SUPPLEMENTARY MATERIAL

Self-heating of biochar during postproduction storage by O_2 chemisorption at low temperatures

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S1. Detail of kinetic parameters measurement and calculation

Figure S1 depicts an example of mass loss curves obtained from TGA for the determination of kinetic parameters. The example shows three repetitions measured at isothermal temperatures of 50, 150, and 300 ºC.

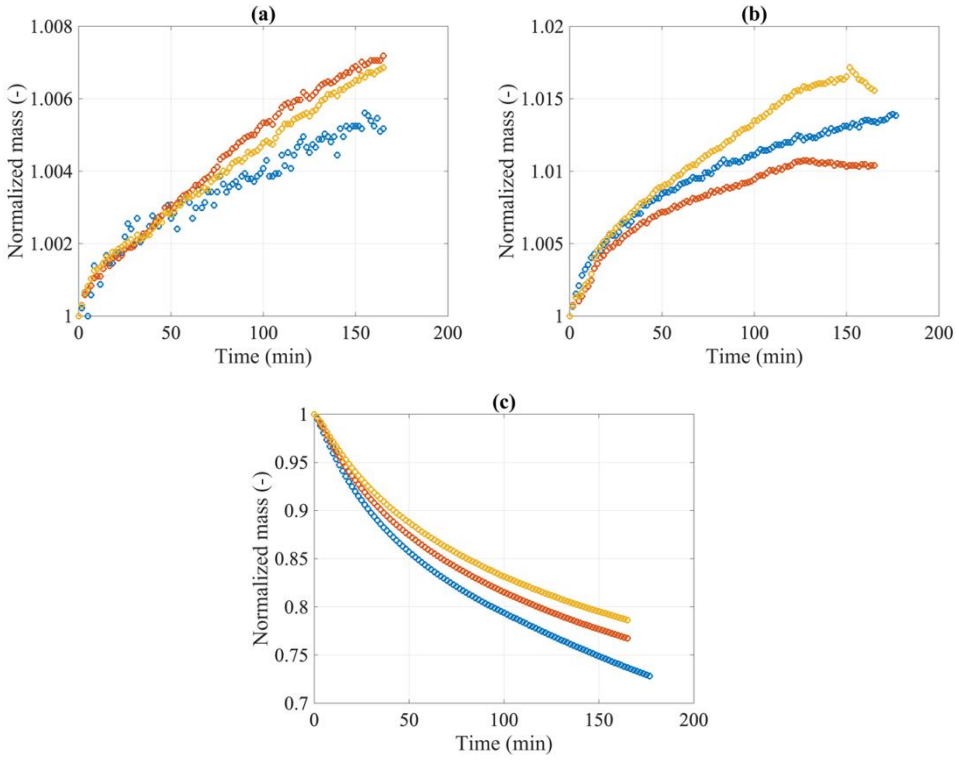

Figure S1. TG curves a) 50 ºC and 20% O_2 b) 150 ºC and 10% O_2 c) 300 ºC and 5% O_2.

Figure S2 depicts the fitting of reaction rates for Reaction 1 and Reaction 2. The figure shows a reasonable fit by applying a first-order reaction equation.

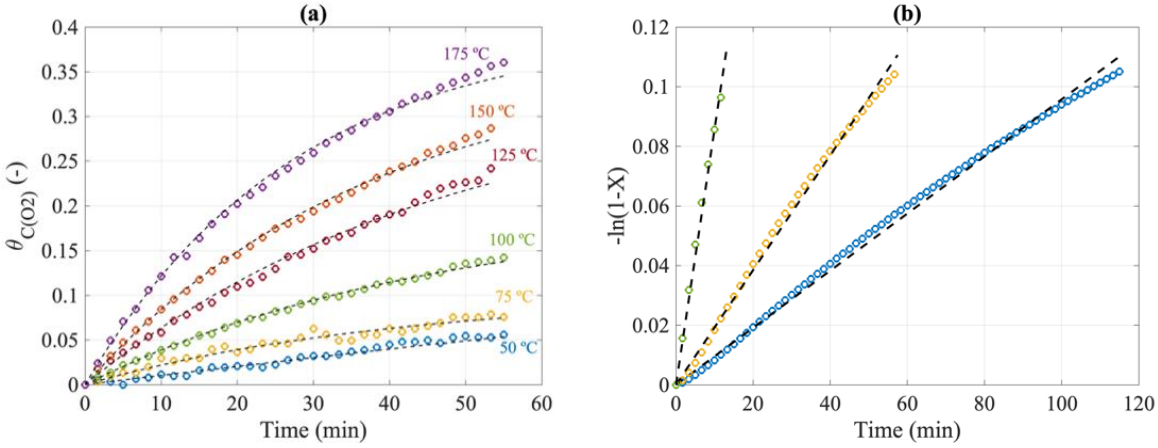

Figure S2. Fitting of Reaction 1 (a) and 2 (b). (Symbol: experiment, line: model)

The fitted rate constants are summarized in Table S1.

Table S1. Fitted rate constants.

Temperature (ºC)	k_{1f} **(1/s/bar)**		
	5% O2	**10% O2**	**20% O2**
50	4.37×10^{-4}	2.40×10^{-4}	1.82×10^{-4}
75	7.48×10^{-4}	4.04×10^{-4}	1.76×10^{-4}
100	1.52×10^{-3}	6.24×10^{-4}	4.09×10^{-4}
125	2.20×10^{-3}	1.35×10^{-3}	5.21×10^{-4}
150	2.86×10^{-3}	1.79×10^{-3}	6.93×10^{-4}
175	4.75×10^{-3}	2.07×10^{-3}	1.51×10^{-3}
Temperature (ºC)	k_{1b} **(1/s)**		
	5% O2	**10% O2**	**20% O2**
50	2.44×10^{-5}	3.46×10^{-5}	4.07×10^{-5}
75	5.63×10^{-6}	2.41×10^{-6}	4.16×10^{-5}
100	2.30×10^{-4}	1.75×10^{-5}	1.76×10^{-5}
125	2.65×10^{-4}	2.56×10^{-4}	4.89×10^{-4}
150	3.36×10^{-4}	3.57×10^{-4}	9.25×10^{-4}
175	3.38×10^{-4}	4.92×10^{-4}	5.24×10^{-4}
Temperature (ºC)	k_2 **(1/s)**		
	5% O2	**10% O2**	**20% O2**
250	1.15×10^{-5}	1.99×10^{-5}	2.21×10^{-5}
275	3.82×10^{-5}	4.29×10^{-5}	4.85×10^{-5}
300	1.04×10^{-4}	1.09×10^{-4}	1.19×10^{-4}

Kinetic parameters were optimized by using the following equation

$$objective\ function = \sum_{j=1}^{N_{exp}} \frac{\sum_{i=1}^{N_{data}} \frac{k_{exp}-k_{model}}{k_{exp}}}{N_{data}}, \quad \text{(S1)}$$

where, N_{data} is the number of experimental data. This step was done using MATLAB's built-in function called fminsearch. Figure S3 shows reaction rates as a function of temperature between experimental data and the model.

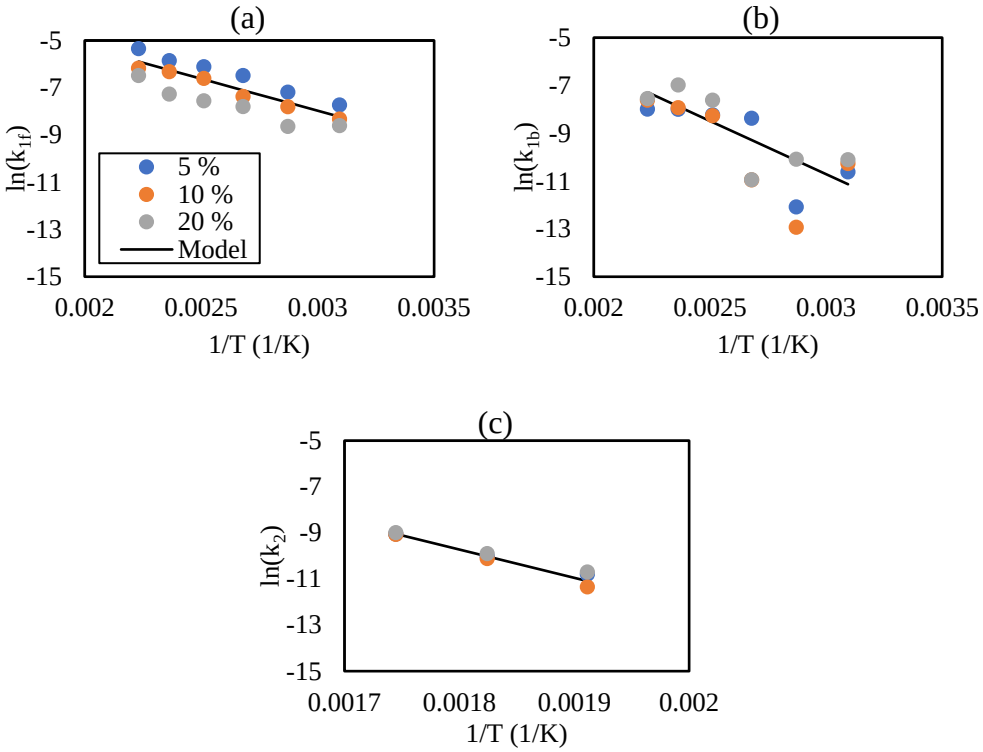

Figure S3. The Arrhenius plots for k_{1f} (a), k_{1b} (b), and k_2 (c).

S2. Sensible heat and specific heat capacity

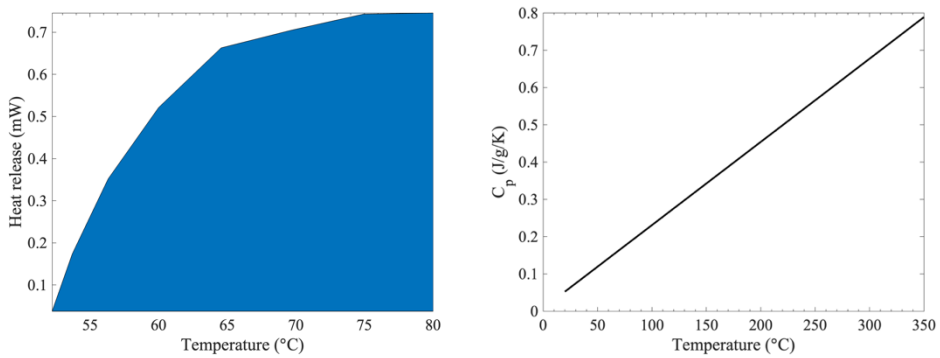

Figure S4. Sensible heat (a) and specific heat capacity (b) of biochar.

S3. Sub-models for physical properties implemented in the numerical model

Table S2. Values and correlations for physical properties

Property	Correlation/value	Refs.
Atmospheric pressure, Pa	$P_{atm} = 101325$	-
Wind speed, m s^{-1}	$u_{wind} = 1$	-
Bed pore diameter, mm	$d_{pore} = 10$	-
Tortuosity of char bed, -	$\tau = 1/\sqrt{\varepsilon}$	[1]
Permeability of char bed, - (Carman-Kozeney equation)	$\varphi = \frac{d_{pore}^2 \varepsilon^3}{180 \cdot (1-\varepsilon^2)}$	[2]
Reynolds number, -	$Re = \frac{2 \cdot u_{wind} \cdot bag\ width}{\mu_{air}}$	-
Prandtl number, -	$Pr = \frac{\alpha_{air}}{D_{AB}}$	-
Schmidt number, -	$Sc = \frac{\mu_{air}}{D_{AB}}$	-
Nusselt number, -	$Nu = 0.332 \cdot \sqrt{Re} \cdot \sqrt[3]{Pr}$	-
Sherwood number, -	$Sh = 0.332 \cdot \sqrt{Re} \cdot \sqrt[3]{Sc}$	-
Effective diffusivity of gas mixture, m^2 s^{-1}	$D_{mix} = (1 - x_A)(\sum \frac{x_i}{D_{Ai}})$	[3]
Specific heat capacity of gas	$\frac{C_{p,i}}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4$	[4]
Dynamic viscosity of gases, kg m^{-2} s^{-1}	$\mu_{N2} = -0.0001T^2 + 0.4428T + 60.145 \times 10^{-7}$ $\mu_{CO2} = (0.3794T + 38.631) \times 10^{-7}$ $\mu_{O2} = (-8 \times 10^5)T^2 + 0.488T + 75.521 \times 10^{-7}$	[5]
Thermal conductivity of gases, W m^{-1} K^{-1}	$\lambda_{CO2} = (0.0782T - 6.7926) \times 10^{-3}$ $\lambda_{N2} = (0.0532T + 11.861) \times 10^{-3}$ $\lambda_{O2} = (0.0605T + 9.7264) \times 10^{-3}$	[5]

S4. Evaluation of intraparticle effectiveness factor

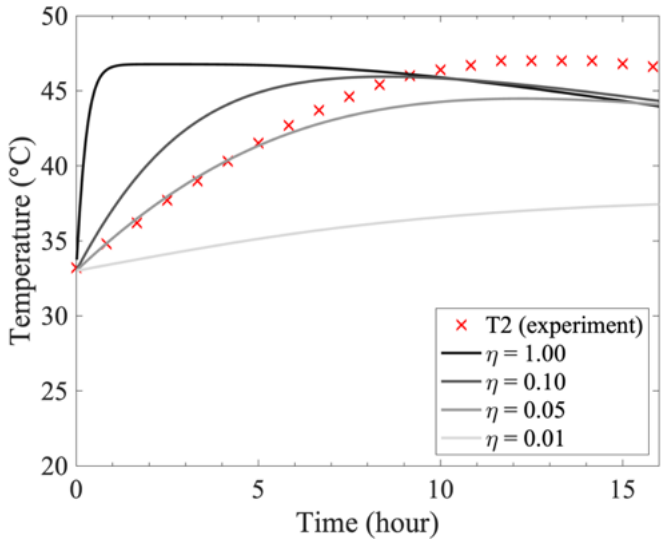

Figure S5. Effect of intraparticle effectiveness factor on time of self-heating.

References

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[5] Incopera FP, Dewitt DP, Bergman TL, Lavine AS. Fudamental Of Heat And Mass Transfer 6th Edition. vol. 53. 2013.