is the first order adsorption rate constant, q_e and q_t are the amounts of carbofuran adsorbed at equilibrium and at time "t", respectively.

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e} \quad \text{(SM2)}$$

Where, k_2 is rate constant of pseudo second order adsorption (g mg^{-1} min^{-1}). k_2 and q_e values were determined from the plots at different temperatures and concentrations. k_2 (g mg^{-1} min^{-1}) can be determined experimentally from the slope and intercept of plot t/q_t versus t.

2. Isotherm models:

Sorption data was fitted using Freundlich,[3] Langmuir,[4] and Temkin[5] isotherm models. The non-linear form of Freundlich model is shown in eqn. SM3

$$q_e = K_F C_e^{1/n} \quad \text{(SM3)}$$

Where q_e is the amount of carbofuran adsorbed per unit biochar weight (mg/g), C_e is the equilibrium carbofuran concentration (mg/L), constant K_F indicates the biochar's relative adsorption capacity (mg/g) and 1/n is the adsorption intensity.

The linear form of Langmuir isotherm however is given in eqn. SM4.

$$q_e = \frac{Q^0 b C_e}{1 + b C_e}$$

(SM4)

Where q_e is the amount of carbofuran adsorbed per unit weight of adsorbent (mg/g), C_e is the carbofuran equilibrium concentration in solution in mg/L, Q° is the monolayer adsorption capacity (mg/g) and b is constant related to the net enthalpy. Non- linear form of Temkin[5] isotherm model is given in eqn. SM5.

$$q_e = \frac{RT}{b_{T_e}} \ln \left(a_{T_e} C_e \right)$$

(SM5)

Where, q_e is amount of carbofuran adsorbed per unit weight of adsorbent (mg/g). $a_{T_e} and\ b_{T_e}$ are the Temkin constants related to heat of sorption (KJ/mol). C_e is the equilibrium carbofuran concentration in mg/L. R is universal gas constant and T is absolute temperature.

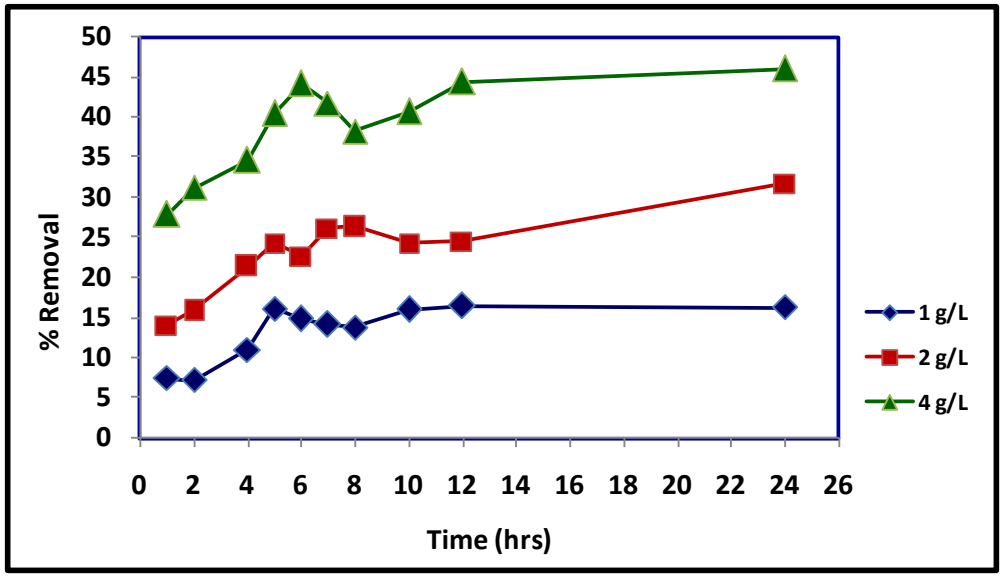

Figure SM1. Effect of different adsorbent dosages on carbofuran adsorption [pH 6.0; Carbofuran concentration= 10 mg/L; particle size=30-50 B.S.S mesh, at 25^{0}C]

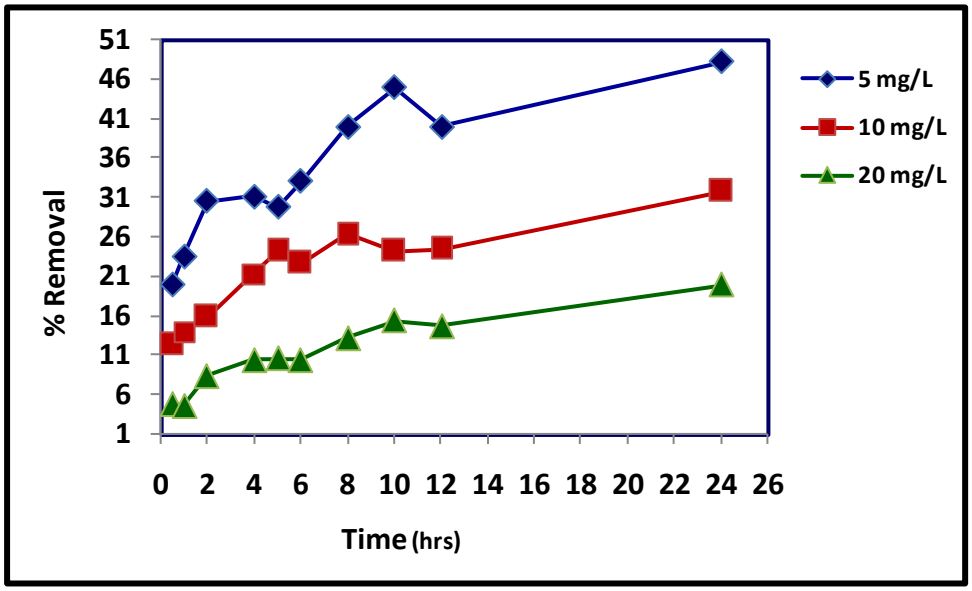

Figure SM2. Effect of different carbofuran concentration on adsorption [pH 6.0; adsorbent (SB500) dose= 2 g/L; particle size=30-50 B.S.S mesh, at 25^{0}C]

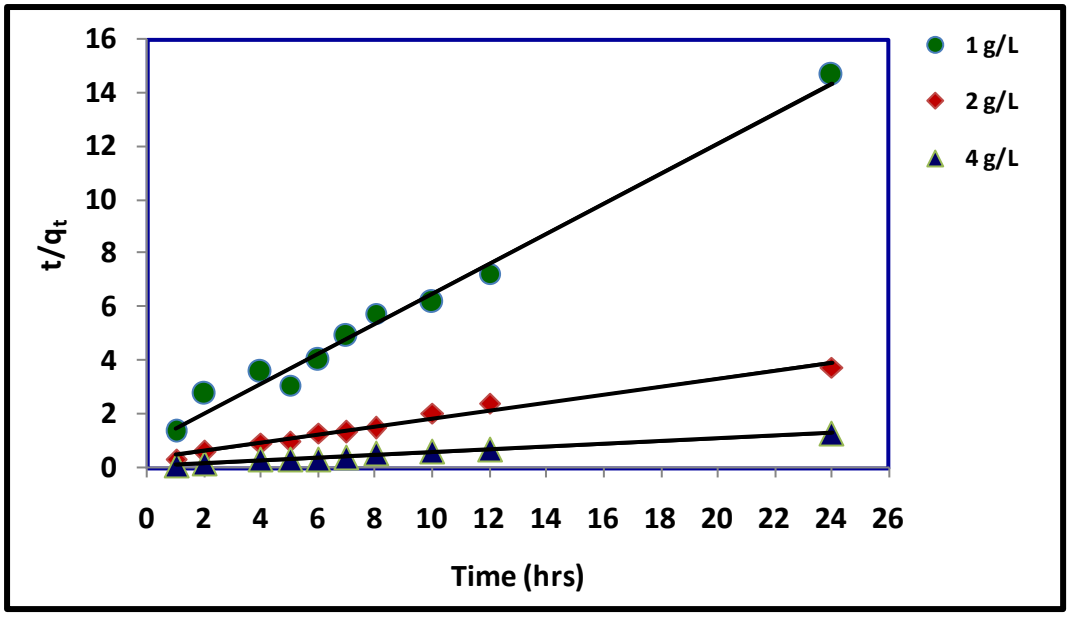

Figure SM3. Pseudo-second order kinetic plots for effect of different adsorbent (SB500) dosages on carbofuran adsorption [pH 6.0; Carbofuran concentration= 10 mg/L; particle size=30-50 B.S.S mesh, at 25^{0}C]

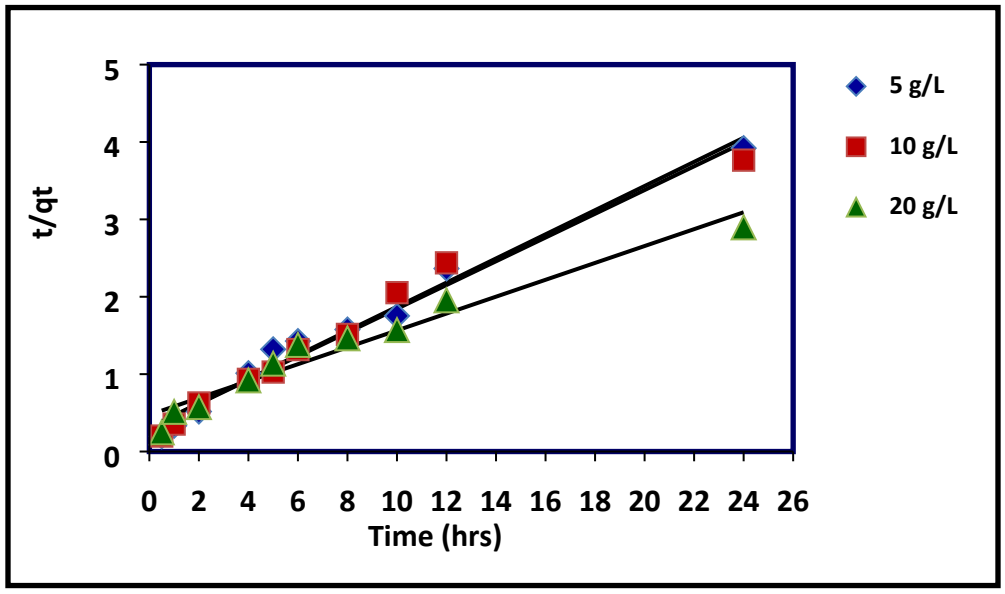

Figure SM4. Pseudo-second order kinetic plot for effect of different carbofuran concentration on adsorption by SB500 [pH 6.0; adsorbent (SB500) dose= 2 g/L; particle size=30-50 B.S.S mesh, at 25^{0}C]

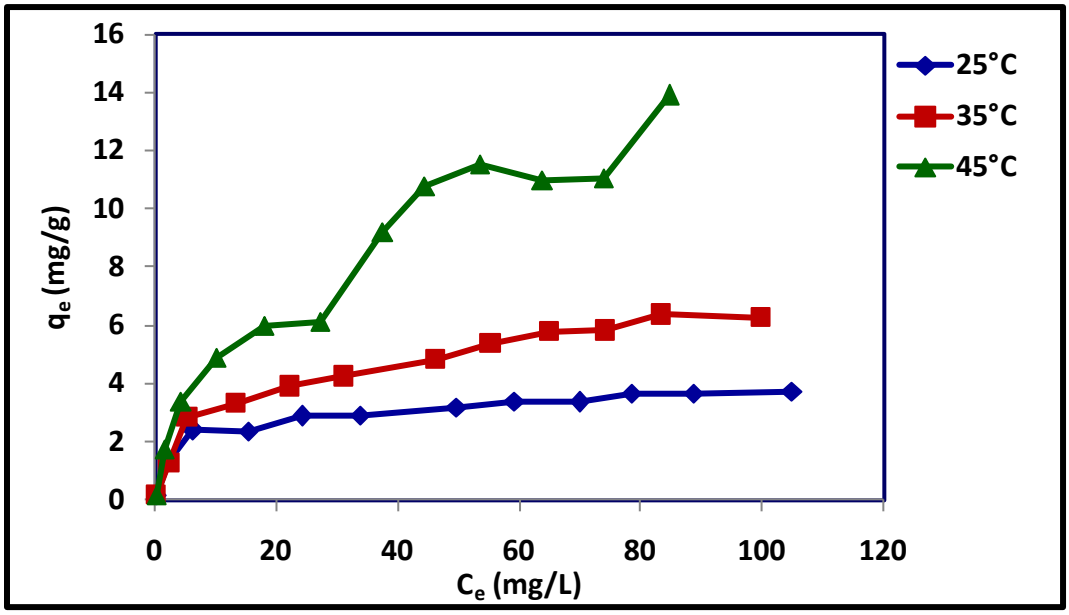

Figure SM5: Adsorption isotherms of carbofuran by SB500 at different temperatures [pH 6.0; adsorbent (SB500) dose=2g/L; carbofuran concentration= 1-100 mg/L; particle size=30-50 B.S.S mesh].

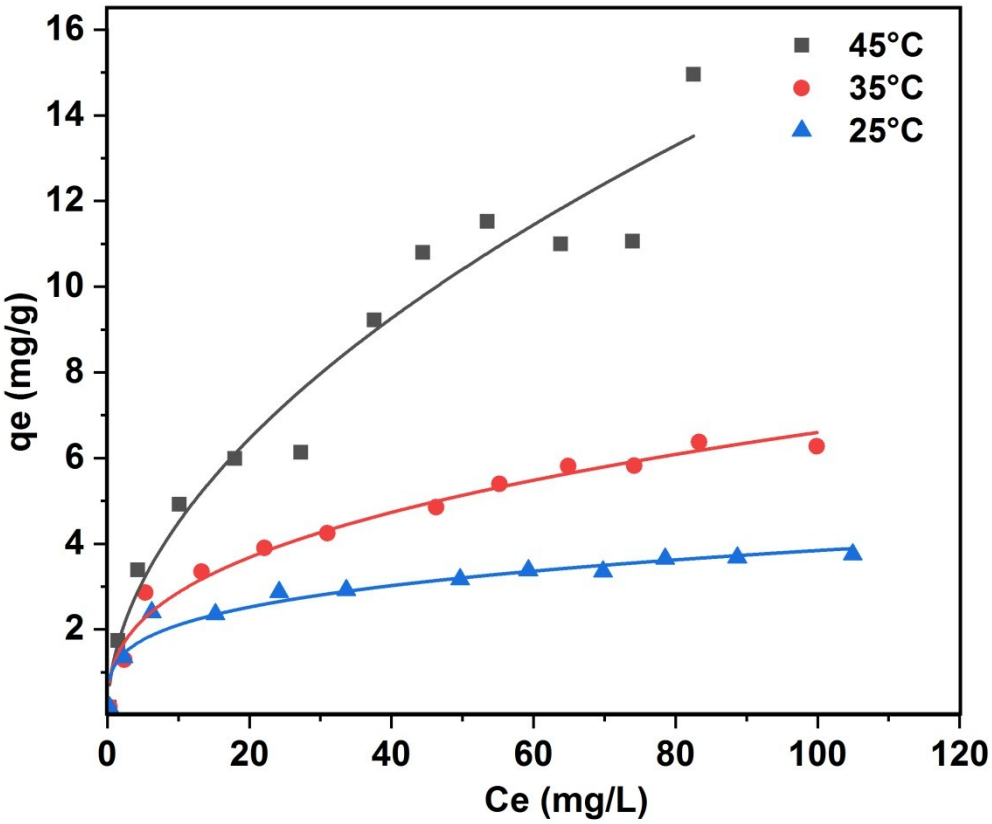

Figure SM6: Freundlich adsorption isotherms of carbofuran by SB500 at different temperatures [pH 6.0; adsorbent (SB500) dose = 2g/L; carbofuran concentration= 1-100 mg/L; particle size of 30-50 B.S.S mesh]. Colored solid lines represent the data fitted by the Freundlich isotherm model

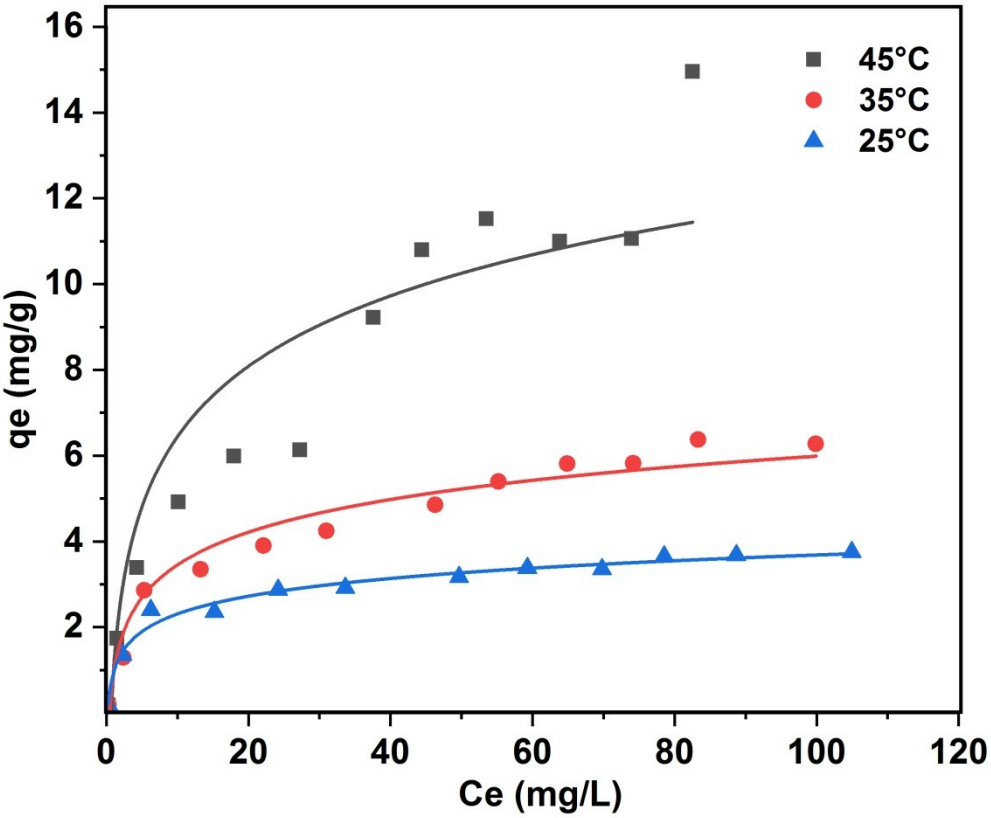

Figure SM7: Temkin adsorption isotherms of carbofuran by SB500 at different temperatures [pH 6.0; adsorbent (SB500) dose = 2g/L; carbofuran concentration= 1-100 mg/L; particle size of 30-50 B.S.S mesh]. Colored solid lines represent the data fitted by the Temkin isotherm model

Table SM1. Pseudo first-order and pseudo-second order rate constants and comparative evaluation of q_e as calculated experimentally and by using pseudo first and pseudo second order rate equations at different SB500 dose.

Dose (g/L)	First order rate constant, k_1 (h^{-1})	R^2	Second order rate constant, k_2 (g mg^{-1} h^{-1})	R^2	q_e experimental (mg/g)	q_e, calculated using first-order kinetic model (mg/g)	q_e , calculated using second-order kinetic model (mg/g)
1	0.362	0.558	0.333	0.986	1.638	1.396	1.786
2	0.099	0.683	0.064	0.978	6.373	3.349	6.666
4	0.195	0.663	0.584	0.994	18.455	8.109	19.120

Table SM2. Pseudo-first order and pseudo-second order rate constants and comparative evaluation of q_e as calculated experimentally and by using pseudo first and pseudo second-order rate equations at different carbofuran concentrations.

Conc. (mg/L)	First order rate constant, k_1 (h^{-1})	R^2	Second order rate constant, k_2 (g mg^{-1} h^{-1})	R^2	q_e experimental (mg/g)	q_e, calculated using first-order kinetic model (mg/g)	q_e , calculated using second-order kinetic model (mg/g)
5	0.1027	0.9381	0.0781	0.979	6.121	6.449	6.410
10	0.0958	0.727	0.0756	0.977	6.373	3.408	6.518
20	0.1443	0.740	0.0251	0.953	8.285	3.677	9.165

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