Supplementary Material for Article

Non-Isothermal Kinetics: Best Fitting Empirical Models Instead of Model Free Methods

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Keywords: Non-isothermal kinetics • Least squares evaluation • Isoconversional methods • Model-free methods • Biomass • Wood • Spruce.

Scope of this document: The least squares evaluation of experimental α(t) curves and experimental dα(t)/dt curves are presented for five TGA experiments on a wood sample. An empirical model was used:

$$d\alpha/dt = A(\alpha)f(\alpha)\exp(-\frac{E}{RT})$$

Note that *E* is constant here; the variation of the reactivity is expressed by function A(α)f(α).

See more info in the paper.

The five TGA experiments were taken from the following work:

- Barta-Rajnai, E.; Várhegyi, G.; Wang, L.; Skreiberg, Ø.; Grønli, M.; Czégény, Zs. Thermal decomposition kinetics of wood and bark and their torrefied products. *Energy Fuels* **2017**, *31*, 4024-4034. *doi*: 10.1021/acs.energyfuels.6b03419 Supporting info Repository

Notation in the Figures:

Experimental curves: oooo;

Curves calculated from the model: ——;

Temperature (when present): - - - .

Contents

S1. Evaluation of the experimental α(t) curves

Model: $d\alpha/dt = \tilde{A}(\alpha)\exp(-E/RT)(1-\alpha)$

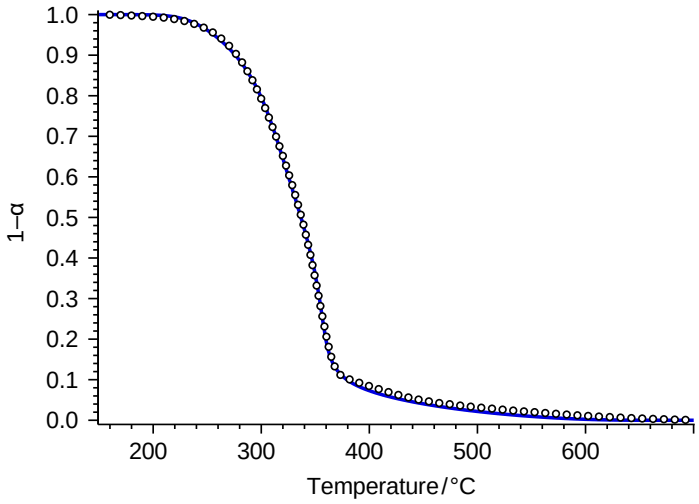
E= 179.29911

$x=2\alpha-1$

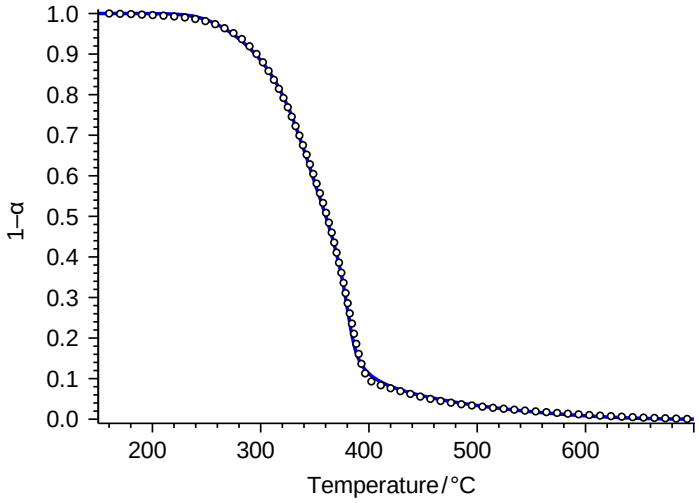
$\log_{10}\tilde{A}(x) = 12.241749 - .66597x + 2.01255x^2 + 2.242752x^3 - 3.154896x^4 - 4.881232x^5$

Expressed by Chebyshev polynomials of the first kind:

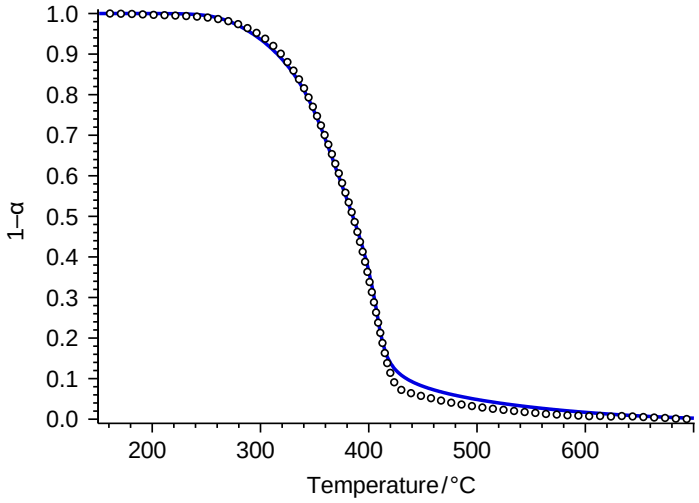
$\log_{10}\tilde{A}(x) = 12.064938T_0(x) - 2.034676T_1(x) - 0.571173T_2(x) - .964697T_3(x) - 0.394362T_4(x) - 0.305077T_5(x)$



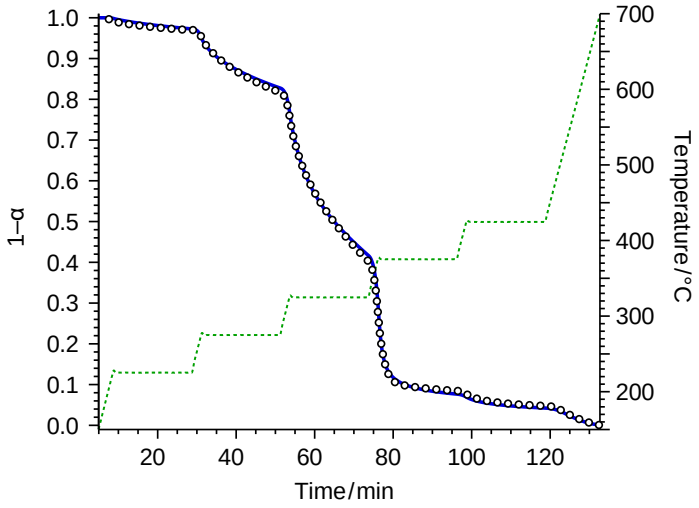
Wood 2.5°C/min 4mg
Relative deviation: 0.72%, Deviation: 23. µg



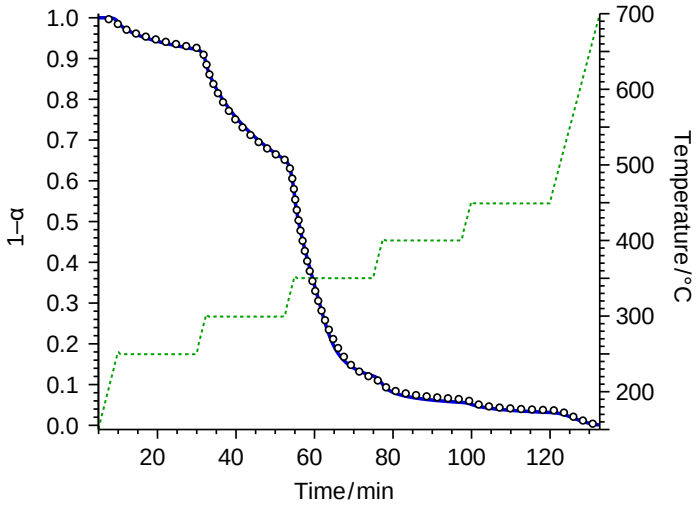
Wood 10°C/min 2mg
Relative deviation: 0.56 (0.56) %, Deviation: 9.3 µg



Wood 40°C/min 0.5mg
Relative deviation: 1.26 (1.26) %, Deviation: 5.1 µg



Wood stepwise T(t) A, 4mg
Relative deviation: 0.61 (0.61) %, Deviation: 20. µg



Wood stepwise T(t) B, 4mg
Relative deviation: 0.51 (0.51) %, Deviation: 19. µg

S2. Evaluation of the experimental dα/dt curves

Model: dα/dt= Ã(α) exp(-E/RT) (1-α)

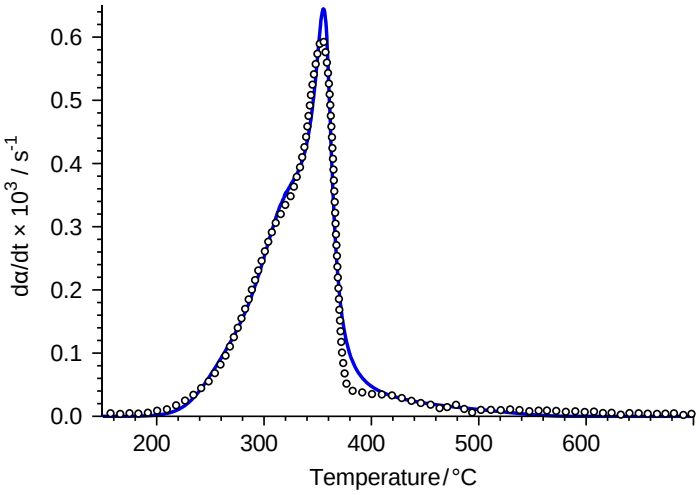
E= 171.81292

x=2α-1

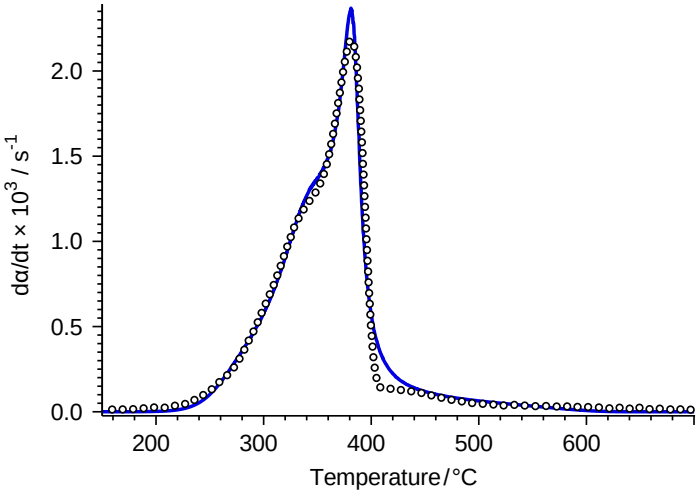
$\log_{10}\tilde{A}(x)= 11.613439 -0.442952x +1.448896x^2 + +0.847084x^3 -2.244368x^4 -2.849616x^5$

Expressed by Chebyshev polynomials of the first kind:

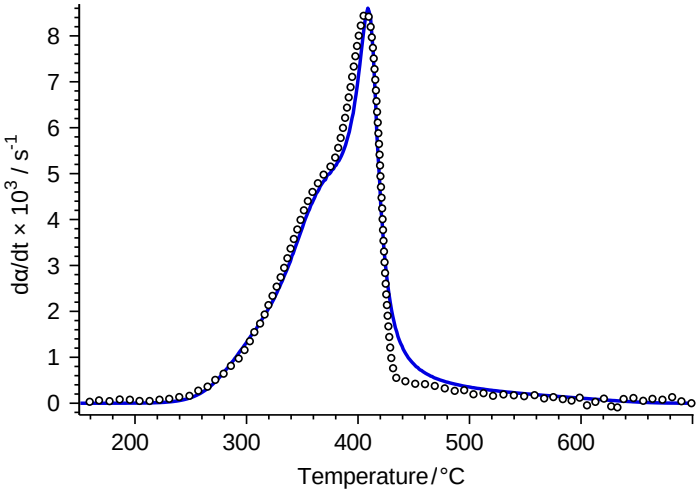
$\log_{10}\tilde{A}(x)= 11.496249T_0(x) -1.588649T_1(x) - -0.397736T_2(x) -0.678734T_3(x) -0.280546T_4(x) - -0.178101T_5(x)$



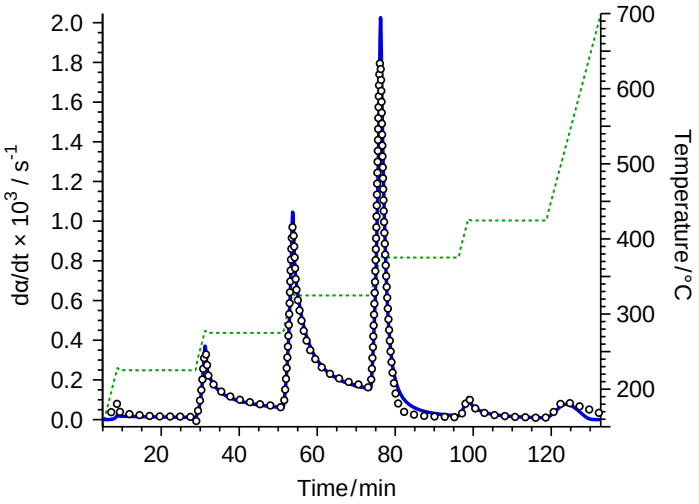
Wood 2.5°C/min 4mg
Relative deviation: 2.29%, Deviation: 0.044 µg/s



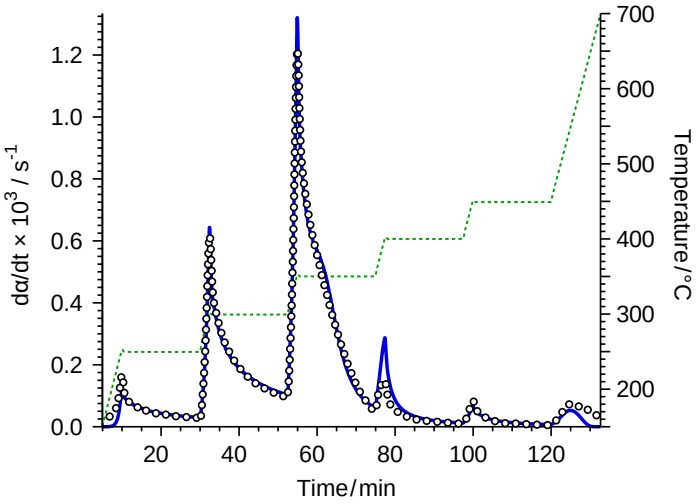
Wood 10°C/min 2mg
Relative deviation: 2.79%, Deviation: 0.10 µg/s



Wood 40°C/min 0.5mg
Relative deviation: 3.01%, Deviation: 0.10 µg/s



Wood stepwise T(t) A, 4mg
Relative deviation: 1.39%, Deviation: 0.082 µg/s



Wood stepwise T(t) B, 4mg
Relative deviation: 1.90%, Deviation: 0.085 µg/s