Supporting Information for Article

Empirical Models with Constant and Variable Activation Energy for Biomass Pyrolysis

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Gábor Várhegyi

Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences, PO Box 286, Budapest, Hungary 1519
Email: varhegyi.gabor@t-online.hu or gvarhegyi@gmail.com

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Scope of this document: Models are presented for 16 different types of biomass. Their performance is illustrated by figures showing the calculated and experimental data. *Such experimental curves are shown here that had also been displayed in the figures of the original papers.* In this way the reader can compare the present fit quality to the ones obtained by other sorts of modelling.

Notation in the Figures: Two models are shown for each biomass: one with $E(\alpha)$ approximated by a third-order polynomial **(red color)**, and another one when E does not depend on α **(blue color)**. This coloring scheme was applied to the plots of $E(\alpha)$ and $\tilde{A}(\alpha)f(\alpha)$ as well as to the figures illustrating the fit quality. In the latter figures the experimental mass loss rate curves ($-dm/dt$) were denoted **by thick gray lines**, while the temperature – time dependences ($T(t)$), when present, were represented by thin dashed green lines.

Each section starts with a figure on the 4 – 9 temperature programs that were employed for the given set of experiments; the selection of the colors in these figures is arbitrary (it aimed only at the discernibility of the 4 – 9 T(t) curves).

Contents

About the Employed Models

Herewith the model is repeated from the article and a few relations are added:

The employed empirical model:

$$d\alpha/dt = A(\alpha)f(\alpha)\exp(-E(\alpha)/RT) \qquad (S1)$$

where α is the reacted fraction (dimensionless), while $[A(\alpha)f(\alpha)]/s^{-1}$ and $E(\alpha)/kJmol^{-1}$ are empirical functions.

In a rearranged form:

$$d\alpha/dt = \tilde{A}(\alpha)(1-\alpha)\exp(-E(\alpha)/RT) \qquad (S2)$$

where the term $(1-\alpha)$ ensures that dα/dt would be 0 at $\alpha=1$. $\tilde{A}(\alpha)=A(\alpha)f(\alpha)/(1-\alpha)$ when $\alpha<1$. (Obviously, the division by $(1-\alpha)$ is not possible at the $\alpha=1$ point. There, however, $\tilde{A}(\alpha)$ may have any finite value so that $\tilde{A}(\alpha)(1-\alpha)$ would be zero at $\alpha=1$.)

A further rearrangement yields:

$$d\alpha/dt = (1-\alpha)\exp(\ln\tilde{A}(\alpha) - E(\alpha)/RT) \qquad (S3)$$

To obtain flexible approximations with limited numbers of unknowns, $\ln\tilde{A}(\alpha)$ and $E(\alpha)$ are approximated by polynomials. For this purpose, the variable $x=2\alpha-1$ is introduced which varies from -1 till +1 as α varies from 0 to 1 and the results will be presented as the following example shows:

$$E(x) = 177.269618 - 37.801456\,x + 26.878364\,x^2 + 93.1628\,x^3 \qquad (S4)$$

Each model will also be expressed by Chebyshev polynomials of the first kind (T_0, $T_1(x)$, $T_2(x)$, …) because they have favorable properties for actual calculations. For example, the above polynomial is also expressed as

$$E(x) = 190.7088\,T_0(x) + 32.070644\,T_1(x) + 13.439182\,T_2(x) + 23.2907\,T_3(x) \qquad (S5)$$

The user is kindly asked to select whichever form he/she likes better.

Pls note that the calculation with the by Chebyshev polynomials of the first kind are fast and simple. There is no need for the actual form of these polynomials because their values can be calculated by a simple recurrence relationship at any *x*. In our case it means the insertion of a few simple program lines in the source code. For example:

```
T0 = 1;
T1 = x;
T2 = 2*x*T1 - T0;
T3 = 2*x*T2 - T1;
E = a[0] + a[1]*T1 + a[2]*T2 + a[3]*T3;
```

where array **a** contains the coefficients of a polynomial of type eq S5 and the program lines are written in C (C++/C#/Java) notation.

S1. Wood shoots from an energy plantation

Source of the data:

[S1] Mészáros, E.; Várhegyi, G.; Jakab, E.; Marosvölgyi, B.: Thermogravimetric and reaction kinetic analysis of biomass samples from an energy plantation. *Energy Fuels* **2004**, *18*, 497-507. *doi:* 10.1021/ef034030%2B Repository

Four TGA experiments were available for each sample. The figure below shows the corresponding temperature programs. It is a redrawn/rearranged version of Figure 1 of the cited paper. Please note that the stepwise programs differed for the different samples; the one in Figure S2.1 was used for the willow shoots.

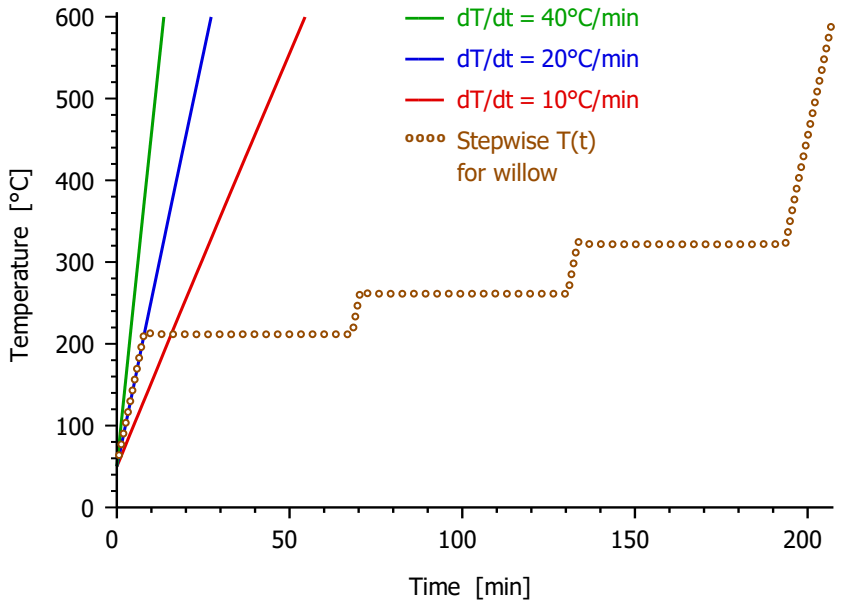


Figure S1.1: Temperature programs used for the TGA experiments of this section.

S1.1. Black locust shoots (Robinia pseudoacacia)

Model with constant E:

Input file: "B_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 201.39157$

$\log_{10}\tilde{A}(x)= 14.767721 -.837505x +.7874086x^2 +.175056x^3 +.0748392x^4 -.806736x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 15.18949T_0(x) -1.210423T_1(x) +.4311239T_2(x) -.208341T_3(x) +.0093549T_4(x) -.050421T_5(x)$

Model with third order E(α):

Input file: "B_3,5_oneC.PAR"

$x=2\alpha-1$

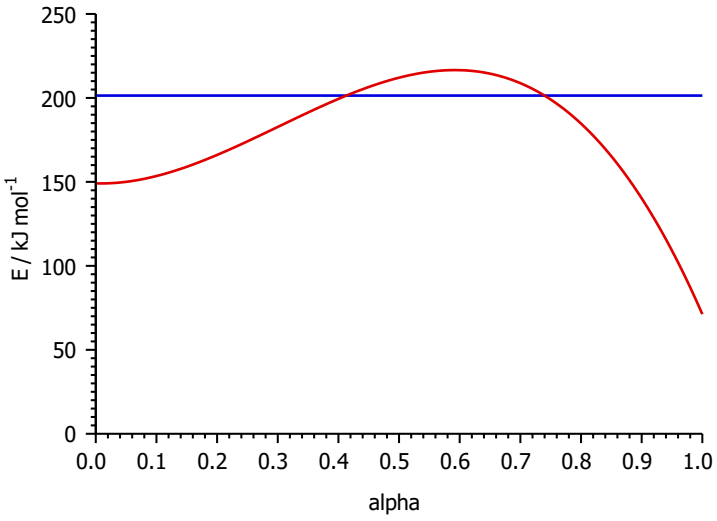
$E(x)= 212.05679 +46.19796x -101.87136x^2 -85.14972x^3$

$\log_{10}\tilde{A}(x)= 15.543158 +2.883188x -7.763372x^2 -5.756672x^3 -.703496x^4 -1.915872x^5$

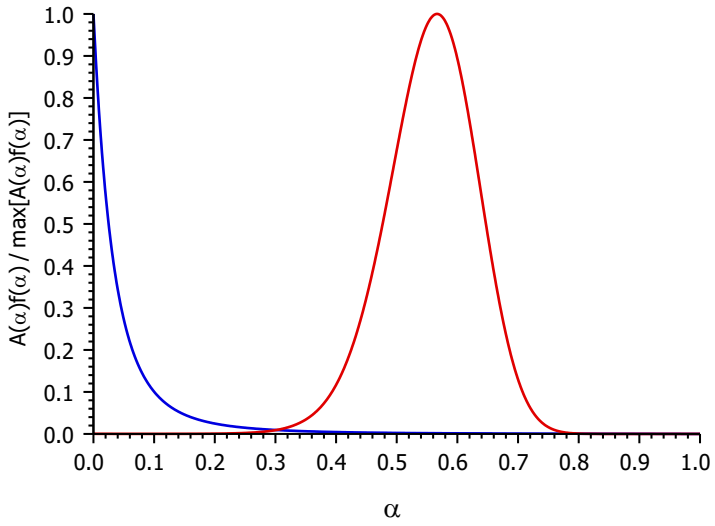
Expressed by Chebyshev polynomials of the first kind:

$E(x)= 161.12111T_0(x) -17.66433T_1(x) -50.93568T_2(x) -21.28743T_3(x)$

$\log_{10}\tilde{A}(x)= 11.397661T_0(x) -2.631736T_1(x) -4.233434T_2(x) -2.037878T_3(x) -.087937T_4(x) -.119742T_5(x)$



E(α) = polynomial of (2α-1)



Plot of A(α)f(α) / max[A(α)f(α)]

Parameter file: B_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 17.10$ $E(0)= 201.4$ $\log_{10}\tilde{A}(1)= 14.16$ $E(1)= 201.4$

mean $\log_{10}\tilde{A}= 15.05$ mean $E= 201.4$

Parameter file: B_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 11.87$ $E(0)= 149.1$ $\log_{10}\tilde{A}(1)= 2.29$ $E(1)= 71.2$

mean $\log_{10}\tilde{A}= 12.81$ mean $E= 178.1$

Parameter file: B_0,5_oneC.PAR

$A(0)f(0)= 1.256E+17$ $E(0)= 201.4$ $A(1)f(1)= 0.00$ $E(1)= 201.4$

mean $A(\alpha)f(\alpha)= 5.498E+15$ mean $E= 201.4$

max $A(\alpha)f(\alpha)= 1.256E+17$ at $\alpha= 0.000$ and $E= 201.4$

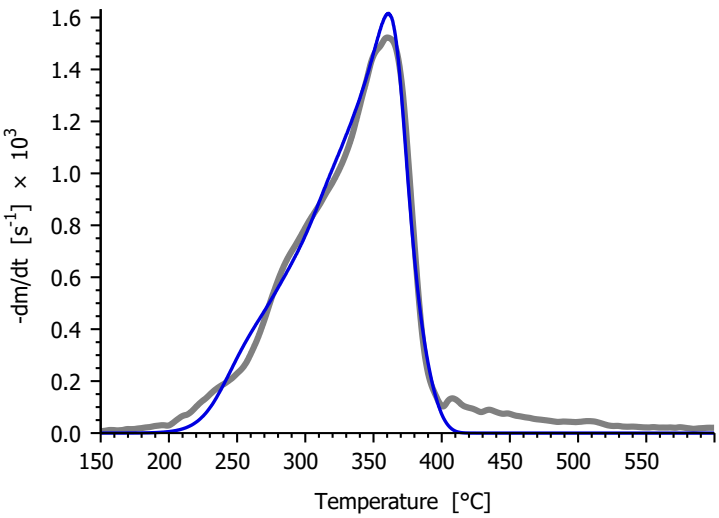
Parameter file: B_3,5_oneC.PAR

$A(0)f(0)= 7.339E+11$ $E(0)= 149.1$ $A(1)f(1)= 0.00$ $E(1)= 71.2$

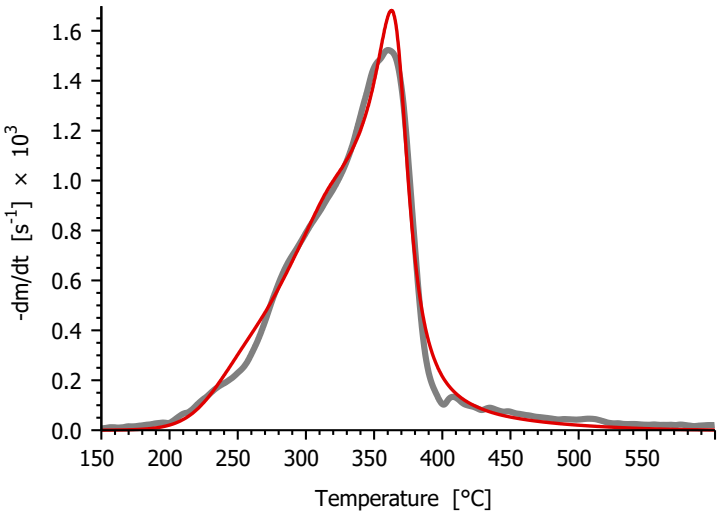
mean $A(\alpha)f(\alpha)= 4.718E+14$ mean $E= 178.1$

max $A(\alpha)f(\alpha)= 2.585E+15$ at $\alpha= 0.567$ and $E= 216.2$

Figures illustrating the fit quality *(cf. Figure 10 in reference [S1])*



Black locust shoots, 10°C/min
Relative deviation: 3.32%, Deviation: 0.20 µg/s
rms rel. dev. of 4 experiments: 3.11%
Model: x=2α-1
E(x) = 201.39
$\log_{10}$ Ã(x) = 15.189T_0(x) -1.21T_1(x) +.431T_2(x) -.208T_3(x)
+.009T_4(x) -.05T_5(x)
c = 0.788



Black locust shoots, 10°C/min
Relative deviation: 2.82%, Deviation: 0.17 µg/s
rms rel. dev. of 4 experiments: 2.65%
Model: x=2α-1
E(x) = 161.12T_0(x) -17.66T_1(x) -50.94T_2(x) -21.29T_3(x)
$\log_{10}$ Ã(x) = 11.398T_0(x) -2.632T_1(x) -4.233T_2(x) -2.038T_3(x)
-.088T_4(x) -.12T_5(x)
c = 0.851

S1.2. Poplar shoots

Model with constant E:

Input file: "P_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 207.00457$

$\log_{10}\tilde{A}(x)= 15.09038 -.657046x +1.360278x^2 -.238448x^3 -2.281232x^4 -2.317552x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 14.915057T_0(x) -2.284352T_1(x) -.460477T_2(x) -.783847T_3(x) -.285154T_4(x) -.144847T_5(x)$

Model with third order E(α):

Input file: "P_3,5_oneC.PAR"

$x=2\alpha-1$

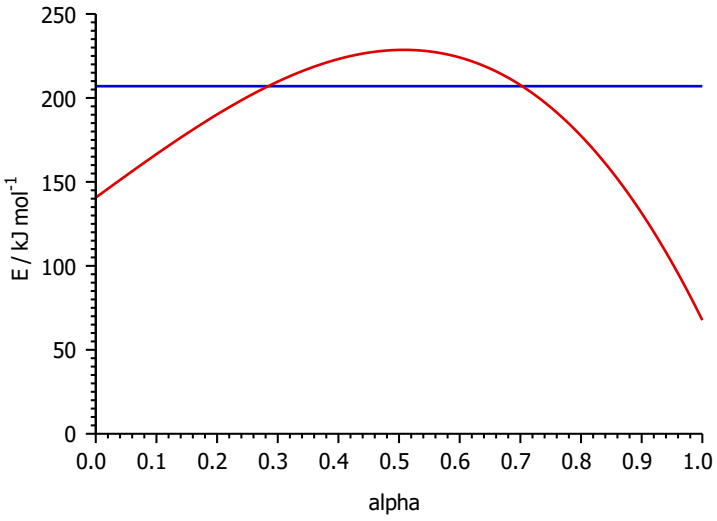
$E(x)= 228.59258 +3.95597x -124.41916x^2 -40.45308x^3$

$\log_{10}\tilde{A}(x)= 16.905634 -.453547x -9.157212x^2 -3.179244x^3 -2.015672x^4 -1.364736x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 166.383T_0(x) -26.38384T_1(x) -62.20958T_2(x) -10.11327T_3(x)$

$\log_{10}\tilde{A}(x)= 11.571151T_0(x) -3.69094T_1(x) -5.586442T_2(x) -1.221291T_3(x) -.251959T_4(x) -.085296T_5(x)$



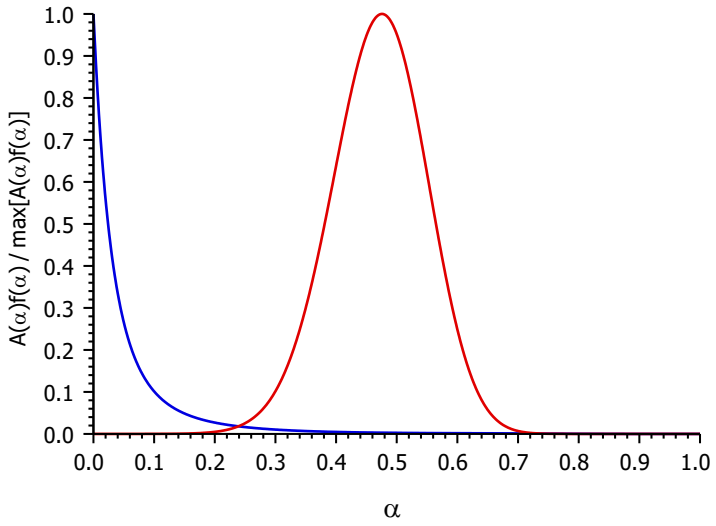
E(α) = polynomial of (2α-1)

Parameter file: P_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 17.38 E(0)= 207.0 $\log_{10}\tilde{A}(1)$= 10.96 E(1)= 207.0
mean $\log_{10}\tilde{A}$= 15.09 mean E= 207.0

Parameter file: P_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 10.73 E(0)= 140.7 $\log_{10}\tilde{A}(1)$= 0.74 E(1)= 67.7
mean $\log_{10}\tilde{A}$= 13.45 mean E= 187.1



Plot of A(α)f(α) / max[A(α)f(α)]

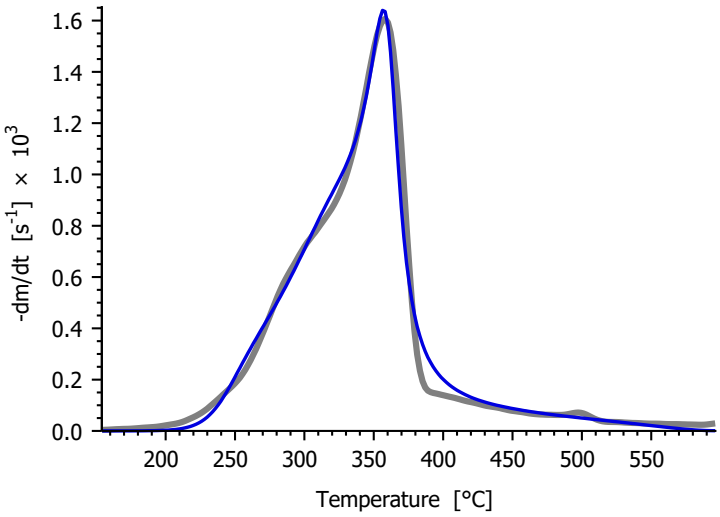
Parameter file: P_0,5_oneC.PAR

A(0)f(0)= 2.413E+17 E(0)= 207.0 A(1)f(1)= 0.00 E(1)= 207.0
mean A(α)f(α)= 1.053E+16 mean E= 207.0
max A(α)f(α)= 2.413E+17 at α= 0.000 and E= 207.0

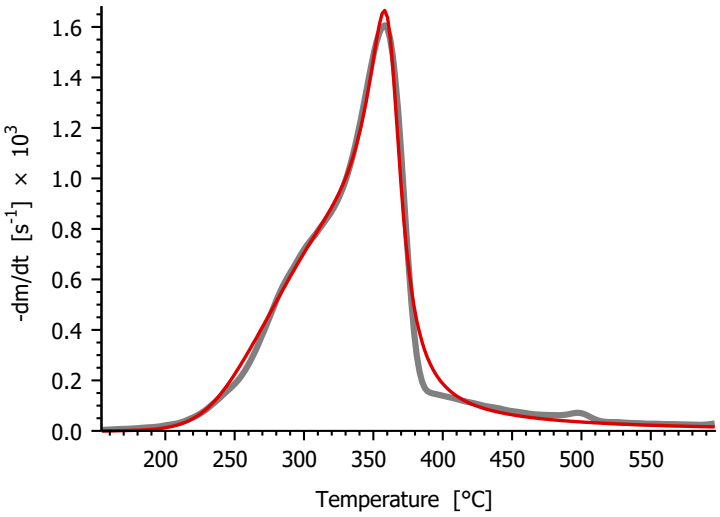
Parameter file: P_3,5_oneC.PAR

A(0)f(0)= 5.374E+10 E(0)= 140.7 A(1)f(1)= 0.00 E(1)= 67.7
mean A(α)f(α)= 8.250E+15 mean E= 187.1
max A(α)f(α)= 4.227E+16 at α= 0.476 and E= 228.1

Figures illustrating the fit quality *(cf. Figure 10 in reference [S1])*



Poplar shoots, 10°C/min
Relative deviation: 2.95%, Deviation: 0.18 µg/s
rms rel. dev. of 4 experiments: 3.78%
Model: x=2α-1
E(x) = 207.0
$\log_{10}$ Ã(x) = 14.915T_0(x) -2.284T_1(x) -.46T_2(x) -.784T_3(x)
-.285T_4(x) -.145T_5(x)
c = 0.791



Poplar shoots, 10°C/min
Relative deviation: 2.24%, Deviation: 0.14 µg/s
rms rel. dev. of 4 experiments: 3.13%
Model: x=2α-1
E(x) = 166.38T_0(x) -26.38T_1(x) -62.21T_2(x) -10.11T_3(x)
$\log_{10}$ Ã(x) = 11.571T_0(x) -3.691T_1(x) -5.586T_2(x) -1.221T_3(x)
-.252T_4(x) -.085T_5(x)
c = 0.804

S1.3. Willow shoots

Model with constant E:

Input file: "W_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 192.30365$

$\log_{10}\tilde{A}(x)= 13.872239 -.914686x +1.330912x^2 +.955792x^3 -1.563432x^4 -2.8156x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 13.951408T_0(x) -1.957592T_1(x) -.11626T_2(x) -.640927T_3(x) -.195429T_4(x) -.175975T_5(x)$

Model with third order E(α):

Input file: "W_3,5_oneC.PAR"

$x=2\alpha-1$

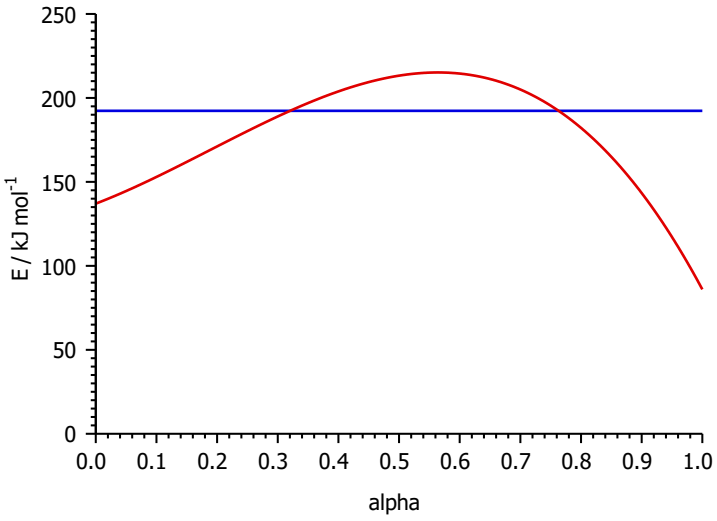
$E(x)= 213.26372 +28.74274x -101.7404x^2 -54.27984x^3$

$\log_{10}\tilde{A}(x)= 15.633178 +1.380063x -7.413694x^2 -3.175292x^3 -1.403592x^4 -2.098592x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 162.39352T_0(x) -11.96714T_1(x) -50.8702T_2(x) -13.56996T_3(x)$

$\log_{10}\tilde{A}(x)= 11.399984T_0(x) -2.313026T_1(x) -4.408643T_2(x) -1.449633T_3(x) -.175449T_4(x) -.131162T_5(x)$



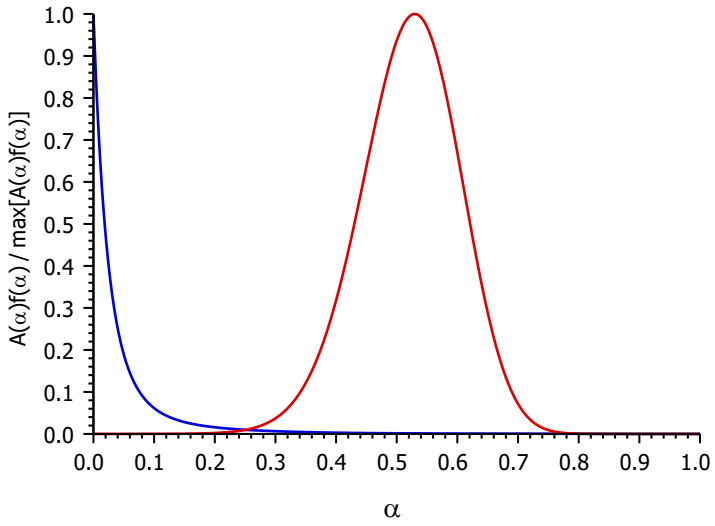
E(α) = polynomial of (2α-1)

Parameter file: W_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)=$ 16.41 E(0)= 192.3 $\log_{10}\tilde{A}(1)=$ 10.87 E(1)= 192.3
mean $\log_{10}\tilde{A}=$ 14.00 mean E= 192.3

Parameter file: W_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)=$ 10.71 E(0)= 137.1 $\log_{10}\tilde{A}(1)=$ 2.92 E(1)= 86.0
mean $\log_{10}\tilde{A}=$ 12.88 mean E= 179.3



Plot of A(α)f(α) / max[A(α)f(α)]

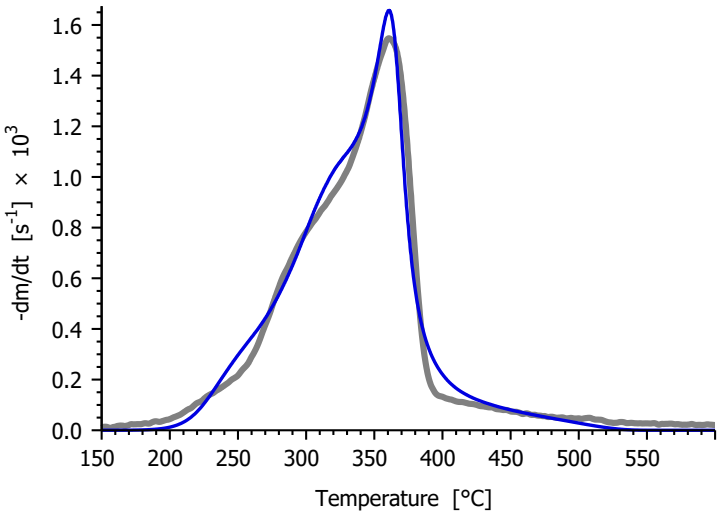
Parameter file: W_0,5_oneC.PAR

A(0)f(0)= 2.595E+16 E(0)= 192.3 A(1)f(1)= 0.00 E(1)= 192.3
mean A(α)f(α)= 8.746E+14 mean E= 192.3
max A(α)f(α)= 2.595E+16 at α= 0.000 and E= 192.3

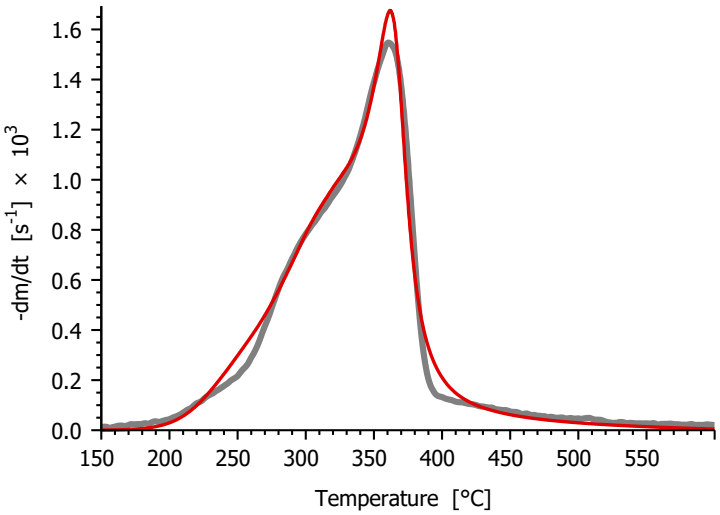
Parameter file: W_3,5_oneC.PAR

A(0)f(0)= 5.125E+10 E(0)= 137.1 A(1)f(1)= 0.00 E(1)= 86.0
mean A(α)f(α)= 4.668E+14 mean E= 179.3
max A(α)f(α)= 2.294E+15 at α= 0.530 and E= 214.6

Figures illustrating the fit quality *(cf. Figure 10 in reference [S1])*



Willow shoots, 10°C/min
Relative deviation: 3.66%, Deviation: 0.23 µg/s
rms rel. dev. of 4 experiments: 3.42%
Model: x=2α-1
E(x) = 192.3
$\log_{10}$ Ã(x) = 13.951T_0(x) -1.958T_1(x) -.116T_2(x) -.641T_3(x)
-.195T_4(x) -.176T_5(x)
c = 0.831



Willow shoots, 10°C/min
Relative deviation: 2.72%, Deviation: 0.17 µg/s
rms rel. dev. of 4 experiments: 2.74%
Model: x=2α-1
E(x) = 162.39T_0(x) -11.97T_1(x) -50.87T_2(x) -13.57T_3(x)
$\log_{10}$ Ã(x) = 11.4T_0(x) -2.313T_1(x) -4.409T_2(x) -1.45T_3(x)
-.175T_4(x) -.131T_5(x)
c = 0.841

S2. Industrial Biomass Wastes

Source of the data:

[S2] Becidan, M.; Várhegyi, G.; Hustad, J. E.; Skreiberg, Ø.: Thermal decomposition of biomass wastes. A kinetic study. *Ind. Eng. Chem. Res.* **2007**, *46*, 2428-2437. *doi:* 10.1021/ie061468z Repository

Five TGA experiments were available for each sample. The figure below shows the corresponding temperature programs. It is a redrawn/rearranged version of Figure 1 of the cited paper. Please note that the CRR ("constant reaction rate") programs were determined by the apparatus separately for each sample. The one in Figure S2.1 belongs to the brewer spent grains.

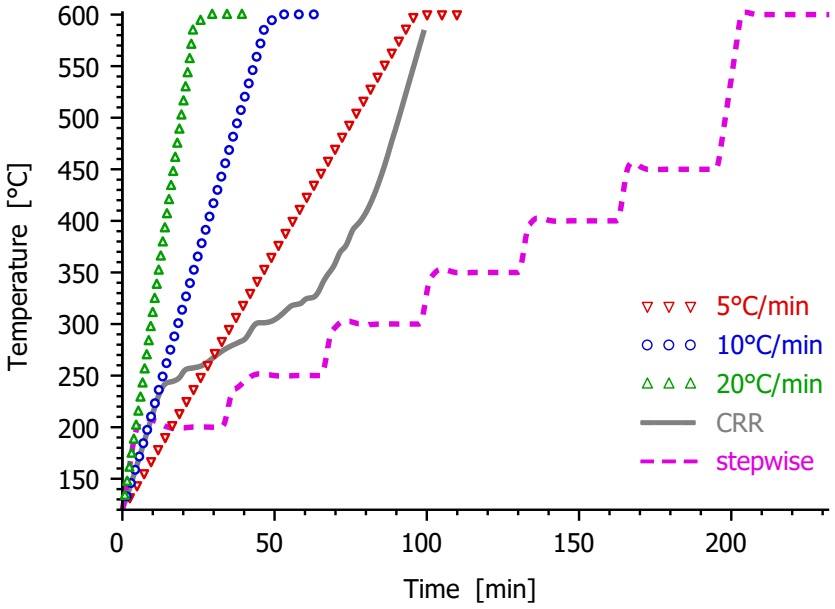


Figure S2.1: Temperature programs used for the TGA experiments of this section.

S2.1. Brewer spent grains

Model with constant E:

Input file: "B_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 205.49138$

$\log_{10}\tilde{A}(x)= 15.480744 -1.943698x +.876088x^2 +.930456x^3 -2.606512x^4 -3.164768x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 14.941346T_0(x) -3.223836T_1(x) -.865212T_2(x) -.756376T_3(x) -.325814T_4(x) -.197798T_5(x)$

Model with third order E(α):

Input file: "B_3,5_oneC.PAR"

$x=2\alpha-1$

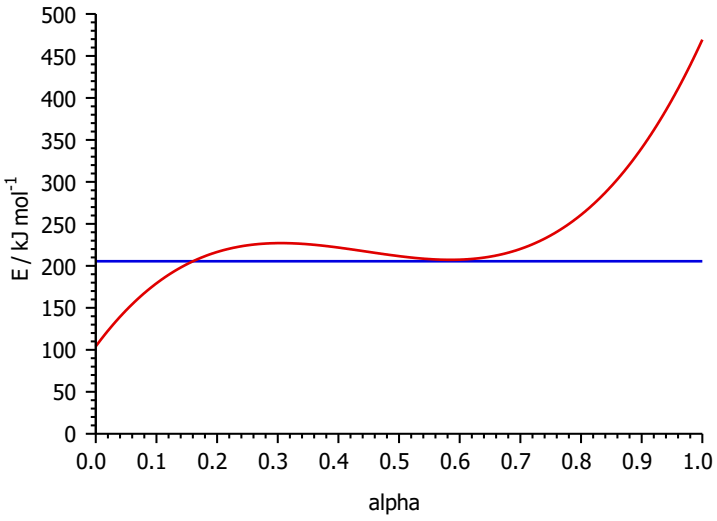
$E(x)= 211.563722 -45.096816x +75.199396x^2 +227.735488x^3$

$\log_{10}\tilde{A}(x)= 16.038065 -6.0397905x +8.675692x^2 +20.7184024x^3 -6.172224x^4 -3.687408x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 249.16342T_0(x) +125.7048T_1(x) +37.599698T_2(x) +56.933872T_3(x)$

$\log_{10}\tilde{A}(x)= 18.061327T_0(x) +7.1943813T_1(x) +1.251734T_2(x) +4.0272856T_3(x) -.771528T_4(x) -.230463T_5(x)$



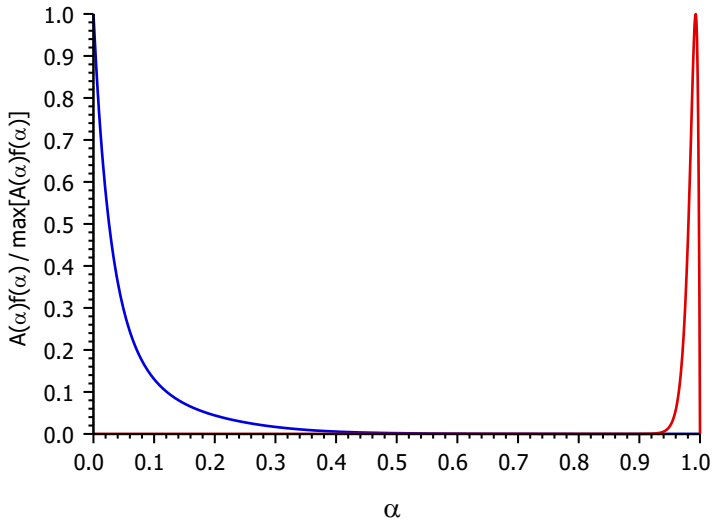
E(α) = polynomial of (2α-1)

Parameter file: B_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)=$ 17.93 E(0)= 205.5 $\log_{10}\tilde{A}(1)=$ 9.57 E(1)= 205.5
mean $\log_{10}\tilde{A}=$ 15.25 mean E= 205.5

Parameter file: B_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)=$ 7.55 E(0)= 104.1 $\log_{10}\tilde{A}(1)=$ 29.53 E(1)= 469.4
mean $\log_{10}\tilde{A}=$ 17.70 mean E= 236.6



Plot of A(α)f(α) / max[A(α)f(α)]

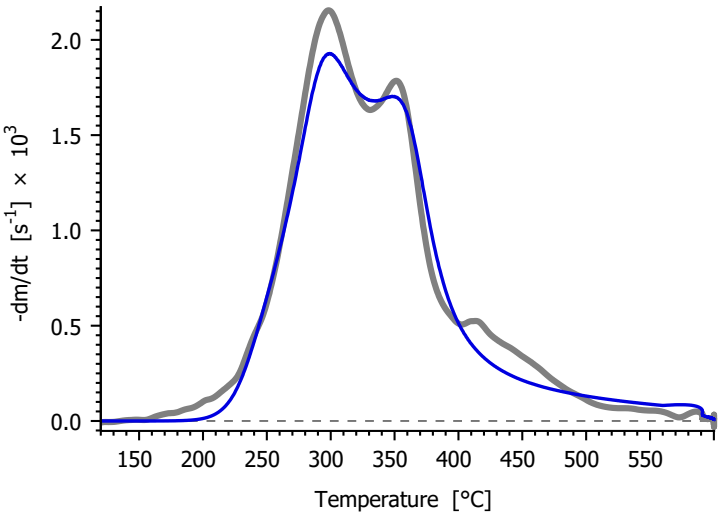
Parameter file: B_0,5_oneC.PAR

A(0)f(0)= 8.479E+17 E(0)= 205.5 A(1)f(1)= 0.00 E(1)= 205.5
mean A(α)f(α)= 4.205E+16 mean E= 205.5
max A(α)f(α)= 8.479E+17 at α= 0.000 and E= 205.5

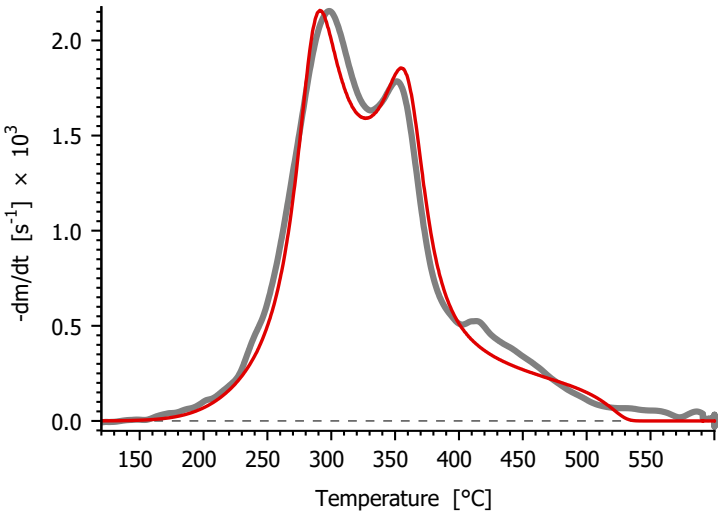
Parameter file: B_3,5_oneC.PAR

A(0)f(0)= 3.551E+07 E(0)= 104.1 A(1)f(1)= 0.00 E(1)= 469.4
mean A(α)f(α)= 1.742E+25 mean E= 236.6
max A(α)f(α)= 8.967E+26 at α= 0.993 and E= 458.4

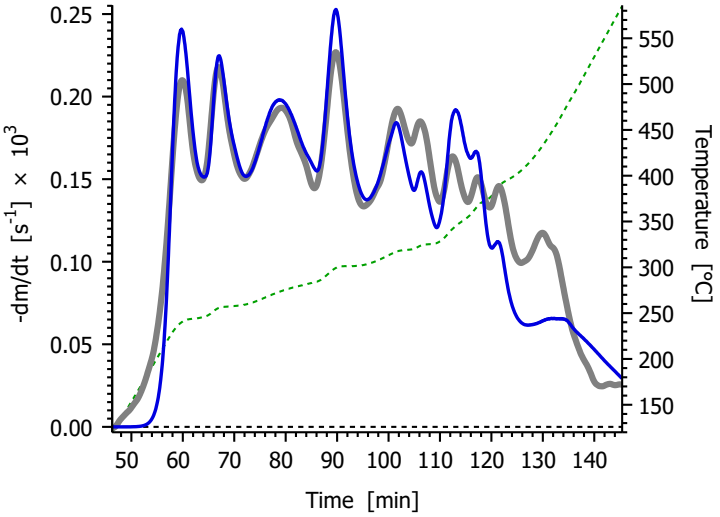
Figures illustrating the fit quality *(cf. Figure 4 in reference [S2])*



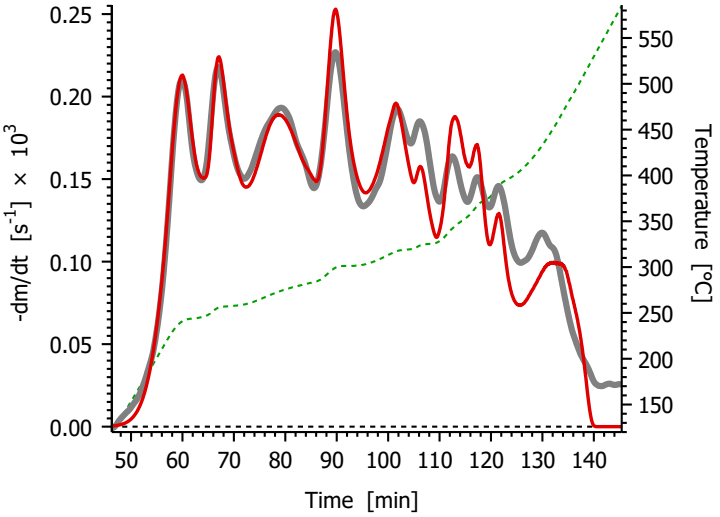
Brewer spent grains, 20°C/min
Relative deviation: 3.22%, Deviation: 0.18 µg/s
rms rel. dev. of 5 experiments: 5.28%
Model: x=2α-1
E(x) = 205.49
$\log_{10}$ Ã(x) = 14.941T_0(x) -3.224T_1(x) -.865T_2(x) -.756T_3(x) -.326T_4(x) -.198T_5(x)
c = 0.759



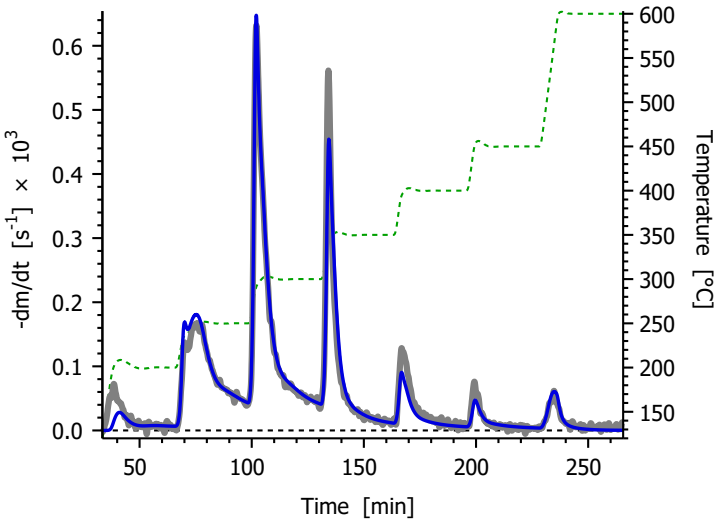
Brewer spent grains, 20°C/min
Relative deviation: 3.01%, Deviation: 0.17 µg/s
rms rel. dev. of 5 experiments: 3.94%
Model: x=2α-1
E(x) = 249.16T_0(x) +125.7T_1(x) +37.6T_2(x) +56.93T_3(x)
$\log_{10}$ Ã(x) = 18.061T_0(x) +7.194T_1(x) +1.252T_2(x) +4.027T_3(x) -.772T_4(x) -.23T_5(x)
c = 0.758



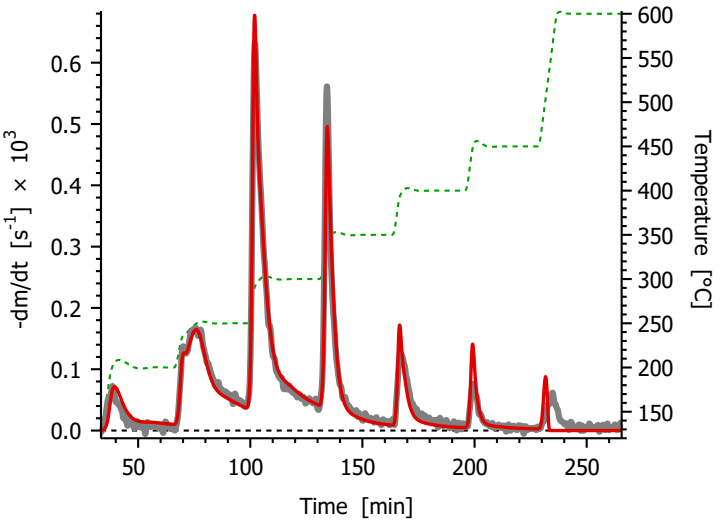
Brewer spent grains, "constant reaction rate" (CRR)
Relative deviation: 9.64%, Deviation: 0.10 µg/s
rms rel. dev. of 5 experiments: 5.28%
Model: x=2α-1
E(x) = 205.49
$\log_{10}$ Ã(x) = 14.941T_0(x) -3.224T_1(x) -.865T_2(x) -.756T_3(x) -.326T_4(x) -.198T_5(x)
c = 0.759



Brewer spent grains, "constant reaction rate" (CRR)
Relative deviation: 6.87%, Deviation: 0.073 µg/s
rms rel. dev. of 5 experiments: 3.94%
Model: x=2α-1
E(x) = 249.16T_0(x) +125.7T_1(x) +37.6T_2(x) +56.93T_3(x)
$\log_{10}$ Ã(x) = 18.061T_0(x) +7.194T_1(x) +1.252T_2(x) +4.027T_3(x) -.772T_4(x) -.23T_5(x)
c = 0.758



Brewer spent grains, Stepwise T(t)
Relative deviation: 2.55%, Deviation: 0.078 µg/s
rms rel. dev. of 5 experiments: 5.28%
Model: x=2α-1
E(x) = 205.49
$\log_{10}$ Ã(x) = 14.941T_0(x) -3.224T_1(x) -.865T_2(x) -.756T_3(x)
-.326T_4(x) -.198T_5(x)
c = 0.759



Brewer spent grains, Stepwise T(t)
Relative deviation: 2.44%, Deviation: 0.075 µg/s
rms rel. dev. of 5 experiments: 3.94%
Model: x=2α-1
E(x) = 249.16T_0(x) +125.7T_1(x) +37.6T_2(x) +56.93T_3(x)
$\log_{10}$ Ã(x) = 18.061T_0(x) +7.194T_1(x) +1.252T_2(x) +4.027T_3(x)
-.772T_4(x) -.23T_5(x)
c = 0.758

S2.2. Coffee waste

Model with constant E:

Input file: "C_0,5_oneC.PAR"

$x=2\alpha-1$

E= 206.20704

$\log_{10}\tilde{A}(x)= 15.69215 -1.090325x -.199498x^2 -3.290896x^3 -1.54684x^4 -.204288x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 15.012336T_0(x) -3.686177T_1(x) -.873169T_2(x) -.886564T_3(x) -.193355T_4(x) -.012768T_5(x)$

Model with third order E(α):

Input file: "C_3,5_oneC.PAR"

$x=2\alpha-1$

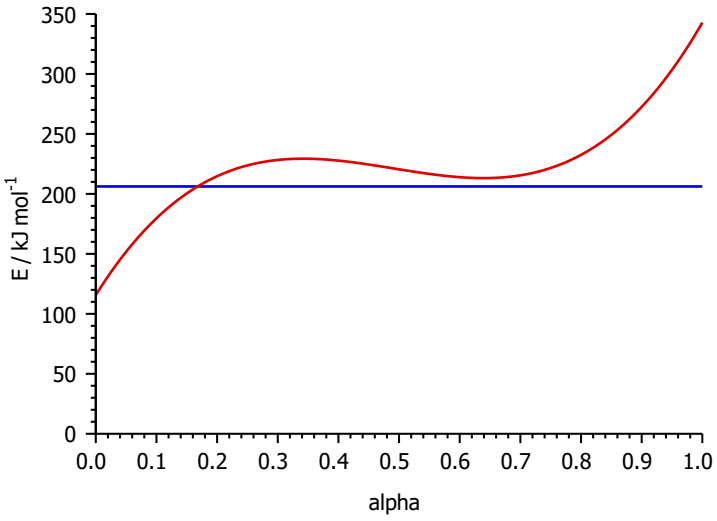
$E(x)= 220.4857005 -40.704909x +8.731879x^2 +154.29576x^3$

$\log_{10}\tilde{A}(x)= 17.015448 -4.8389645x +1.855026x^2 +10.371016x^3 -4.78824x^4 -.356224x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 224.85164T_0(x) +75.016911T_1(x) +4.3659395T_2(x) +38.57394T_3(x)$

$\log_{10}\tilde{A}(x)= 16.147371T_0(x) +2.7166575T_1(x) -1.466607T_2(x) +2.481434T_3(x) -.59853T_4(x) -.022264T_5(x)$



E(α) = polynomial of (2α-1)

Parameter file: C_0,5_oneC.PAR

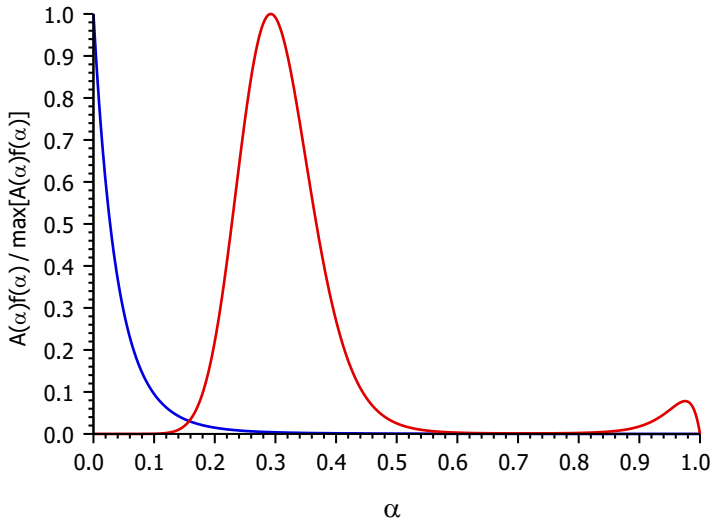
$\log_{10}\tilde{A}(0)$= 18.53 E(0)= 206.2 $\log_{10}\tilde{A}(1)$= 9.36 E(1)= 206.2

mean $\log_{10}\tilde{A}$= 15.32 mean E= 206.2

Parameter file: C_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 8.91 E(0)= 115.6 $\log_{10}\tilde{A}(1)$= 19.26 E(1)= 342.8

mean $\log_{10}\tilde{A}$= 16.68 mean E= 223.4



Plot of A(α)f(α) / max[A(α)f(α)]

Parameter file: C_0,5_oneC.PAR

A(0)f(0)= 3.399E+18 E(0)= 206.2 A(1)f(1)= 0.00 E(1)= 206.2

mean A(α)f(α)= 1.444E+17 mean E= 206.2

max A(α)f(α)= 3.399E+18 at α= 0.000 and E= 206.2

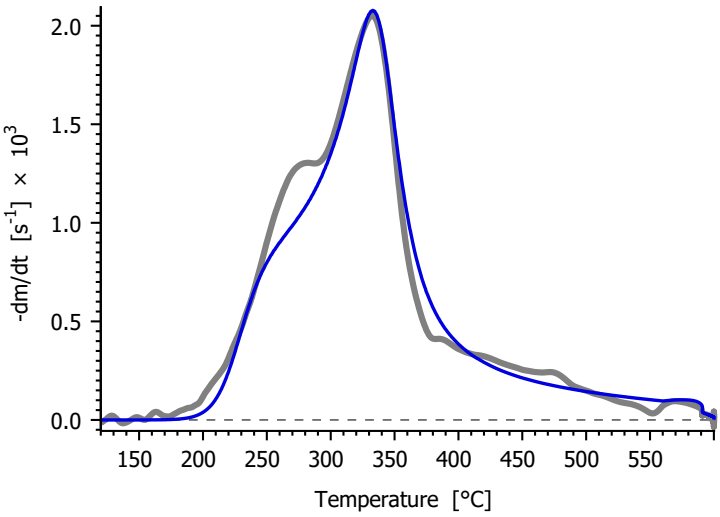
Parameter file: C_3,5_oneC.PAR

A(0)f(0)= 8.061E+08 E(0)= 115.6 A(1)f(1)= 0.00 E(1)= 342.8

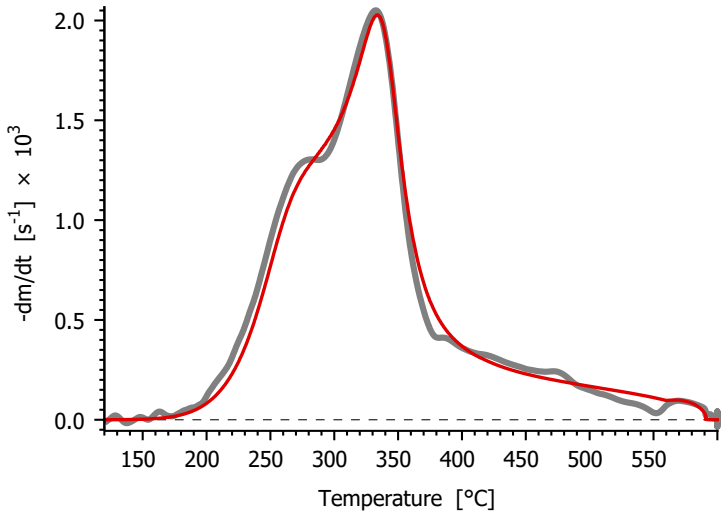
mean A(α)f(α)= 3.238E+17 mean E= 223.4

max A(α)f(α)= 2.060E+18 at α= 0.292 and E= 227.8

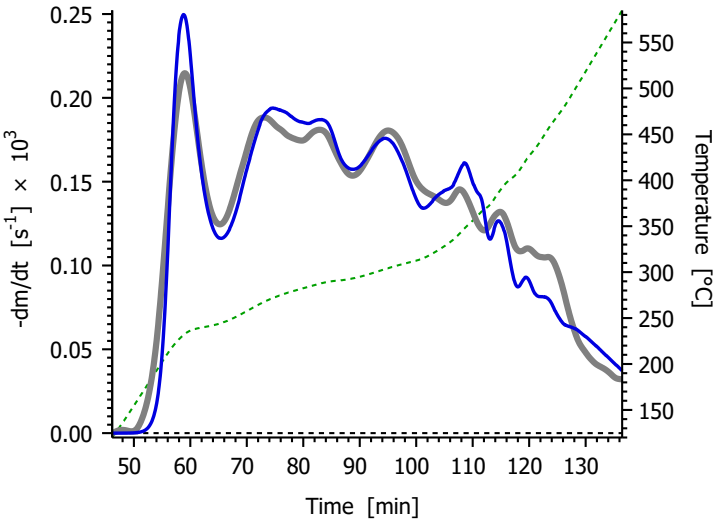
Figures illustrating the fit quality *(cf. Figure 5 in reference [S2])*



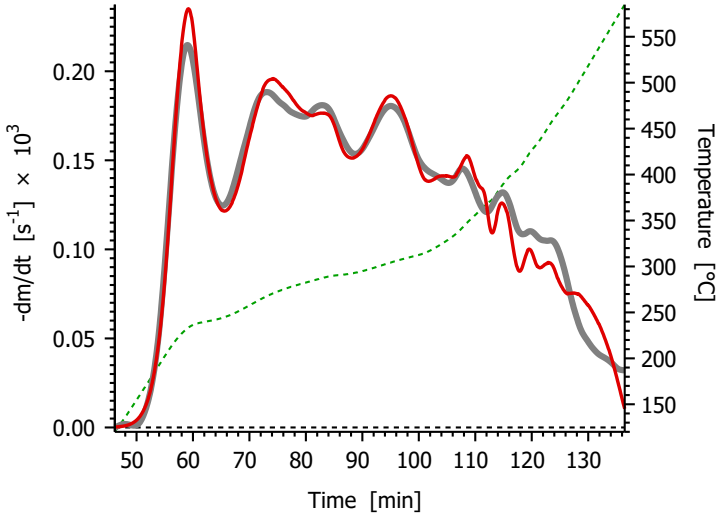
Coffee waste, 20°C/min
Relative deviation: 3.22%, Deviation: 0.16 µg/s
rms rel. dev. of 5 experiments: 3.76%
Model: x=2α-1
E(x) = 206.21
$\log_{10}$ Ã(x) = 15.012T_0(x) -3.686T_1(x) -.873T_2(x) -.887T_3(x) -.193T_4(x) -.013T_5(x)
c = 0.689



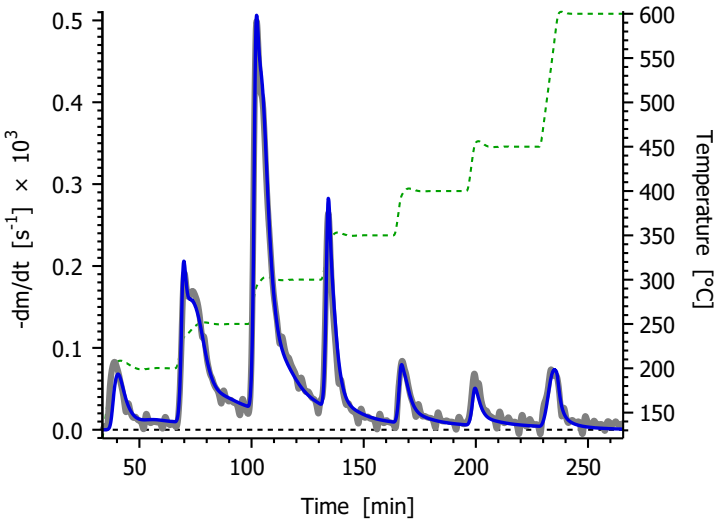
Coffee waste, 20°C/min
Relative deviation: 2.22%, Deviation: 0.11 µg/s
rms rel. dev. of 5 experiments: 2.65%
Model: x=2α-1
E(x) = 224.85T_0(x) +75.02T_1(x) +4.37T_2(x) +38.57T_3(x)
$\log_{10}$ Ã(x) = 16.147T_0(x) +2.717T_1(x) -1.467T_2(x) +2.481T_3(x) -.599T_4(x) -.022T_5(x)
c = 0.687



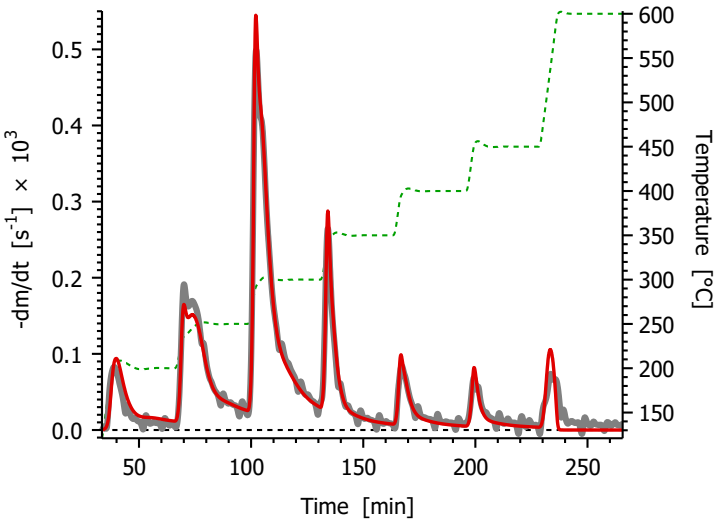
Coffee waste, "constant reaction rate" (CRR)
Relative deviation: 6.57%, Deviation: 0.069 µg/s
rms rel. dev. of 5 experiments: 3.76%
Model: x=2α-1
E(x) = 206.21
$\log_{10}$ Ã(x) = 15.012T_0(x) -3.686T_1(x) -.873T_2(x) -.887T_3(x) -.193T_4(x) -.013T_5(x)
c = 0.689



Coffee waste, "constant reaction rate" (CRR)
Relative deviation: 4.24%, Deviation: 0.045 µg/s
rms rel. dev. of 5 experiments: 2.65%
Model: x=2α-1
E(x) = 224.85T_0(x) +75.02T_1(x) +4.37T_2(x) +38.57T_3(x)
$\log_{10}$ Ã(x) = 16.147T_0(x) +2.717T_1(x) -1.467T_2(x) +2.481T_3(x) -.599T_4(x) -.022T_5(x)
c = 0.687



Coffee waste, Stepwise T(t)
Relative deviation: 2.03%, Deviation: 0.050 µg/s
rms rel. dev. of 5 experiments: 3.76%
Model: x=2α-1
E(x) = 206.21
$\log_{10}$ Ã(x) = 15.012T_0(x) -3.686T_1(x) -.873T_2(x) -.887T_3(x)
-.193T_4(x) -.013T_5(x)
c = 0.689



Coffee waste, Stepwise T(t)
Relative deviation: 2.17%, Deviation: 0.053 µg/s
rms rel. dev. of 5 experiments: 2.65%
Model: x=2α-1
E(x) = 224.85T_0(x) +75.02T_1(x) +4.37T_2(x) +38.57T_3(x)
$\log_{10}$ Ã(x) = 16.147T_0(x) +2.717T_1(x) -1.467T_2(x) +2.481T_3(x)
-.599T_4(x) -.022T_5(x)
c = 0.687

S2.3. Medium density fiberboard

Model with constant E:

Input file: "F_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 178.76916$

$\log_{10}\tilde{A}(x)= 12.799454 -.925107x +1.25016x^2 +1.629328x^3 -1.983728x^4 -4.327232x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 12.680636T_0(x) -2.407631T_1(x) -.366784T_2(x) -.944928T_3(x) -.247966T_4(x) -.270452T_5(x)$

Model with third order E(α):

Input file: "F_3,5_oneC.PAR"

$x=2\alpha-1$

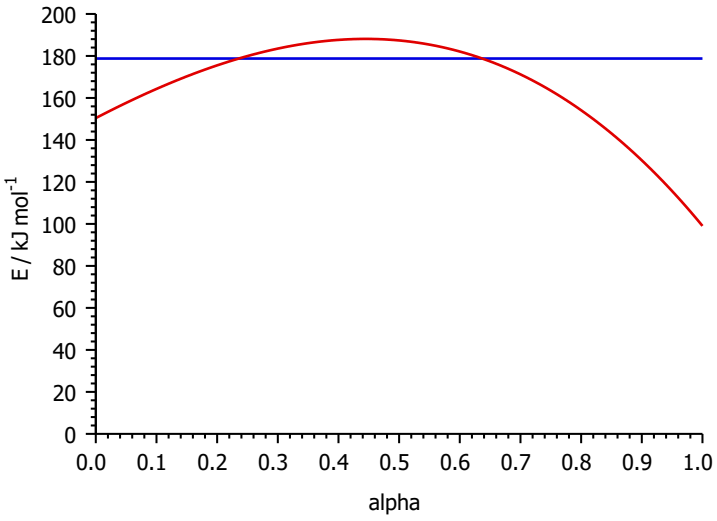
$E(x)= 187.38753 -13.38397x -62.65204x^2 -12.29512x^3$

$\log_{10}\tilde{A}(x)= 13.555281 -2.124616x -4.26881x^2 +.462856x^3 -1.82284x^4 -3.499696x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 156.06151T_0(x) -22.60531T_1(x) -31.32602T_2(x) -3.07378T_3(x)$

$\log_{10}\tilde{A}(x)= 10.737311T_0(x) -3.964784T_1(x) -3.045825T_2(x) -.977941T_3(x) -.227855T_4(x) -.218731T_5(x)$



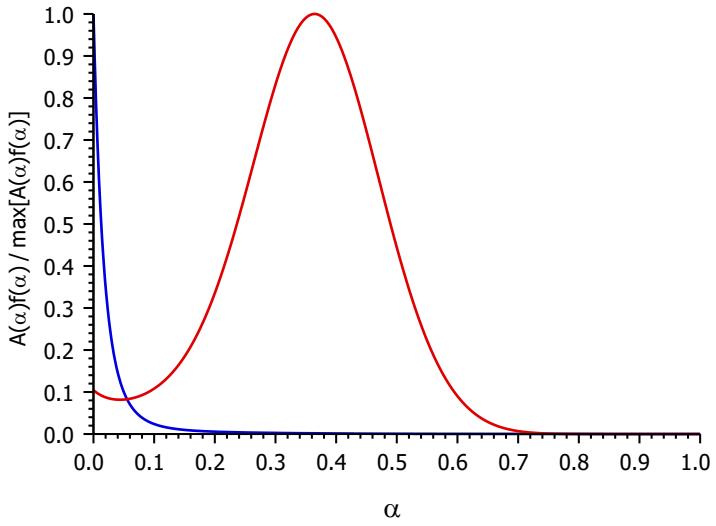
E(α) = polynomial of (2α-1)

Parameter file: F_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 15.69 E(0)= 178.8 $\log_{10}\tilde{A}(1)$= 8.44 E(1)= 178.8
mean $\log_{10}\tilde{A}$= 12.82 mean E= 178.8

Parameter file: F_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 12.63 E(0)= 150.4 $\log_{10}\tilde{A}(1)$= 2.30 E(1)= 99.1
mean $\log_{10}\tilde{A}$= 11.77 mean E= 166.5



Plot of A(α)f(α) / max[A(α)f(α)]

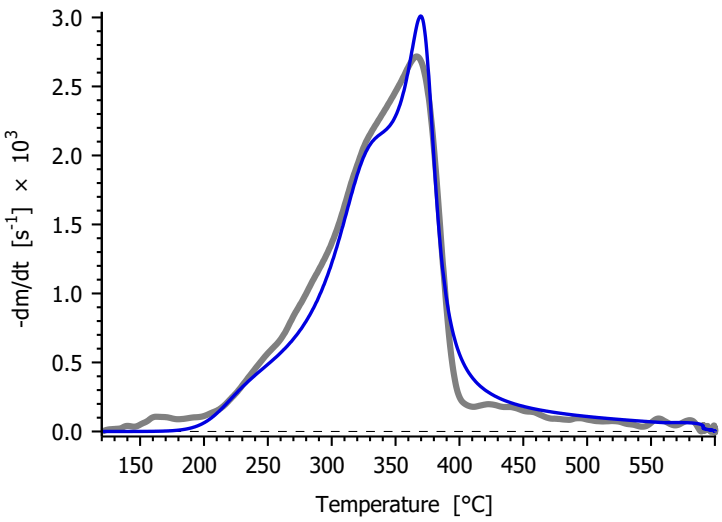
Parameter file: F_0,5_oneC.PAR

A(0)f(0)= 4.885E+15 E(0)= 178.8 A(1)f(1)= 0.00 E(1)= 178.8
mean A(α)f(α)= 1.097E+14 mean E= 178.8
max A(α)f(α)= 4.885E+15 at α= 0.000 and E= 178.8

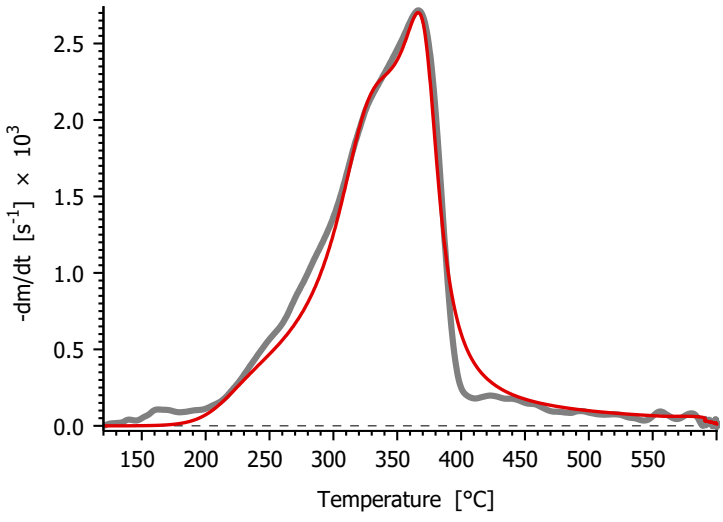
Parameter file: F_3,5_oneC.PAR

A(0)f(0)= 4.218E+12 E(0)= 150.4 A(1)f(1)= 0.00 E(1)= 99.1
mean A(α)f(α)= 1.134E+13 mean E= 166.5
max A(α)f(α)= 4.043E+13 at α= 0.364 and E= 186.7

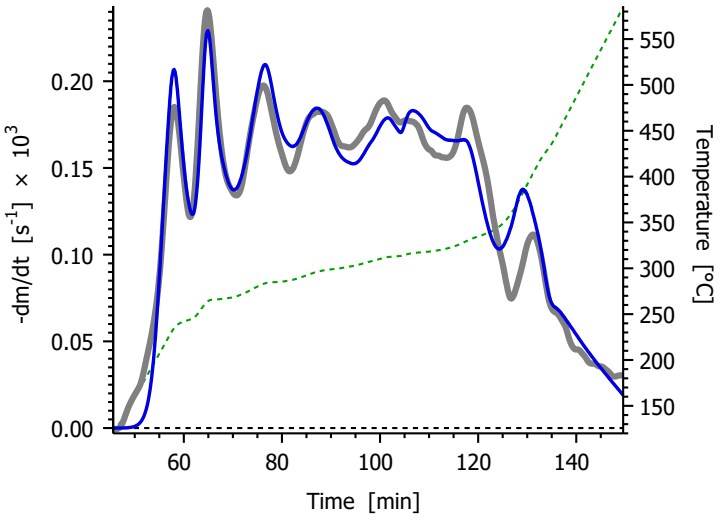
Figures illustrating the fit quality *(cf. Figure 6 in reference [S2])*



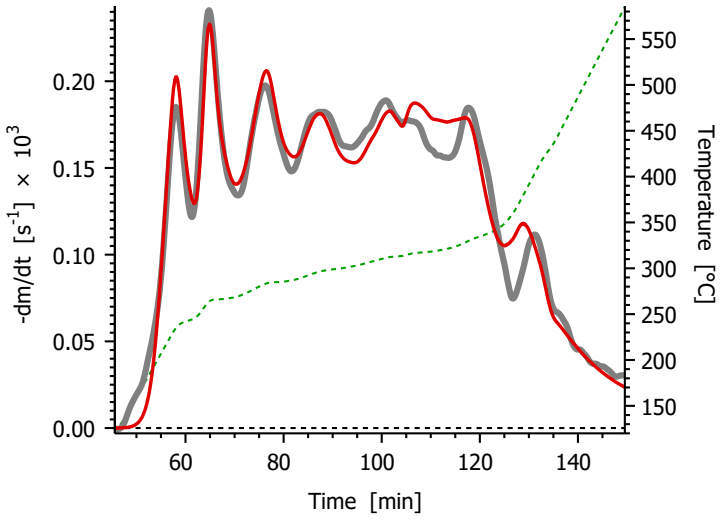
Fiberboard, 20°C/min
Relative deviation: 2.93%, Deviation: 0.20 µg/s
rms rel. dev. of 5 experiments: 3.56%
Model: x=2α-1
E(x) = 178.77
$\log_{10}$ Ã(x) = 12.681T_0(x) -2.408T_1(x) -.367T_2(x) -.945T_3(x) -.248T_4(x) -.27T_5(x)
c = 0.813



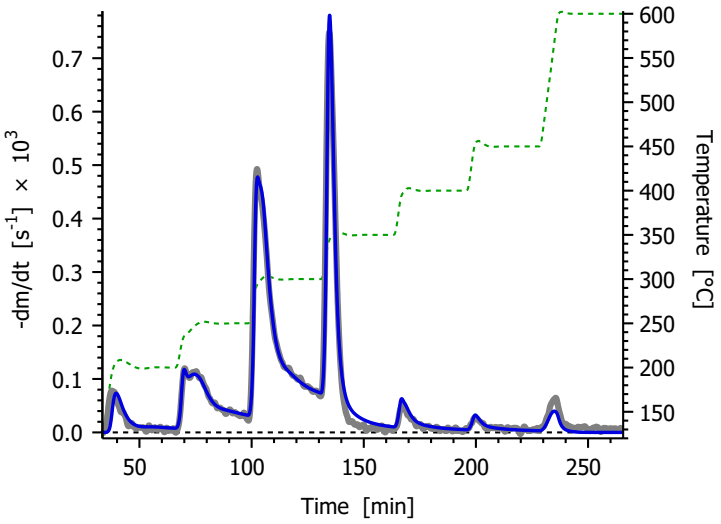
Fiberboard, 20°C/min
Relative deviation: 2.71%, Deviation: 0.18 µg/s
rms rel. dev. of 5 experiments: 3.08%
Model: x=2α-1
E(x) = 156.06T_0(x) -22.61T_1(x) -31.33T_2(x) -3.07T_3(x)
$\log_{10}$ Ã(x) = 10.737T_0(x) -3.965T_1(x) -3.046T_2(x) -.978T_3(x) -.228T_4(x) -.219T_5(x)
c = 0.827



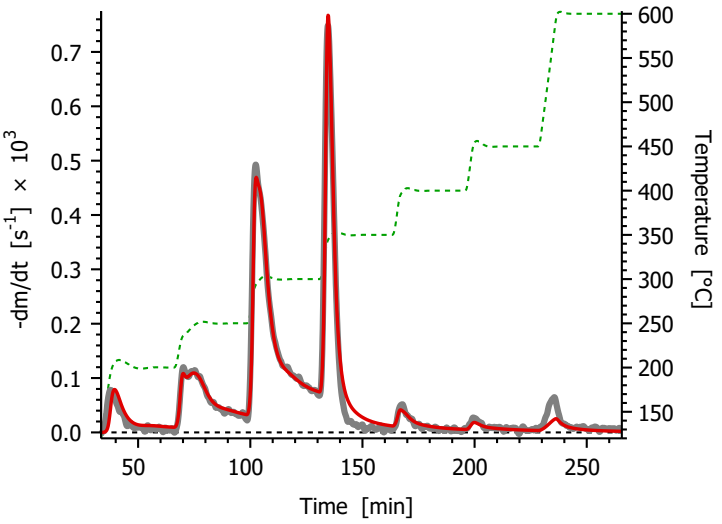
Fiberboard, "constant reaction rate" (CRR)
Relative deviation: 5.93%, Deviation: 0.067 µg/s
rms rel. dev. of 5 experiments: 3.56%
Model: x=2α-1
E(x) = 178.77
$\log_{10}$ Ã(x) = 12.681T_0(x) -2.408T_1(x) -.367T_2(x) -.945T_3(x) -.248T_4(x) -.27T_5(x)
c = 0.813



Fiberboard, "constant reaction rate" (CRR)
Relative deviation: 4.77%, Deviation: 0.054 µg/s
rms rel. dev. of 5 experiments: 3.08%
Model: x=2α-1
E(x) = 156.06T_0(x) -22.61T_1(x) -31.33T_2(x) -3.07T_3(x)
$\log_{10}$ Ã(x) = 10.737T_0(x) -3.965T_1(x) -3.046T_2(x) -.978T_3(x) -.228T_4(x) -.219T_5(x)
c = 0.827



Fiberboard, stepwise T(t)
Relative deviation: 2.02%, Deviation: 0.073 µg/s
rms rel. dev. of 5 experiments: 3.56%
Model: x=2α-1
E(x) = 178.77
$\log_{10}$ Ã(x) = 12.681T_0(x) -2.408T_1(x) -.367T_2(x) -.945T_3(x) -.248T_4(x) -.27T_5(x)
c = 0.813



Fiberboard, stepwise T(t)
Relative deviation: 2.09%, Deviation: 0.076 µg/s
rms rel. dev. of 5 experiments: 3.08%
Model: x=2α-1
E(x) = 156.06T_0(x) -22.61T_1(x) -31.33T_2(x) -3.07T_3(x)
$\log_{10}$ Ã(x) = 10.737T_0(x) -3.965T_1(x) -3.046T_2(x) -.978T_3(x) -.228T_4(x) -.219T_5(x)
c = 0.827

S3. Four Agricultural Residues

Source of the data:

[S3] Várhegyi, G.; Bobály, B.; Jakab, E.; Chen, H.: Thermogravimetric study of biomass pyrolysis kinetics. A distributed activation energy model with prediction tests. *Energy Fuels* **2011**, *25*, 24-32. *doi:* 10.1021/ef101079r Supporting Info Repository

Four TGA experiments were available for each sample. The figures below show the corresponding temperature programs. It is a redrawn/rearranged version of Figure 2 of the cited paper. The Supporting Information of the cited paper contains all the experimental curves with different evaluations. (It is available free-of-charge at the internet links given in the above reference.)

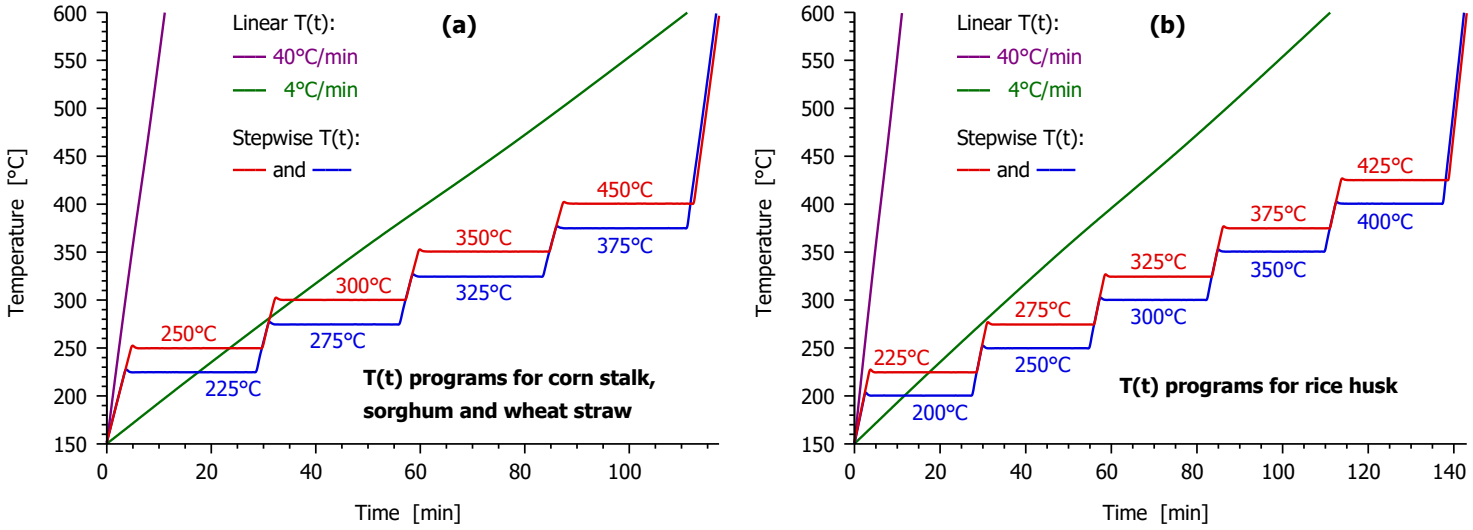


Figure S3.1: Temperature programs used for the TGA experiments of this section.

S3.1. Corn stalk

Model with constant E:

Input file: "C_0,5_oneC.PAR"

x=2α-1

E= 187.97731

$\log_{10}\tilde{A}(x)$= 13.775727 -.36308x +.381556x^2 -3.726592x^3 -4.469088x^4 -3.221648x^5

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)$= 12.290597$T_0(x)$ -5.171554$T_1(x)$ -2.043766$T_2(x)$ -1.938413$T_3(x)$ -.558636$T_4(x)$ -.201353$T_5(x)$

Model with third order E(α):

Input file: "C_3,5_oneC.PAR"

x=2α-1

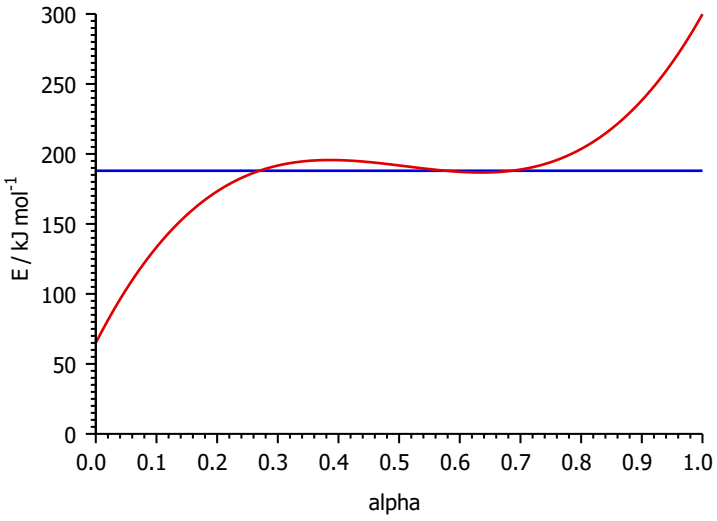
E(x)= 191.764335 -26.613237x -9.33327x^2 +144.055868x^3

$\log_{10}\tilde{A}(x)$= 14.190545 -2.7887559x +1.070722x^2 +10.1355028x^3 -5.115208x^4 -1.183872x^5

Expressed by Chebyshev polynomials of the first kind:

E(x)= 187.0977$T_0(x)$ +81.428664$T_1(x)$ -4.666635$T_2(x)$ +36.013967$T_3(x)$

$\log_{10}\tilde{A}(x)$= 12.807703$T_0(x)$ +4.0729512$T_1(x)$ -2.022243$T_2(x)$ +2.1639157$T_3(x)$ -.639401$T_4(x)$ -.073992$T_5(x)$



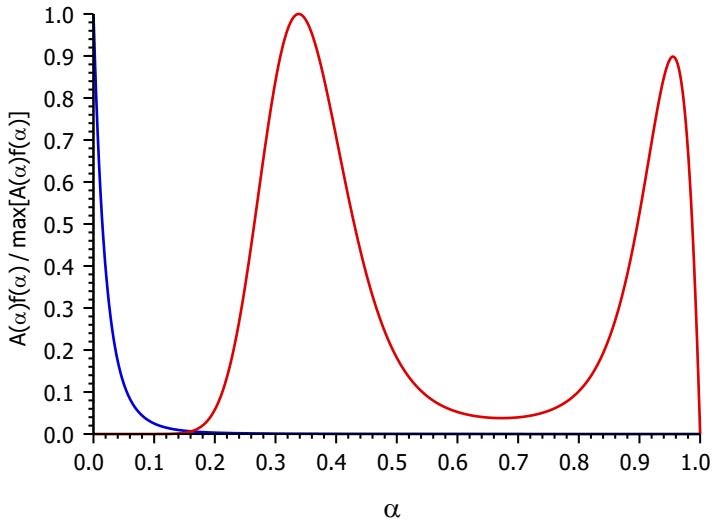
E(α) = polynomial of (2α-1)

Parameter file: C_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 17.00 E(0)= 188.0 $\log_{10}\tilde{A}(1)$= 2.38 E(1)= 188.0
mean $\log_{10}\tilde{A}$= 13.01 mean E= 188.0

Parameter file: C_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 3.98 E(0)= 65.0 $\log_{10}\tilde{A}(1)$= 16.31 E(1)= 299.9
mean $\log_{10}\tilde{A}$= 13.52 mean E= 188.7



Plot of A(α)f(α) / max[A(α)f(α)]

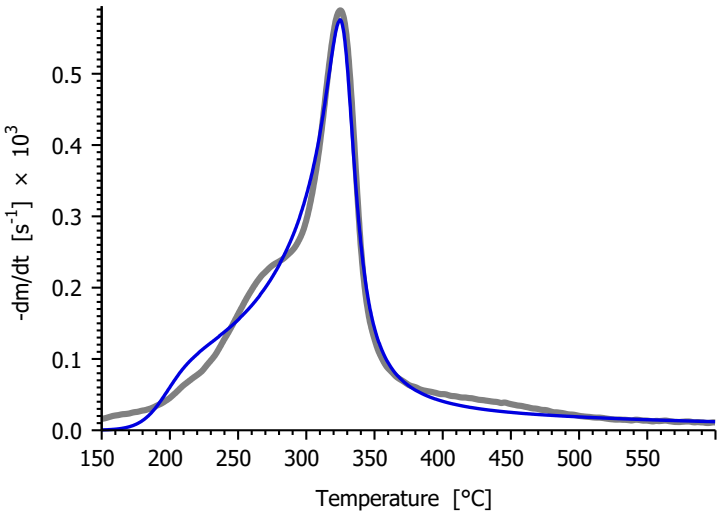
Parameter file: C_0,5_oneC.PAR

A(0)f(0)= 9.989E+16 E(0)= 188.0 A(1)f(1)= 0.00 E(1)= 188.0
mean A(α)f(α)= 2.389E+15 mean E= 188.0
max A(α)f(α)= 9.989E+16 at α= 0.000 and E= 188.0

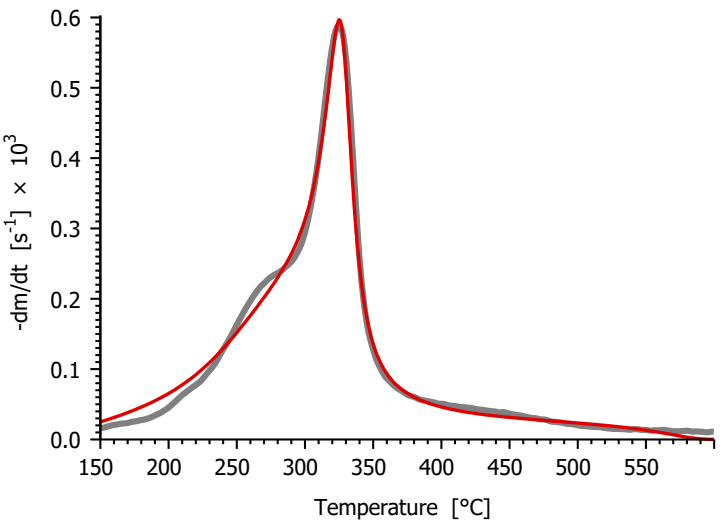
Parameter file: C_3,5_oneC.PAR

A(0)f(0)= 9.620E+03 E(0)= 65.0 A(1)f(1)= 0.00 E(1)= 299.9
mean A(α)f(α)= 1.223E+14 mean E= 188.7
max A(α)f(α)= 4.271E+14 at α= 0.338 and E= 194.5

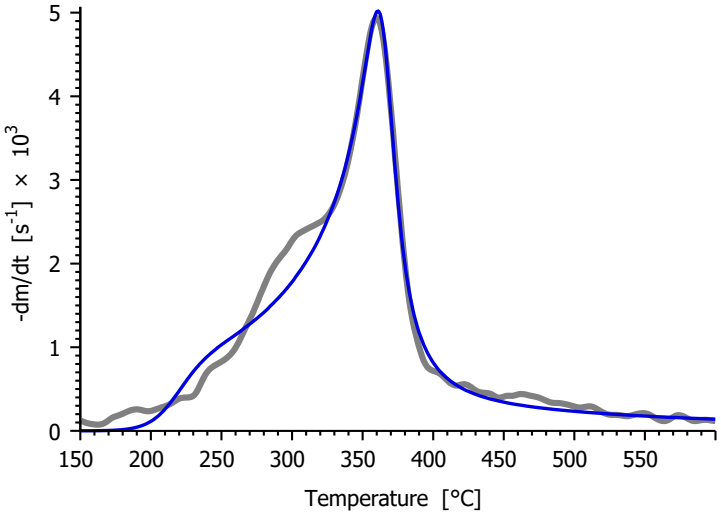
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S3])*



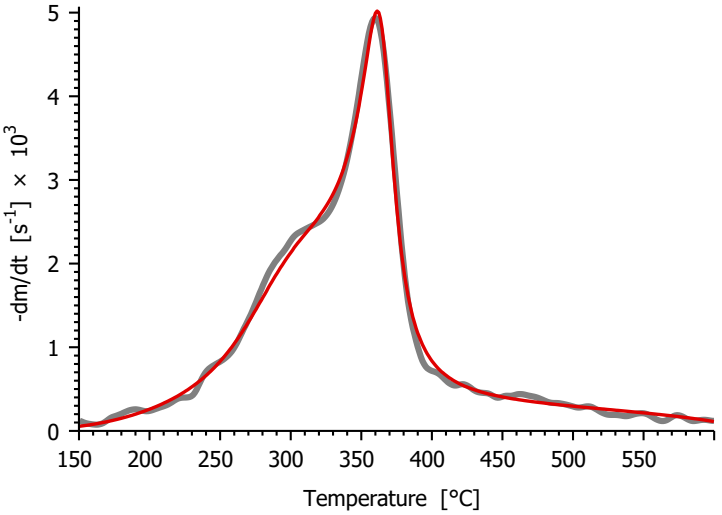
Corn stalk, 4mg, 4°C/min
Relative deviation: 2.40%, Deviation: 0.054 µg/s
rms rel. dev. of 4 experiments: 2.99%
Model: x=2α-1
E(x) = 187.98
$\log_{10}$ Ã(x) = 12.291T_0(x) -5.172T_1(x) -2.044T_2(x) -1.938T_3(x)
-.559T_4(x) -.201T_5(x)
c = 0.721



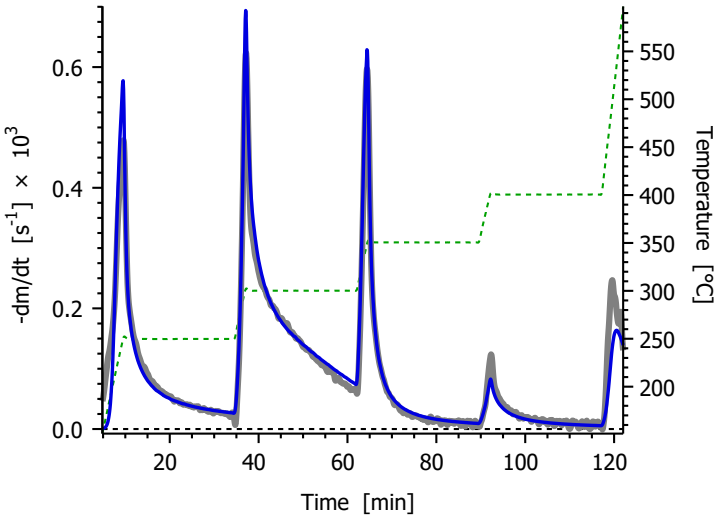
Corn stalk, 4mg, 4°C/min
Relative deviation: 1.94%, Deviation: 0.044 µg/s
rms rel. dev. of 4 experiments: 1.83%
Model: x=2α-1
E(x) = 187.1T_0(x) +81.43T_1(x) -4.67T_2(x) +36.01T_3(x)
$\log_{10}$ Ã(x) = 12.808T_0(x) +4.073T_1(x) -2.022T_2(x) +2.164T_3(x)
-.639T_4(x) -.074T_5(x)
c = 0.690



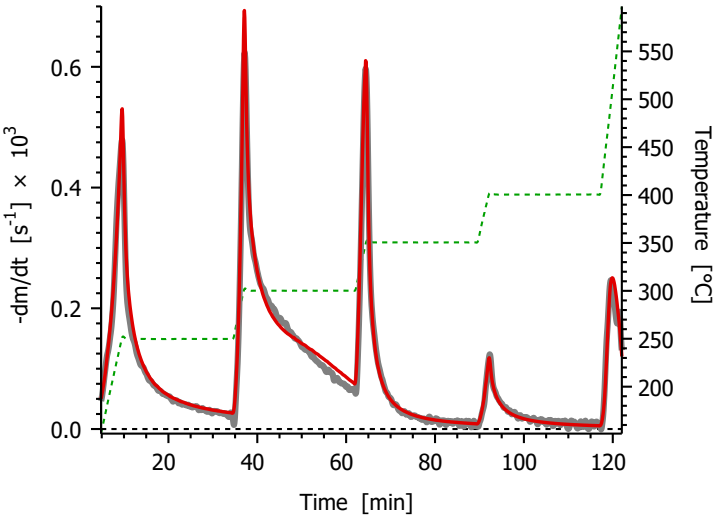
Corn stalk, 0.5mg, 40°C/min
Relative deviation: 3.26%, Deviation: 0.082 µg/s
rms rel. dev. of 4 experiments: 2.99%
Model: x=2α-1
E(x) = 187.98
$\log_{10}$ Ã(x) = 12.291T_0(x) -5.172T_1(x) -2.044T_2(x) -1.938T_3(x)
-.559T_4(x) -.201T_5(x)
c = 0.721



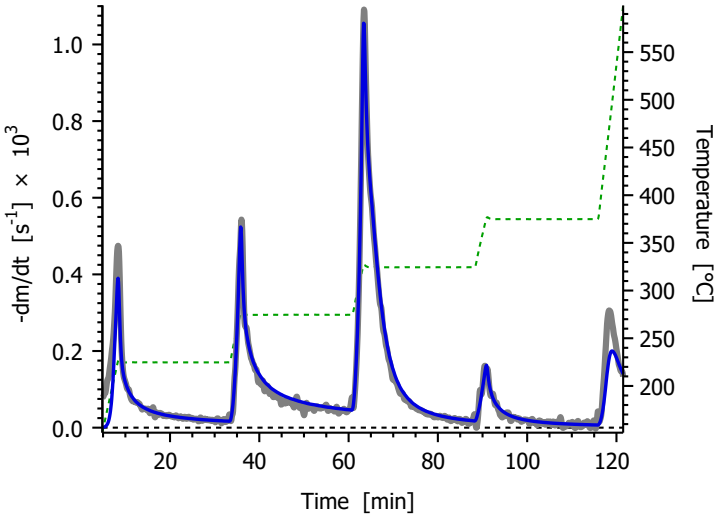
Corn stalk, 0.5mg, 40°C/min
Relative deviation: 1.53%, Deviation: 0.039 µg/s
rms rel. dev. of 4 experiments: 1.83%
Model: x=2α-1
E(x) = 187.1T_0(x) +81.43T_1(x) -4.67T_2(x) +36.01T_3(x)
$\log_{10}$ Ã(x) = 12.808T_0(x) +4.073T_1(x) -2.022T_2(x) +2.164T_3(x)
-.639T_4(x) -.074T_5(x)
c = 0.690



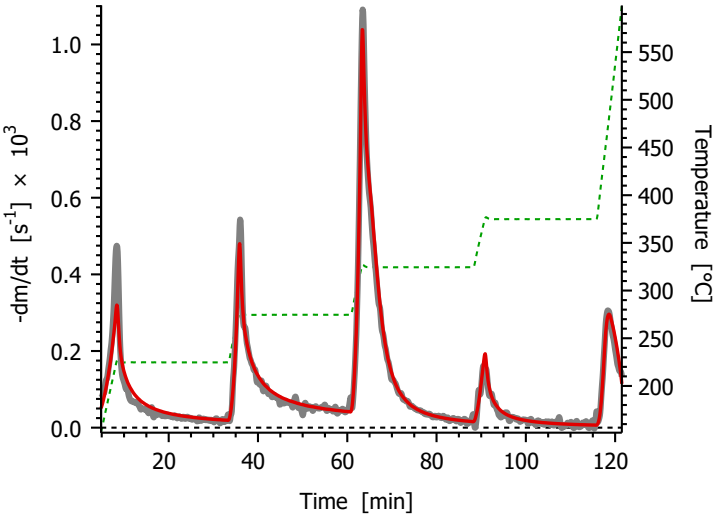
Corn stalk, 2mg, steps: 250 - 400°C
Relative deviation: 3.69%, Deviation: 0.045 µg/s
rms rel. dev. of 4 experiments: 2.99%
Model: x=2α-1
E(x) = 187.98
$\log_{10}$ Ã(x) = 12.291T_0(x) -5.172T_1(x) -2.044T_2(x) -1.938T_3(x) -.559T_4(x) -.201T_5(x)
c = 0.721



Corn stalk, 2mg, steps: 250 - 400°C
Relative deviation: 1.98%, Deviation: 0.024 µg/s
rms rel. dev. of 4 experiments: 1.83%
Model: x=2α-1
E(x) = 187.1T_0(x) +81.43T_1(x) -4.67T_2(x) +36.01T_3(x)
$\log_{10}$ Ã(x) = 12.808T_0(x) +4.073T_1(x) -2.022T_2(x) +2.164T_3(x) -.639T_4(x) -.074T_5(x)
c = 0.690



Corn stalk, 2mg, steps: 225 - 375°C
Relative deviation: 2.40%, Deviation: 0.051 µg/s
rms rel. dev. of 4 experiments: 2.99%
Model: x=2α-1
E(x) = 187.98
$\log_{10}$ Ã(x) = 12.291T_0(x) -5.172T_1(x) -2.044T_2(x) -1.938T_3(x) -.559T_4(x) -.201T_5(x)
c = 0.721



Corn stalk, 2mg, steps: 225 - 375°C
Relative deviation: 1.85%, Deviation: 0.040 µg/s
rms rel. dev. of 4 experiments: 1.83%
Model: x=2α-1
E(x) = 187.1T_0(x) +81.43T_1(x) -4.67T_2(x) +36.01T_3(x)
$\log_{10}$ Ã(x) = 12.808T_0(x) +4.073T_1(x) -2.022T_2(x) +2.164T_3(x) -.639T_4(x) -.074T_5(x)
c = 0.690

S3.2. Rice husk

Model with constant E:

Input file: "R_0,5_oneC.PAR"

$x=2\alpha-1$

E= 181.0715

$\log_{10}\tilde{A}(x)= 13.079498 -.763766x +1.471146x^2 -.472292x^3 -6.014304x^4 -7.5068x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 11.559707T_0(x) -5.809735T_1(x) -2.271579T_2(x) -2.463948T_3(x) -.751788T_4(x) -.469175T_5(x)$

Model with third order E(α):

Input file: "R_3,5_oneC.PAR"

$x=2\alpha-1$

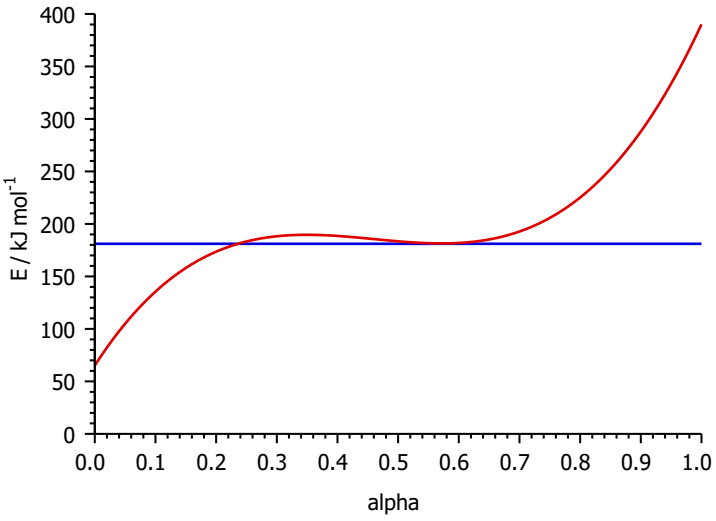
$E(x)= 183.434091 -24.200095x +44.197618x^2 +186.6883x^3$

$\log_{10}\tilde{A}(x)= 13.361836 -2.8951496x +5.813892x^2 +15.4994652x^3 -5.885848x^4 -3.849584x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 205.5329T_0(x) +115.81613T_1(x) +22.098809T_2(x) +46.672075T_3(x)$

$\log_{10}\tilde{A}(x)= 14.061589T_0(x) +6.3234593T_1(x) -.035978T_2(x) +2.6718713T_3(x) -.735731T_4(x) -.240599T_5(x)$



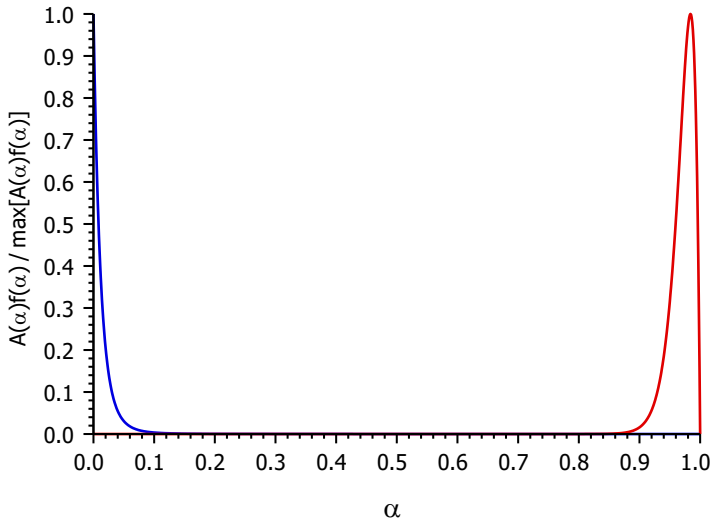
E(α) = polynomial of (2α-1)

Parameter file: R_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 17.28 E(0)= 181.1 $\log_{10}\tilde{A}(1)$= -0.21 E(1)= 181.1
mean $\log_{10}\tilde{A}$= 12.37 mean E= 181.1

Parameter file: R_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 4.54 E(0)= 65.1 $\log_{10}\tilde{A}(1)$= 22.04 E(1)= 390.1
mean $\log_{10}\tilde{A}$= 14.12 mean E= 198.2



Plot of A(α)f(α) / max[A(α)f(α)]

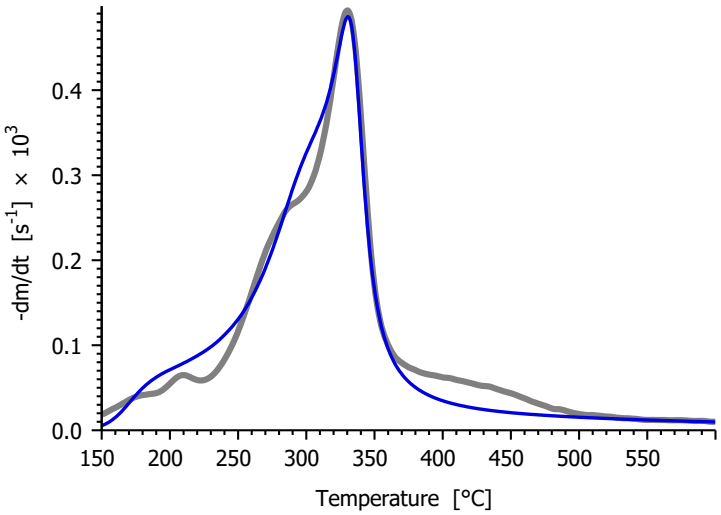
Parameter file: R_0,5_oneC.PAR

A(0)f(0)= 1.902E+17 E(0)= 181.1 A(1)f(1)= 0.00 E(1)= 181.1
mean A(α)f(α)= 2.516E+15 mean E= 181.1
max A(α)f(α)= 1.902E+17 at α= 0.000 and E= 181.1

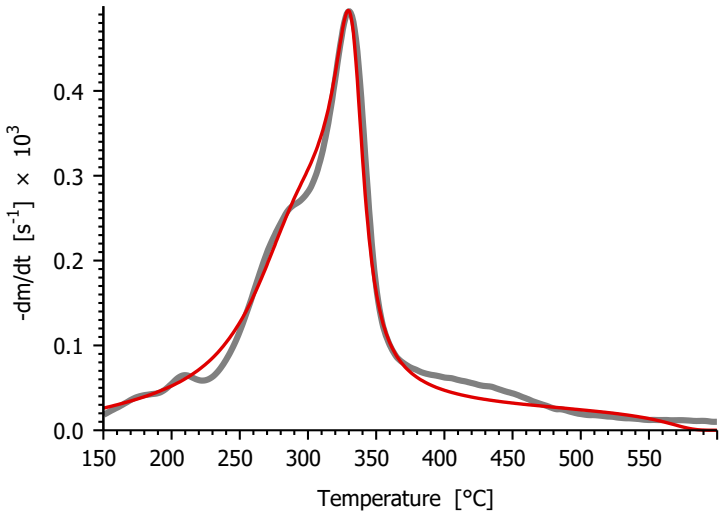
Parameter file: R_3,5_oneC.PAR

A(0)f(0)= 3.429E+04 E(0)= 65.1 A(1)f(1)= 0.00 E(1)= 390.1
mean A(α)f(α)= 2.702E+18 mean E= 198.2
max A(α)f(α)= 6.763E+19 at α= 0.984 and E= 370.9

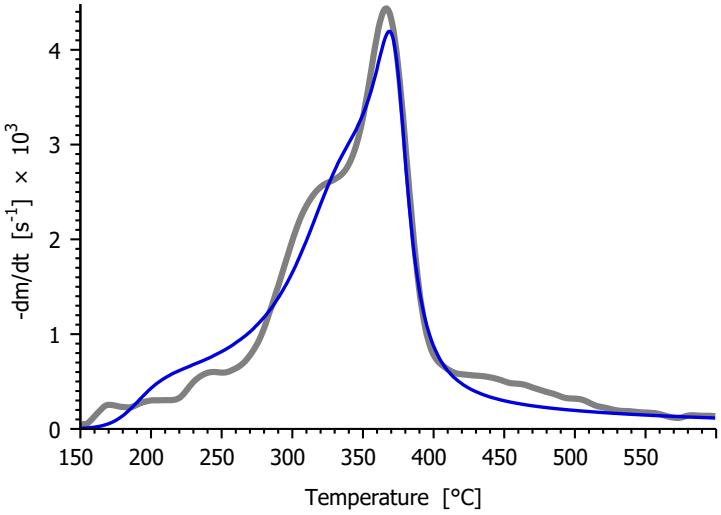
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S3])*



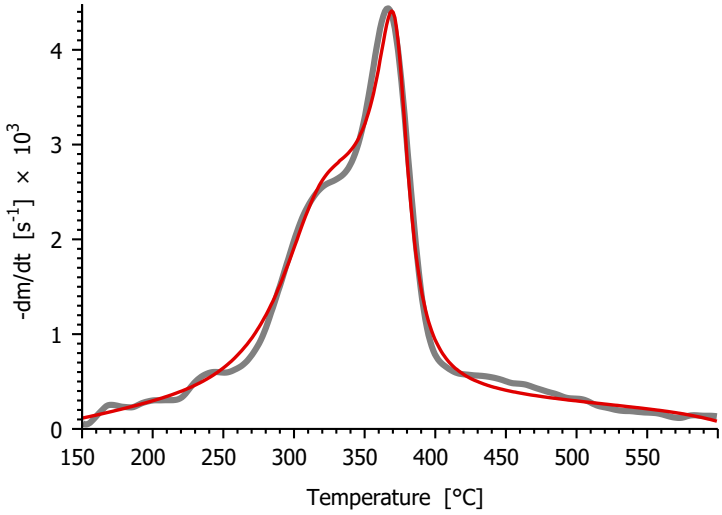
Rice husk, 4mg, 4°C/min
Relative deviation: 3.79%, Deviation: 0.074 µg/s
rms rel. dev. of 4 experiments: 3.54%
Model: $x=2\alpha-1$
$E(x) = 181.07$
$\log_{10} \tilde{A}(x) = 11.56T_0(x) -5.81T_1(x) -2.272T_2(x) -2.464T_3(x)$
$-.752T_4(x) -.469T_5(x)$
$c = 0.696$



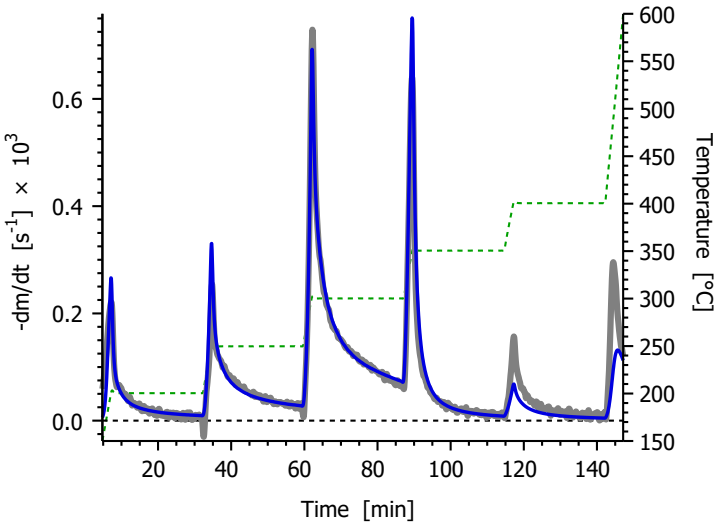
Rice husk, 4mg, 4°C/min
Relative deviation: 2.56%, Deviation: 0.050 µg/s
rms rel. dev. of 4 experiments: 2.17%
Model: $x=2\alpha-1$
$E(x) = 205.53T_0(x) +115.82T_1(x) +22.1T_2(x) +46.67T_3(x)$
$\log_{10} \tilde{A}(x) = 14.062T_0(x) +6.323T_1(x) -.036T_2(x) +2.672T_3(x)$
$-.736T_4(x) -.241T_5(x)$
$c = 0.662$



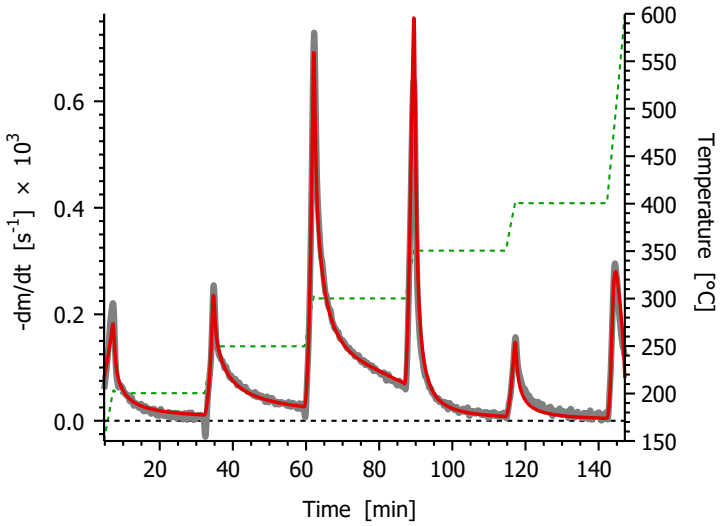
Rice husk, 1mg, 40°C/min
Relative deviation: 3.82%, Deviation: 0.16 µg/s
rms rel. dev. of 4 experiments: 3.54%
Model: $x=2\alpha-1$
$E(x) = 181.07$
$\log_{10} \tilde{A}(x) = 11.56T_0(x) -5.81T_1(x) -2.272T_2(x) -2.464T_3(x)$
$-.752T_4(x) -.469T_5(x)$
$c = 0.696$



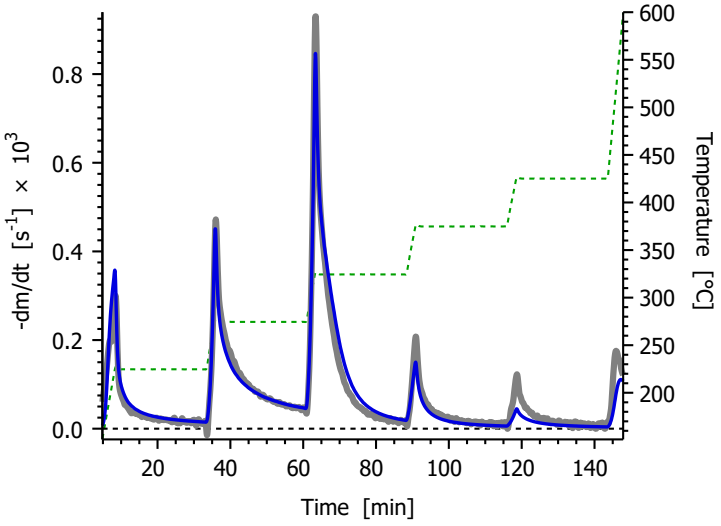
Rice husk, 1mg, 40°C/min
Relative deviation: 2.08%, Deviation: 0.085 µg/s
rms rel. dev. of 4 experiments: 2.17%
Model: $x=2\alpha-1$
$E(x) = 205.53T_0(x) +115.82T_1(x) +22.1T_2(x) +46.67T_3(x)$
$\log_{10} \tilde{A}(x) = 14.062T_0(x) +6.323T_1(x) -.036T_2(x) +2.672T_3(x)$
$-.736T_4(x) -.241T_5(x)$
$c = 0.662$



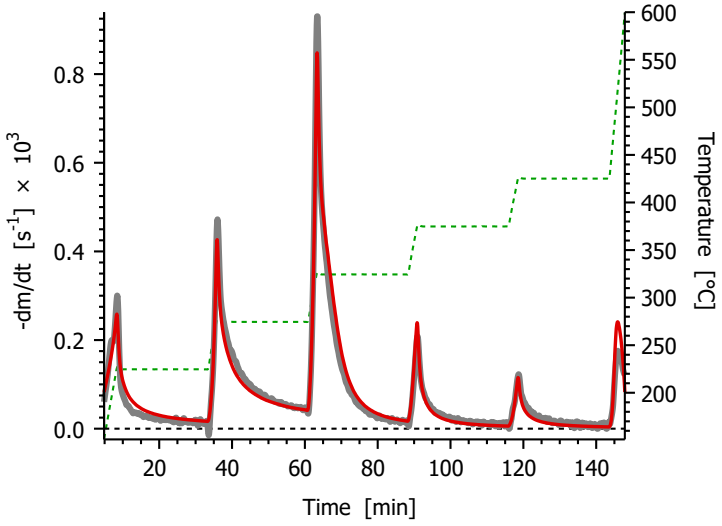
Rice husk, 2mg, steps: 200 - 400°C
Relative deviation: 3.79%, Deviation: 0.055 µg/s
rms rel. dev. of 4 experiments: 3.54%
Model: x=2α-1
E(x) = 181.07
$\log_{10}$ Ã(x) = 11.56T_0(x) -5.81T_1(x) -2.272T_2(x) -2.464T_3(x) -.752T_4(x) -.469T_5(x)
c = 0.696



Rice husk, 2mg, steps: 200 - 400°C
Relative deviation: 1.97%, Deviation: 0.028 µg/s
rms rel. dev. of 4 experiments: 2.17%
Model: x=2α-1
E(x) = 205.53T_0(x) +115.82T_1(x) +22.1T_2(x) +46.67T_3(x)
$\log_{10}$ Ã(x) = 14.062T_0(x) +6.323T_1(x) -.036T_2(x) +2.672T_3(x) -.736T_4(x) -.241T_5(x)
c = 0.662



Rice husk, 2mg, steps: 225 - 425°C
Relative deviation: 2.63%, Deviation: 0.048 µg/s
rms rel. dev. of 4 experiments: 3.54%
Model: x=2α-1
E(x) = 181.07
$\log_{10}$ Ã(x) = 11.56T_0(x) -5.81T_1(x) -2.272T_2(x) -2.464T_3(x) -.752T_4(x) -.469T_5(x)
c = 0.696



Rice husk, 2mg, steps: 225 - 425°C
Relative deviation: 2.02%, Deviation: 0.037 µg/s
rms rel. dev. of 4 experiments: 2.17%
Model: x=2α-1
E(x) = 205.53T_0(x) +115.82T_1(x) +22.1T_2(x) +46.67T_3(x)
$\log_{10}$ Ã(x) = 14.062T_0(x) +6.323T_1(x) -.036T_2(x) +2.672T_3(x) -.736T_4(x) -.241T_5(x)
c = 0.662

S3.3. Sorghum

Model with constant E:

Input file: "S_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 188.21119$

$\log_{10}\tilde{A}(x)= 13.536254 -.570222x -.819662x^2 -3.352008x^3 -3.716208x^4 -2.973456x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 11.732845T_0(x) -4.942638T_1(x) -2.267935T_2(x) -1.767207T_3(x) -.464526T_4(x) -.185841T_5(x)$

Model with third order E(α):

Input file: "S_3,5_oneC.PAR"

$x=2\alpha-1$

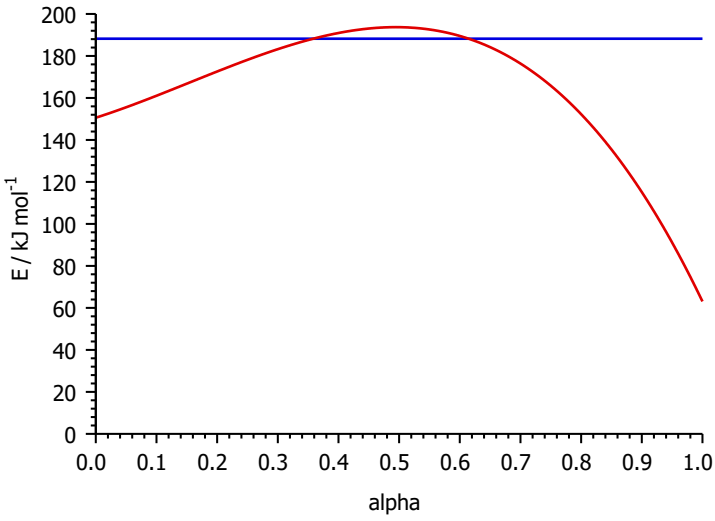
$E(x)= 193.70388 -1.86176x -86.8737x^2 -41.89796x^3$

$\log_{10}\tilde{A}(x)= 13.9385846 -.966972x -9.080428x^2 -7.695572x^3 -3.409552x^4 -1.814272x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 150.26703T_0(x) -33.28523T_1(x) -43.43685T_2(x) -10.47449T_3(x)$

$\log_{10}\tilde{A}(x)= 8.1197886T_0(x) -7.872571T_1(x) -6.24499T_2(x) -2.490853T_3(x) -.426194T_4(x) -.113392T_5(x)$



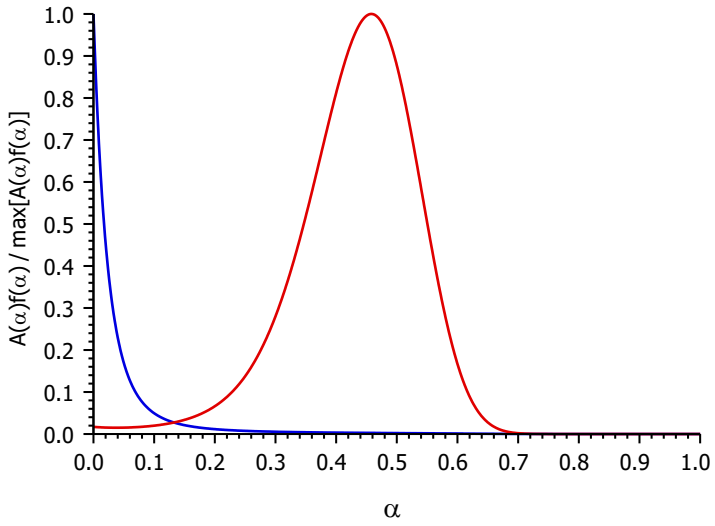
E(α) = polynomial of (2α-1)

Parameter file: S_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 15.90 E(0)= 188.2 $\log_{10}\tilde{A}(1)$= 2.10 E(1)= 188.2
mean $\log_{10}\tilde{A}$= 12.52 mean E= 188.2

Parameter file: S_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 11.93 E(0)= 150.6 $\log_{10}\tilde{A}(1)$= -9.03 E(1)= 63.1
mean $\log_{10}\tilde{A}$= 10.23 mean E= 164.7



Plot of A(α)f(α) / max[A(α)f(α)]

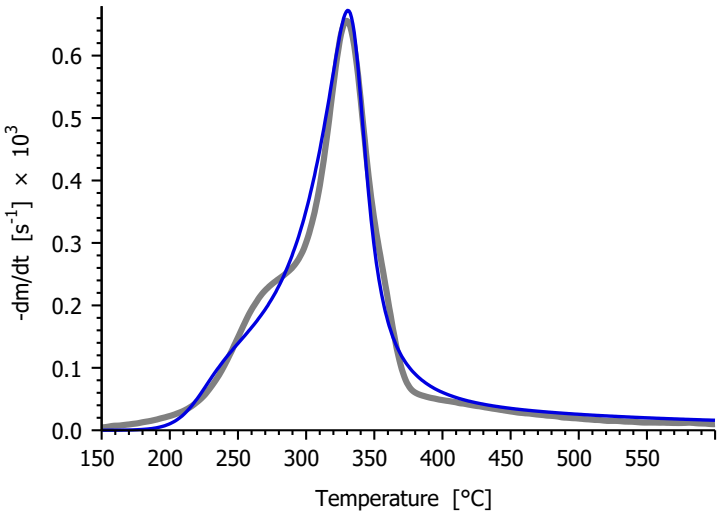
Parameter file: S_0,5_oneC.PAR

A(0)f(0)= 7.872E+15 E(0)= 188.2 A(1)f(1)= 0.00 E(1)= 188.2
mean A(α)f(α)= 2.445E+14 mean E= 188.2
max A(α)f(α)= 7.872E+15 at α= 0.000 and E= 188.2

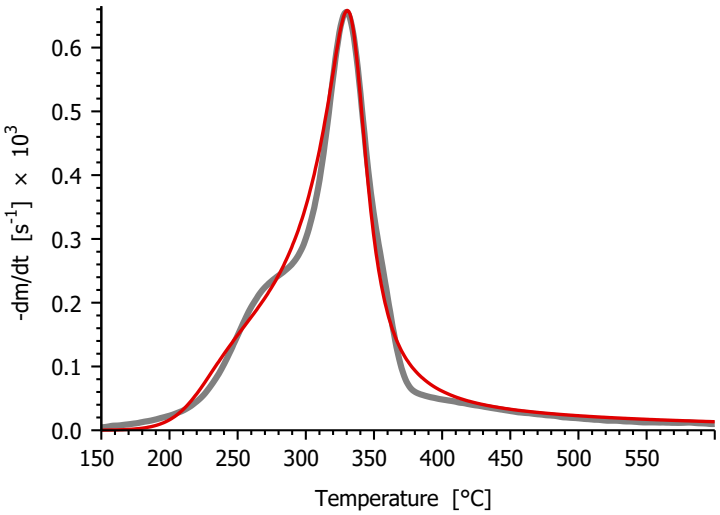
Parameter file: S_3,5_oneC.PAR

A(0)f(0)= 8.422E+11 E(0)= 150.6 A(1)f(1)= 0.00 E(1)= 63.1
mean A(α)f(α)= 1.104E+13 mean E= 164.7
max A(α)f(α)= 4.945E+13 at α= 0.458 and E= 193.3

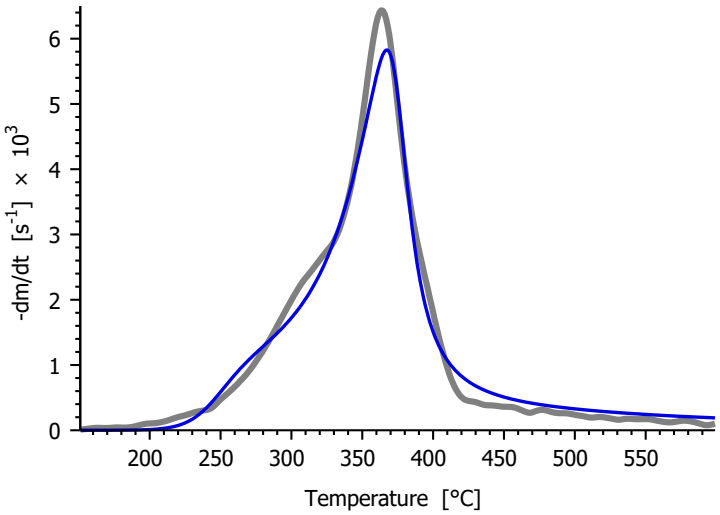
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S3])*



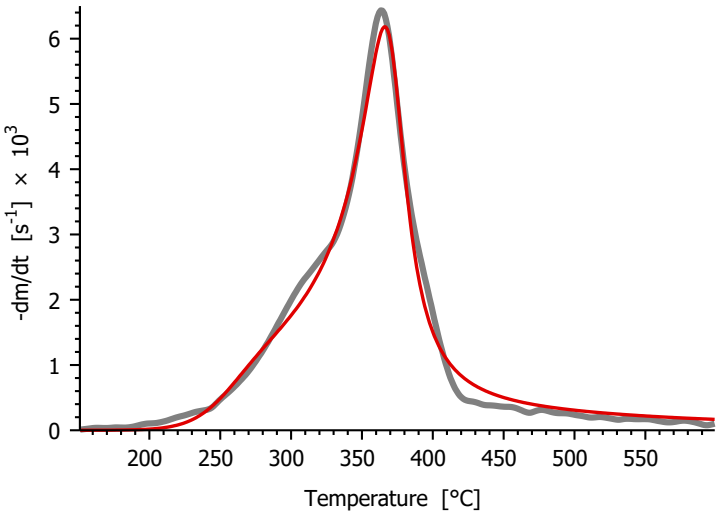
Sorghum, 4mg, 4°C/min
Relative deviation: 2.86%, Deviation: 0.074 µg/s
rms rel. dev. of 4 experiments: 2.49%
Model: x=2α-1
E(x) = 188.21
$\log_{10}$ Ã(x) = 11.733T_0(x) -4.943T_1(x) -2.268T_2(x) -1.767T_3(x)
-.465T_4(x) -.186T_5(x)
c = 0.851



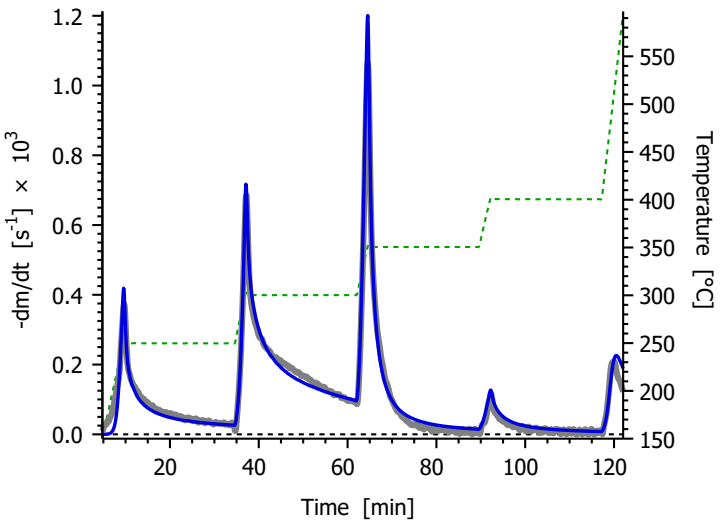
Sorghum, 4mg, 4°C/min
Relative deviation: 2.50%, Deviation: 0.065 µg/s
rms rel. dev. of 4 experiments: 2.23%
Model: x=2α-1
E(x) = 150.27T_0(x) -33.29T_1(x) -43.44T_2(x) -10.47T_3(x)
$\log_{10}$ Ã(x) = 8.12T_0(x) -7.873T_1(x) -6.245T_2(x) -2.491T_3(x)
-.426T_4(x) -.113T_5(x)
c = 0.902



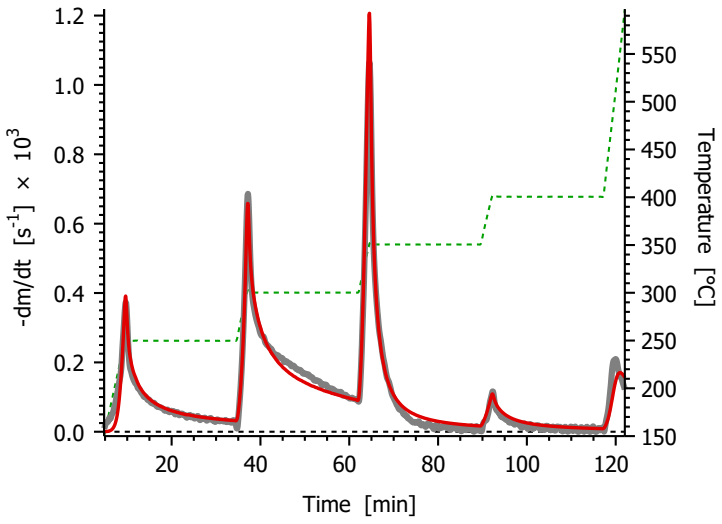
Sorghum, 1mg, 40°C/min
Relative deviation: 3.16%, Deviation: 0.19 µg/s
rms rel. dev. of 4 experiments: 2.49%
Model: x=2α-1
E(x) = 188.21
$\log_{10}$ Ã(x) = 11.733T_0(x) -4.943T_1(x) -2.268T_2(x) -1.767T_3(x)
-.465T_4(x) -.186T_5(x)
c = 0.851



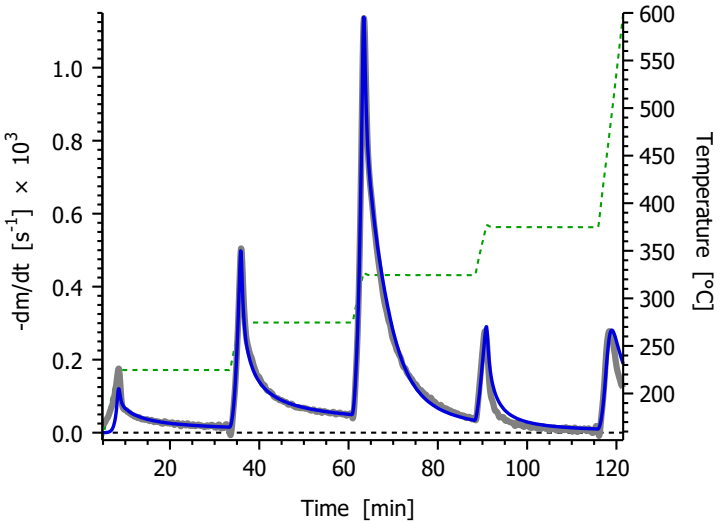
Sorghum, 1mg, 40°C/min
Relative deviation: 2.46%, Deviation: 0.14 µg/s
rms rel. dev. of 4 experiments: 2.23%
Model: x=2α-1
E(x) = 150.27T_0(x) -33.29T_1(x) -43.44T_2(x) -10.47T_3(x)
$\log_{10}$ Ã(x) = 8.12T_0(x) -7.873T_1(x) -6.245T_2(x) -2.491T_3(x)
-.426T_4(x) -.113T_5(x)
c = 0.902



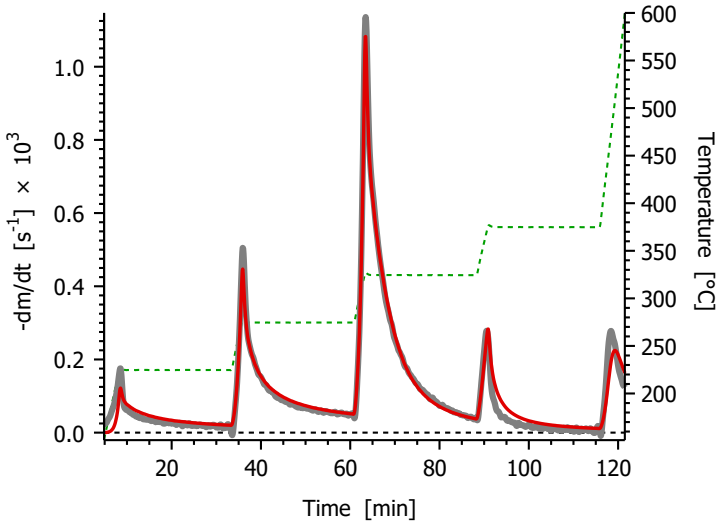
Sorghum, 2mg, steps: 250 - 400°C
Relative deviation: 1.89%, Deviation: 0.040 µg/s
rms rel. dev. of 4 experiments: 2.49%
Model: x=2α-1
E(x) = 188.21
$\log_{10}$ Ã(x) = 11.733T_0(x) -4.943T_1(x) -2.268T_2(x) -1.767T_3(x)
-.465T_4(x) -.186T_5(x)
c = 0.851



Sorghum, 2mg, steps: 250 - 400°C
Relative deviation: 1.99%, Deviation: 0.043 µg/s
rms rel. dev. of 4 experiments: 2.23%
Model: x=2α-1
E(x) = 150.27T_0(x) -33.29T_1(x) -43.44T_2(x) -10.47T_3(x)
$\log_{10}$ Ã(x) = 8.12T_0(x) -7.873T_1(x) -6.245T_2(x) -2.491T_3(x)
-.426T_4(x) -.113T_5(x)
c = 0.902



Sorghum, 2mg, steps: 225-375°C
Relative deviation: 1.72%, Deviation: 0.039 µg/s
rms rel. dev. of 4 experiments: 2.49%
Model: x=2α-1
E(x) = 188.21
$\log_{10}$ Ã(x) = 11.733T_0(x) -4.943T_1(x) -2.268T_2(x) -1.767T_3(x)
-.465T_4(x) -.186T_5(x)
c = 0.851



Sorghum, 2mg, steps: 225-375°C
Relative deviation: 1.92%, Deviation: 0.043 µg/s
rms rel. dev. of 4 experiments: 2.23%
Model: x=2α-1
E(x) = 150.27T_0(x) -33.29T_1(x) -43.44T_2(x) -10.47T_3(x)
$\log_{10}$ Ã(x) = 8.12T_0(x) -7.873T_1(x) -6.245T_2(x) -2.491T_3(x)
-.426T_4(x) -.113T_5(x)
c = 0.902

S3.4. Wheat straw

Model with constant E:

Input file: "W_0,5_oneC.PAR"

x=2α-1

E= 187.61656

$\log_{10}\tilde{A}(x) = 13.748554 - .519708x + .056052x^2 - 1.713088x^3 - 4.838784x^4 - 4.340992x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x) = 11.962036T_0(x) - 4.517644T_1(x) - 2.391366T_2(x) - 1.784832T_3(x) - .604848T_4(x) - .271312T_5(x)$

Model with third order E(α):

Input file: "W_3,5_oneC.PAR"

x=2α-1

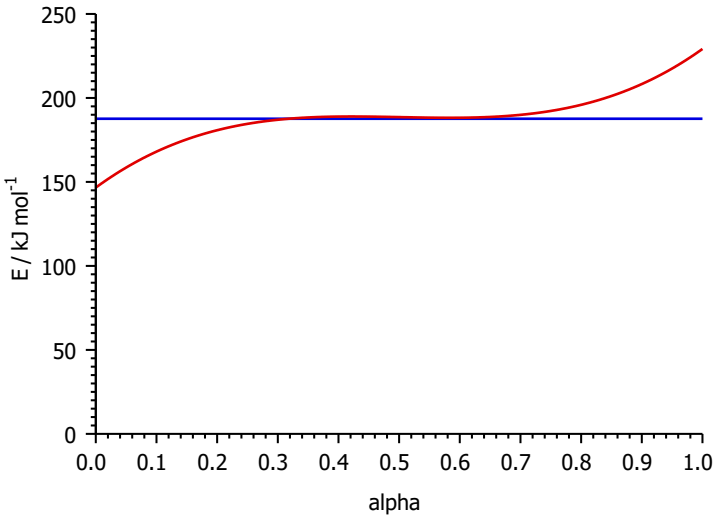
$E(x) = 188.588694 - 3.516947x - .681028x^2 + 44.79034x^3$

$\log_{10}\tilde{A}(x) = 13.838112 - .797866x + .118542x^2 + 1.97342x^3 - 5.190192x^4 - 3.850752x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x) = 188.24818T_0(x) + 30.075808T_1(x) - .340514T_2(x) + 11.197585T_3(x)$

$\log_{10}\tilde{A}(x) = 11.951061T_0(x) - 1.724521T_1(x) - 2.535825T_2(x) - .710005T_3(x) - .648774T_4(x) - .240672T_5(x)$



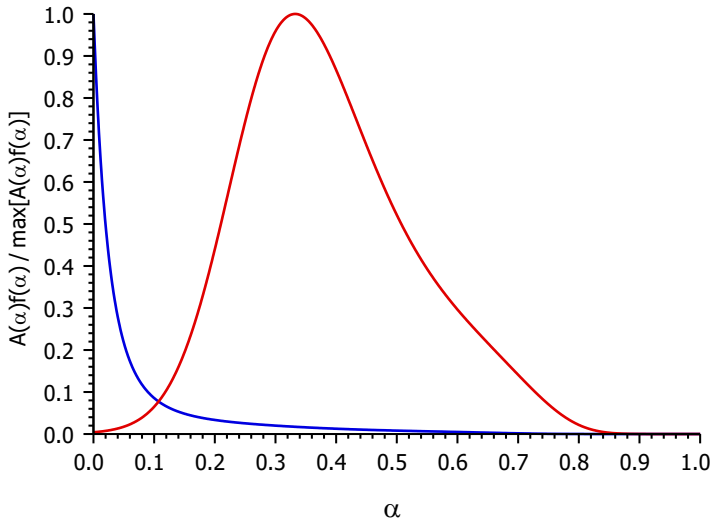
E(α) = polynomial of (2α-1)

Parameter file: W_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 15.54 E(0)= 187.6 $\log_{10}\tilde{A}(1)$= 2.39 E(1)= 187.6
mean $\log_{10}\tilde{A}$= 12.80 mean E= 187.6

Parameter file: W_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 11.44 E(0)= 146.6 $\log_{10}\tilde{A}(1)$= 6.09 E(1)= 229.2
mean $\log_{10}\tilde{A}$= 12.84 mean E= 188.4



Plot of A(α)f(α) / max[A(α)f(α)]

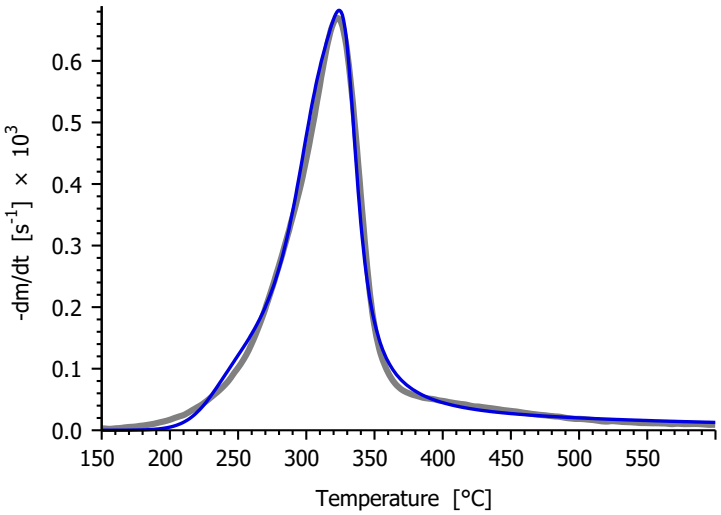
Parameter file: W_0,5_oneC.PAR

A(0)f(0)= 3.464E+15 E(0)= 187.6 A(1)f(1)= 0.00 E(1)= 187.6
mean A(α)f(α)= 1.470E+14 mean E= 187.6
max A(α)f(α)= 3.464E+15 at α= 0.000 and E= 187.6

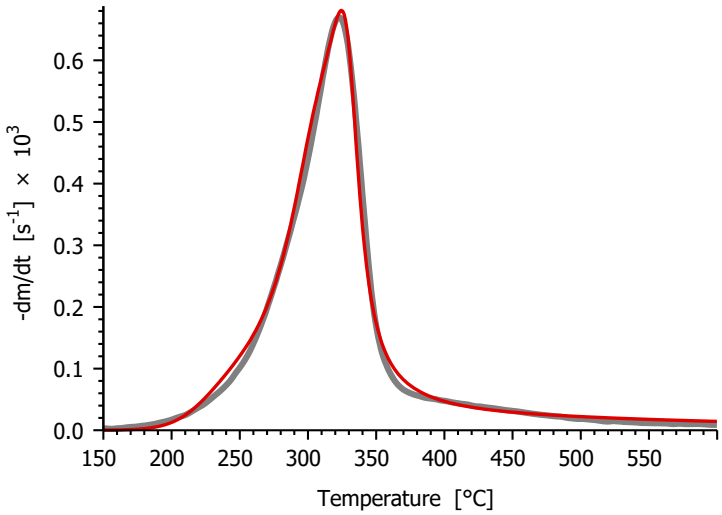
Parameter file: W_3,5_oneC.PAR

A(0)f(0)= 2.765E+11 E(0)= 146.6 A(1)f(1)= 0.00 E(1)= 229.2
mean A(α)f(α)= 2.189E+13 mean E= 188.4
max A(α)f(α)= 6.604E+13 at α= 0.333 and E= 188.0

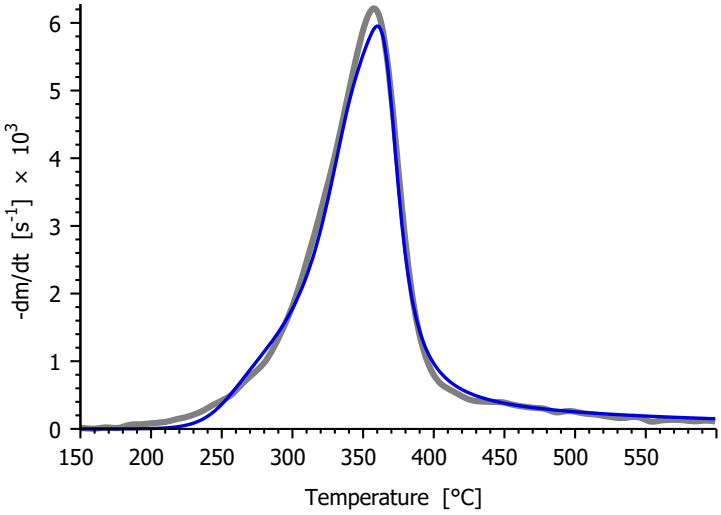
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S3])*



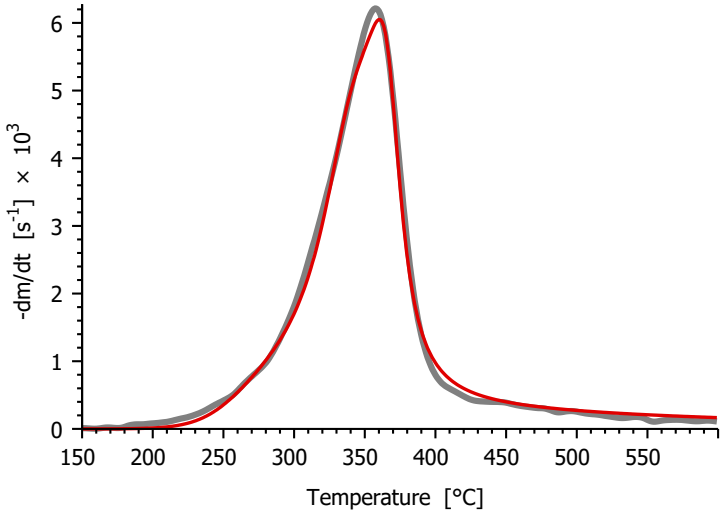
Wheat straw, 4mg, 4°C/min
Relative deviation: 1.80%, Deviation: 0.047 µg/s
rms rel. dev. of 4 experiments: 1.76%
Model: x=2α-1
E(x) = 187.62
$\log_{10}$ Ã(x) = 11.962T_0(x) -4.518T_1(x) -2.391T_2(x) -1.785T_3(x) -.605T_4(x) -.271T_5(x)
c = 0.790



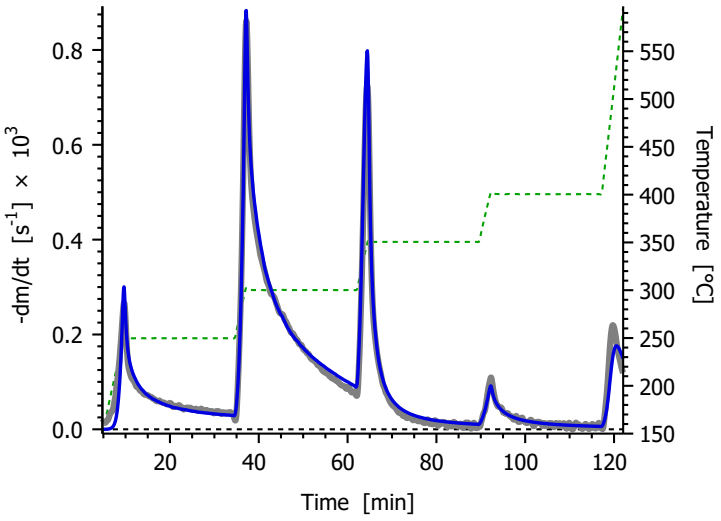
Wheat straw, 4mg, 4°C/min
Relative deviation: 1.76%, Deviation: 0.046 µg/s
rms rel. dev. of 4 experiments: 1.60%
Model: x=2α-1
E(x) = 188.25T_0(x) +30.08T_1(x) -.34T_2(x) +11.2T_3(x)
$\log_{10}$ Ã(x) = 11.951T_0(x) -1.725T_1(x) -2.536T_2(x) -.71T_3(x) -.649T_4(x) -.241T_5(x)
c = 0.791



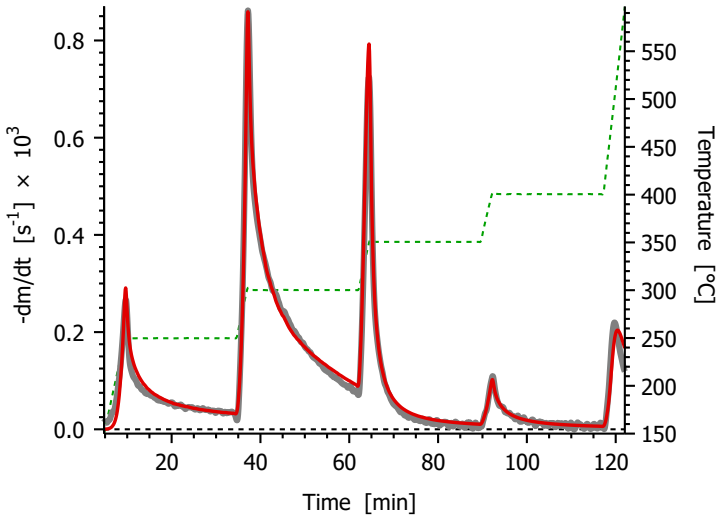
Wheat straw, 1mg, 40°C/min
Relative deviation: 1.91%, Deviation: 0.11 µg/s
rms rel. dev. of 4 experiments: 1.76%
Model: x=2α-1
E(x) = 187.62
$\log_{10}$ Ã(x) = 11.962T_0(x) -4.518T_1(x) -2.391T_2(x) -1.785T_3(x) -.605T_4(x) -.271T_5(x)
c = 0.790



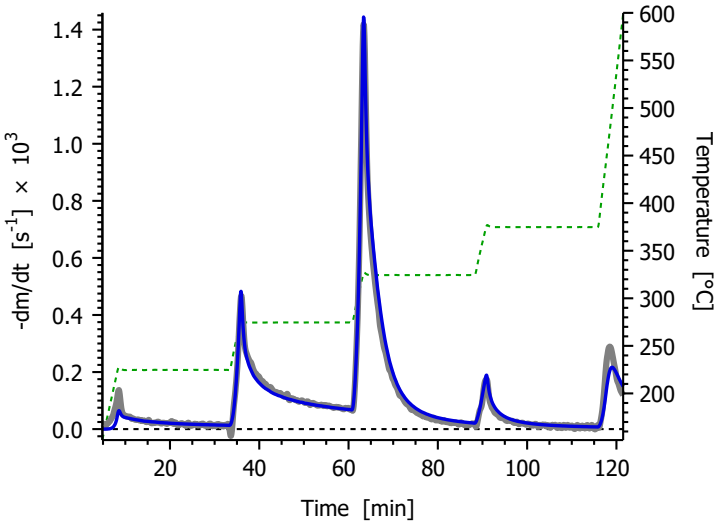
Wheat straw, 1mg, 40°C/min
Relative deviation: 1.57%, Deviation: 0.089 µg/s
rms rel. dev. of 4 experiments: 1.60%
Model: x=2α-1
E(x) = 188.25T_0(x) +30.08T_1(x) -.34T_2(x) +11.2T_3(x)
$\log_{10}$ Ã(x) = 11.951T_0(x) -1.725T_1(x) -2.536T_2(x) -.71T_3(x) -.649T_4(x) -.241T_5(x)
c = 0.791



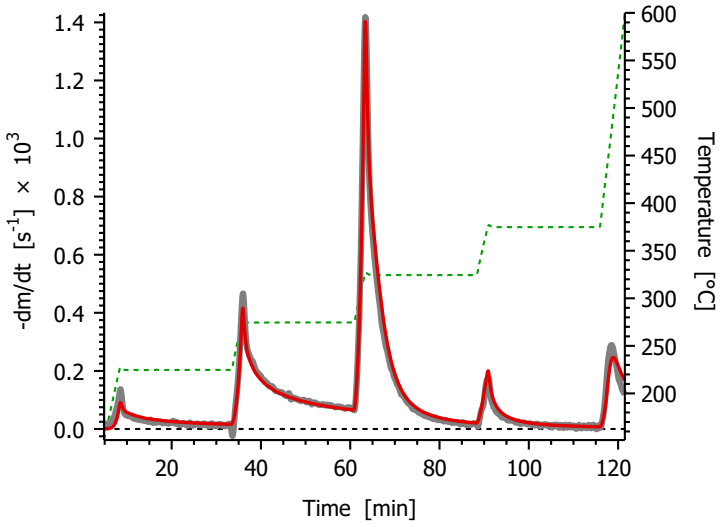
Wheat straw, 2mg, steps: 250 - 400°C
Relative deviation: 1.88%, Deviation: 0.032 µg/s
rms rel. dev. of 4 experiments: 1.76%
Model: x=2α-1
E(x) = 187.62
$\log_{10} \tilde{A}(x) = 11.962T_0(x) -4.518T_1(x) -2.391T_2(x) -1.785T_3(x) -.605T_4(x) -.271T_5(x)$
c = 0.790



Wheat straw, 2mg, steps: 250 - 400°C
Relative deviation: 1.71%, Deviation: 0.029 µg/s
rms rel. dev. of 4 experiments: 1.60%
Model: x=2α-1
E(x) = 188.25T_0(x) +30.08T_1(x) -.34T_2(x) +11.2T_3(x)
$\log_{10} \tilde{A}(x) = 11.951T_0(x) -1.725T_1(x) -2.536T_2(x) -.71T_3(x) -.649T_4(x) -.241T_5(x)$
c = 0.791



Wheat straw, 2mg, steps: 225 - 375°C
Relative deviation: 1.42%, Deviation: 0.040 µg/s
rms rel. dev. of 4 experiments: 1.76%
Model: x=2α-1
E(x) = 187.62
$\log_{10} \tilde{A}(x) = 11.962T_0(x) -4.518T_1(x) -2.391T_2(x) -1.785T_3(x) -.605T_4(x) -.271T_5(x)$
c = 0.790



Wheat straw, 2mg, steps: 225 - 375°C
Relative deviation: 1.33%, Deviation: 0.038 µg/s
rms rel. dev. of 4 experiments: 1.60%
Model: x=2α-1
E(x) = 188.25T_0(x) +30.08T_1(x) -.34T_2(x) +11.2T_3(x)
$\log_{10} \tilde{A}(x) = 11.951T_0(x) -1.725T_1(x) -2.536T_2(x) -.71T_3(x) -.649T_4(x) -.241T_5(x)$
c = 0.791

S4. Two Corncob Samples

Source of the data:

[S4] Trninić, M.; Wang, L.; Várhegyi, G.; Grønli, M.; Skreiberg, Ø.: Kinetics of corncob pyrolysis. *Energy Fuels* **2012**, *26*, 2005-2013. *doi:* 10.1021/ef3002668 Repository

Four TGA experiments were available for each sample. The figure below shows the corresponding temperature programs. It is a redrawn/rearranged version of Figure 1 of the cited paper.

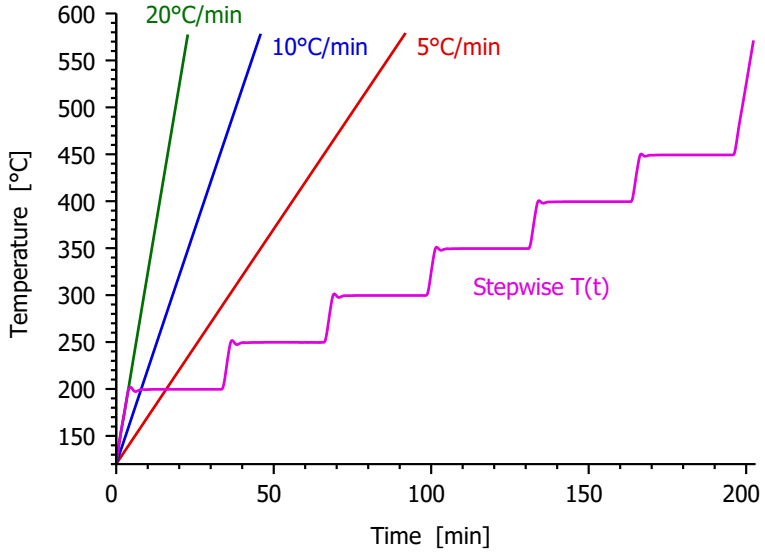


Figure S4.1: Temperature programs used for the TGA experiments of this section.

S4.1. A corncob sample from Oahu, Hawaii

Model with constant E:

Input file: "P_0,5_oneC.PAR"

x=2α-1

E= 184.58533

$\log_{10}\tilde{A}(x)$= 13.791489 -1.424139x +2.858664x^2 +2.334976x^3 -6.331752x^4 -7.615808x^5

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)$= 12.846414$T_0(x)$ -4.432787$T_1(x)$ -1.736544$T_2(x)$ -1.796196$T_3(x)$ -.791469$T_4(x)$ -.475988$T_5(x)$

Model with third order E(α):

Input file: "P_3,5_oneC.PAR"

x=2α-1

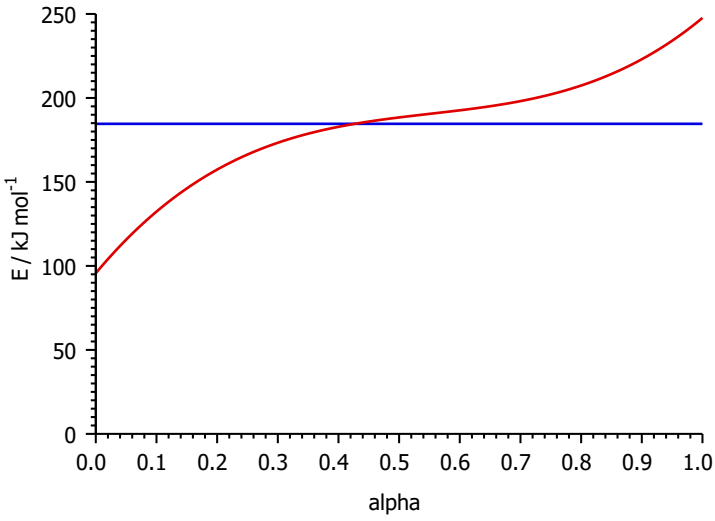
E(x)= 188.396709 +22.413672x -16.740878x^2 +53.57418x^3

$\log_{10}\tilde{A}(x)$= 14.144895 +.6288517x +1.089066x^2 +6.700328x^3 -6.351632x^4 -5.549744x^5

Expressed by Chebyshev polynomials of the first kind:

E(x)= 180.02627$T_0(x)$ +62.594307$T_1(x)$ -8.370439$T_2(x)$ +13.393545$T_3(x)$

$\log_{10}\tilde{A}(x)$= 12.307566$T_0(x)$ +2.1855077$T_1(x)$ -2.631283$T_2(x)$ -.059213$T_3(x)$ -.793954$T_4(x)$ -.346859$T_5(x)$



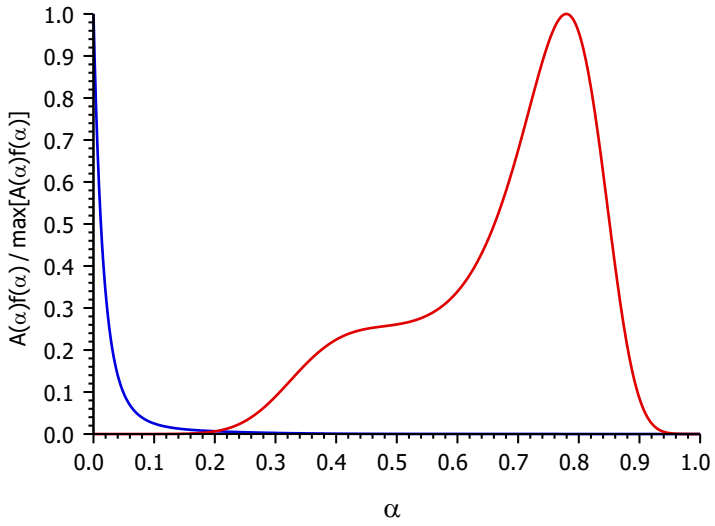
E(α) = polynomial of (2α-1)

Parameter file: P_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 17.02 E(0)= 184.6 $\log_{10}\tilde{A}(1)$= 3.61 E(1)= 184.6
mean $\log_{10}\tilde{A}$= 13.48 mean E= 184.6

Parameter file: P_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 7.10 E(0)= 95.7 $\log_{10}\tilde{A}(1)$= 10.66 E(1)= 247.6
mean $\log_{10}\tilde{A}$= 13.24 mean E= 182.8



Plot of A(α)f(α) / max[A(α)f(α)]

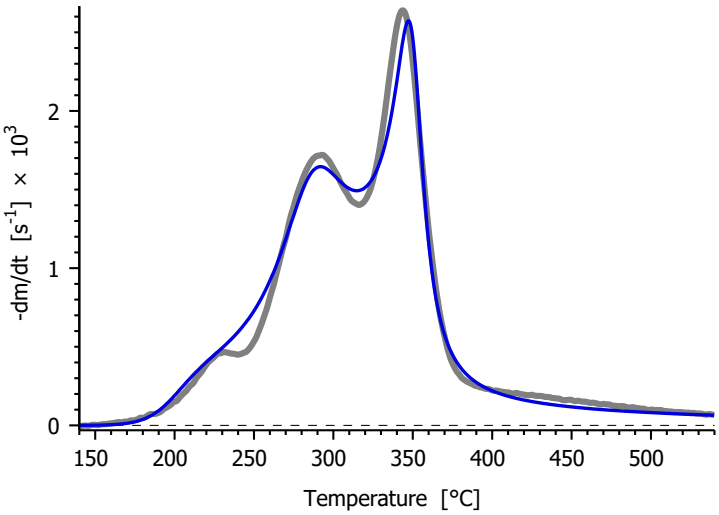
Parameter file: P_0,5_oneC.PAR

A(0)f(0)= 1.055E+17 E(0)= 184.6 A(1)f(1)= 0.00 E(1)= 184.6
mean A(α)f(α)= 2.323E+15 mean E= 184.6
max A(α)f(α)= 1.055E+17 at α= 0.000 and E= 184.6

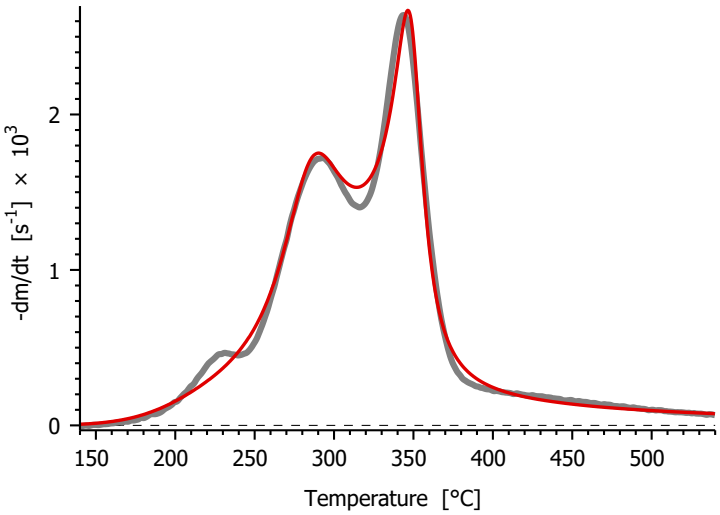
Parameter file: P_3,5_oneC.PAR

A(0)f(0)= 1.267E+07 E(0)= 95.7 A(1)f(1)= 0.00 E(1)= 247.6
mean A(α)f(α)= 7.053E+13 mean E= 182.8
max A(α)f(α)= 2.676E+14 at α= 0.779 and E= 205.0

Figures illustrating the fit quality *(cf. Figure 4 in reference [S4])*



Corncob (Pioneer Hi-Bred, Oahu), 20°C/min
Relative deviation: 2.98%, Deviation: 0.40 µg/s
rms rel. dev. of 4 experiments: 3.09%
Model: $x=2\alpha-1$
$E(x) = 184.59$
$\log_{10} \tilde{A}(x) = 12.846T_0(x) -4.433T_1(x) -1.737T_2(x) -1.796T_3(x) -.791T_4(x) -.476T_5(x)$
$c = 0.741$



Corncob (Pioneer Hi-Bred, Oahu), 20°C/min
Relative deviation: 2.21%, Deviation: 0.30 µg/s
rms rel. dev. of 4 experiments: 2.44%
Model: $x=2\alpha-1$
$E(x) = 180.03T_0(x) +62.59T_1(x) -8.37T_2(x) +13.39T_3(x)$
$\log_{10} \tilde{A}(x) = 12.308T_0(x) +2.186T_1(x) -2.631T_2(x) -.059T_3(x) -.794T_4(x) -.347T_5(x)$
$c = 0.730$

S4.2. A corncob sample from Serbia

Model with constant E:

Input file: "S_0,5_oneC.PAR"

The model:

$x=2\alpha-1$

E= 186.56647

$\log_{10}\tilde{A}(x)= 13.85819 -.8057x +1.842452x^2 +.374848x^3 -3.729488x^4 -3.0152x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 13.380858T_0(x) -2.409064T_1(x) -.943518T_2(x) -.848538T_3(x) -.466186T_4(x) -.18845T_5(x)$

Model with third order E(α):

Input file: "S_3,5_oneC.PAR"

$x=2\alpha-1$

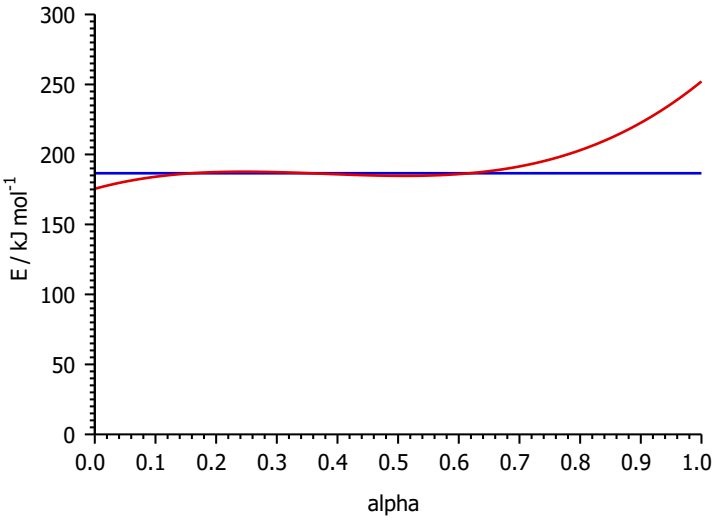
$E(x)= 184.718266 -1.2145034x +29.088348x^2 +39.5551832x^3$

$\log_{10}\tilde{A}(x)= 13.626923 -.81002x +4.619062x^2 +2.860636x^3 -5.76796x^4 -3.881776x^5$

Expressed by Chebyshev polynomials of the first kind:

$E(x)= 199.26244T_0(x) +28.451884T_1(x) +14.544174T_2(x) +9.8887958T_3(x)$

$\log_{10}\tilde{A}(x)= 13.773469T_0(x) -1.090653T_1(x) -.574449T_2(x) -.497896T_3(x) -.720995T_4(x) -.242611T_5(x)$



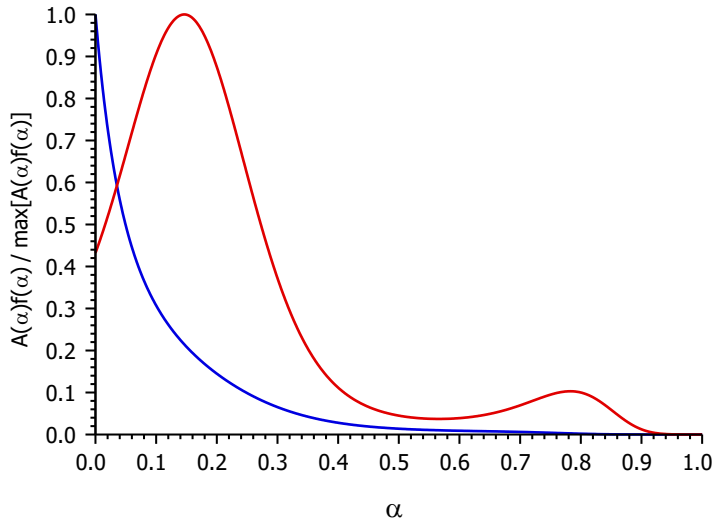
E(α) = polynomial of (2α-1)

Parameter file: S_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 15.42 E(0)= 186.6 $\log_{10}\tilde{A}(1)$= 8.53 E(1)= 186.6
mean $\log_{10}\tilde{A}$= 13.73 mean E= 186.6

Parameter file: S_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 14.31 E(0)= 175.5 $\log_{10}\tilde{A}(1)$= 10.65 E(1)= 252.1
mean $\log_{10}\tilde{A}$= 14.01 mean E= 194.4



Plot of A(α)f(α) / max[A(α)f(α)]

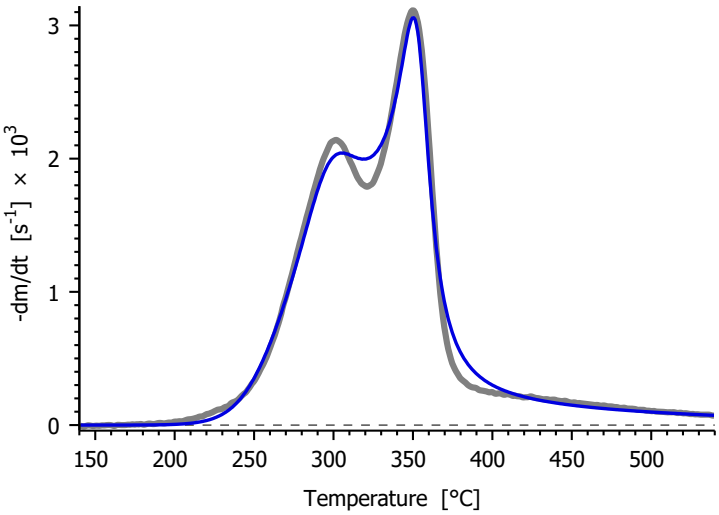
Parameter file: S_0,5_oneC.PAR

A(0)f(0)= 2.613E+15 E(0)= 186.6 A(1)f(1)= 0.00 E(1)= 186.6
mean A(α)f(α)= 2.478E+14 mean E= 186.6
max A(α)f(α)= 2.613E+15 at α= 0.000 and E= 186.6

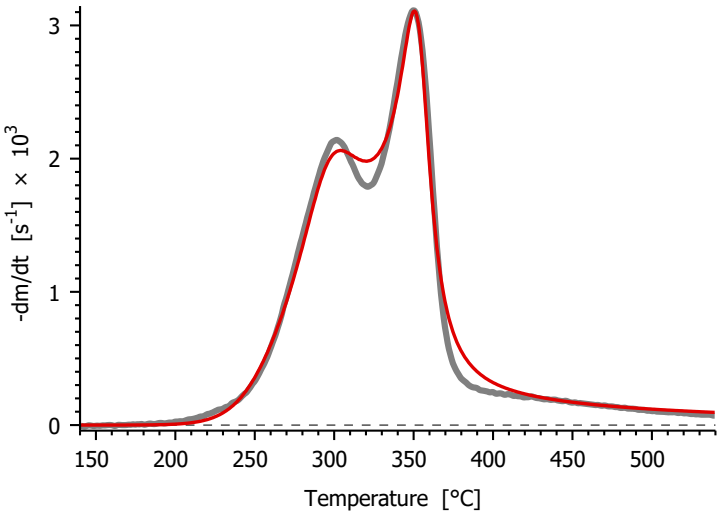
Parameter file: S_3,5_oneC.PAR

A(0)f(0)= 2.038E+14 E(0)= 175.5 A(1)f(1)= 0.00 E(1)= 252.1
mean A(α)f(α)= 1.310E+14 mean E= 194.4
max A(α)f(α)= 4.713E+14 at α= 0.146 and E= 186.1

Figures illustrating the fit quality *(cf. Figure 4 in reference [S4])*



Corncob (ZP Maize Hybrid 505, Serbia), 20°C/min
Relative deviation: 2.46%, Deviation: 0.39 µg/s
rms rel. dev. of 4 experiments: 2.21%
Model: x=2α-1
E(x) = 186.57
$\log_{10}$ Ã(x) = 13.381T_0(x) -2.409T_1(x) -.944T_2(x) -.849T_3(x) -.466T_4(x) -.188T_5(x)
c = 0.766



Corncob (ZP Maize Hybrid 505, Serbia), 20°C/min
Relative deviation: 2.37%, Deviation: 0.38 µg/s
rms rel. dev. of 4 experiments: 2.17%
Model: x=2α-1
E(x) = 199.26T_0(x) +28.45T_1(x) +14.54T_2(x) +9.89T_3(x)
$\log_{10}$ Ã(x) = 13.773T_0(x) -1.091T_1(x) -.574T_2(x) -.498T_3(x) -.721T_4(x) -.243T_5(x)
c = 0.799

S5. Birch and Spruce

Source of the data:

[S5] Tapasvi, D.; Khalil, R.; Várhegyi, G.; Tran, K.-Q.; Grønli, M.; Skreiberg, Ø. Thermal decomposition kinetics of woods with an emphasis on torrefaction. *Energy Fuels* **2013**, *27*, 6134-6145. *doi:* 10.1021/ef4016075 Repository

The birch and spruce samples were taken from standard Norwegian construction boards. Nine TGA experiments were available for each sample: four with linear heating (5, 10, 20 and 40 °C/min); two with stepwise heating; a modulated *T(t)*; a "constant reaction rate" (CRR) *T(t)*; and an isothermal *T(t)* at 275°C. (The latter was evaluated together with its heat-up section, as shown in the next pages.) The figure below shows the corresponding temperature programs. It is a redrawn/rearranged version of Figure 1 of the cited paper. Note that the "constant reaction rate" temperature programs are determined by the apparatus and they differ from sample to sample. The dashed line and the dotted line in Figure S5.1 belong to the birch and the wood samples, respectively.

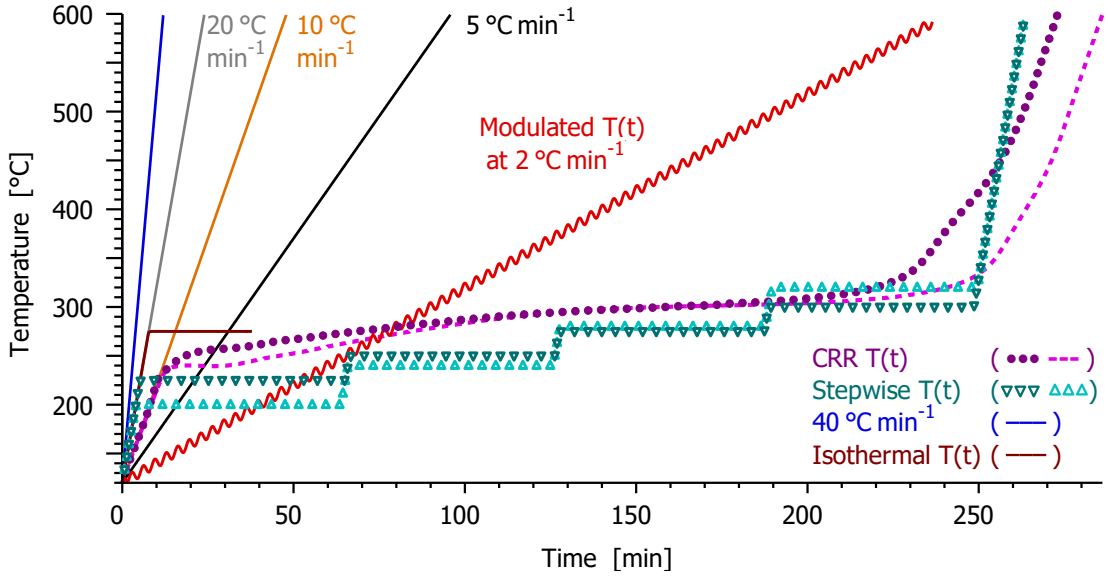


Figure S5.1: Temperature programs used for the TGA experiments of this section.

S5.1. Birch

Model with constant E:

Input file: "B_0,5_oneC.PAR"

x=2α-1

E= 171.15347

$\log_{10}\tilde{A}(x)$= 11.76219 -.555777x +2.408056x^2 +.40424x^3 -2.620136x^4 -1.930992x^5

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)$= 11.983667$T_0(x)$ -1.459467$T_1(x)$ -.10604$T_2(x)$ -.502375$T_3(x)$ -.327517$T_4(x)$ -.120687$T_5(x)$

Model with third order E(α):

Input file: "B_3,5_oneC.PAR"

x=2α-1

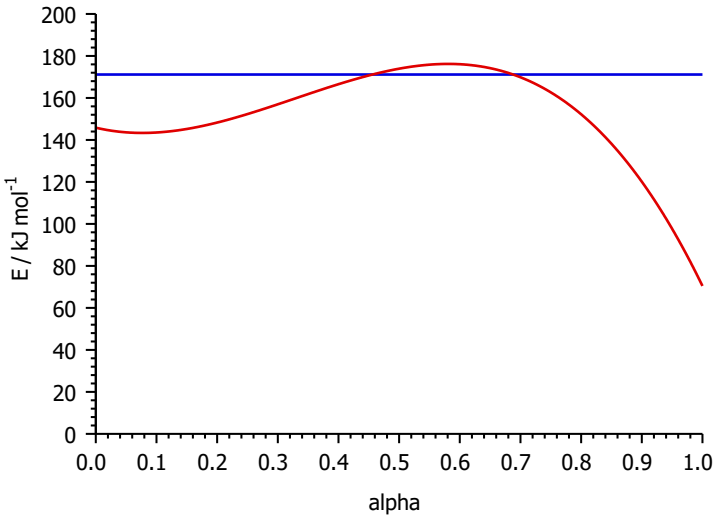
E(x)= 173.93757 +26.34408x -65.79054x^2 -64.03504x^3

$\log_{10}\tilde{A}(x)$= 12.0004161 +1.90238x -3.923592x^2 -5.51472x^3 -1.860768x^4 -1.133216x^5

Expressed by Chebyshev polynomials of the first kind:

E(x)= 141.0423$T_0(x)$ -21.6822$T_1(x)$ -32.89527$T_2(x)$ -16.00876$T_3(x)$

$\log_{10}\tilde{A}(x)$= 9.3408321$T_0(x)$ -2.94192$T_1(x)$ -2.89218$T_2(x)$ -1.73281$T_3(x)$ -.232596$T_4(x)$ -.070826$T_5(x)$



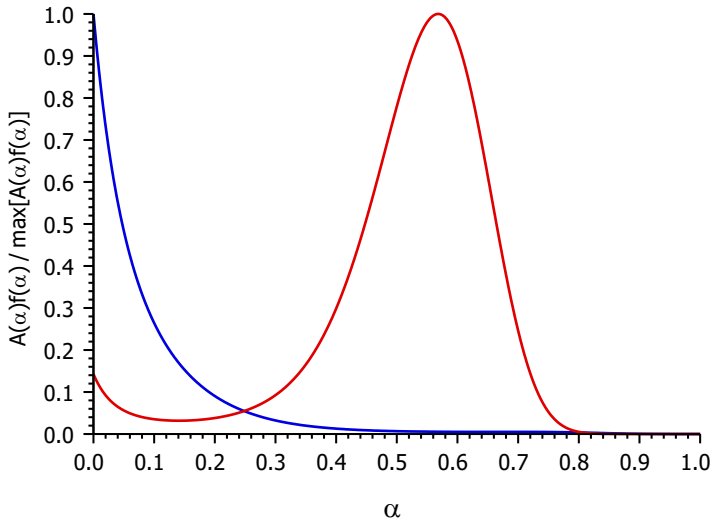
E(α) = polynomial of (2α-1)

Parameter file: B_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 13.63 E(0)= 171.2 $\log_{10}\tilde{A}(1)$= 9.47 E(1)= 171.2
mean $\log_{10}\tilde{A}$= 12.04 mean E= 171.2

Parameter file: B_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 10.96 E(0)= 145.8 $\log_{10}\tilde{A}(1)$= 1.47 E(1)= 70.5
mean $\log_{10}\tilde{A}$= 10.32 mean E= 152.0



Plot of A(α)f(α) / max[A(α)f(α)]

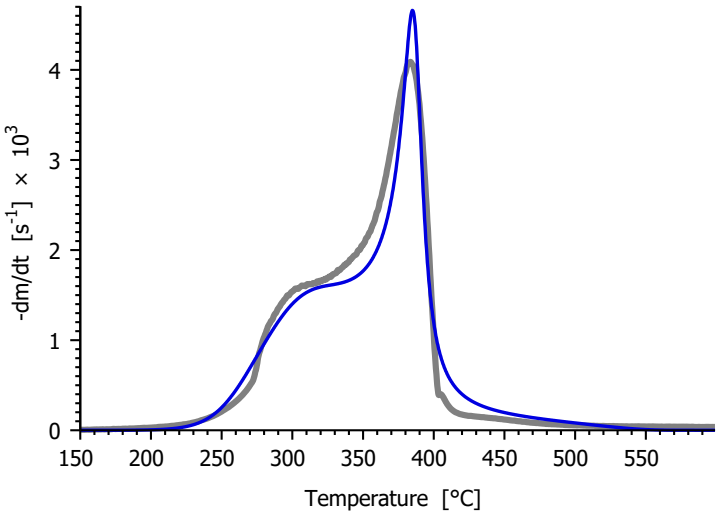
Parameter file: B_0,5_oneC.PAR

A(0)f(0)= 4.292E+13 E(0)= 171.2 A(1)f(1)= 0.00 E(1)= 171.2
mean A(α)f(α)= 3.416E+12 mean E= 171.2
max A(α)f(α)= 4.292E+13 at α= 0.000 and E= 171.2

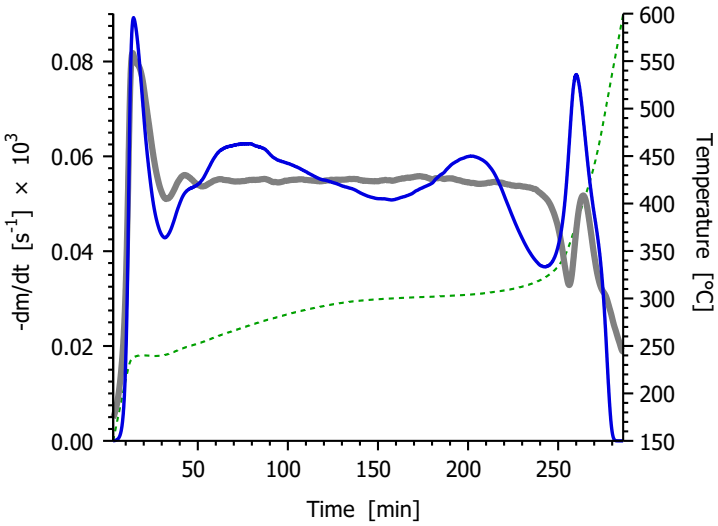
Parameter file: B_3,5_oneC.PAR

A(0)f(0)= 9.154E+10 E(0)= 145.8 A(1)f(1)= 0.00 E(1)= 70.5
mean A(α)f(α)= 1.591E+11 mean E= 152.0
max A(α)f(α)= 6.419E+11 at α= 0.568 and E= 176.1

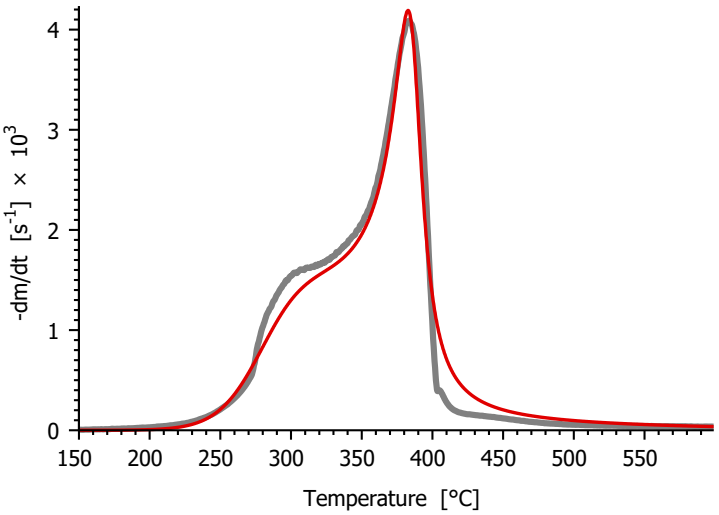
Figures illustrating the fit quality *(cf. Figure 5 in reference [S5])*



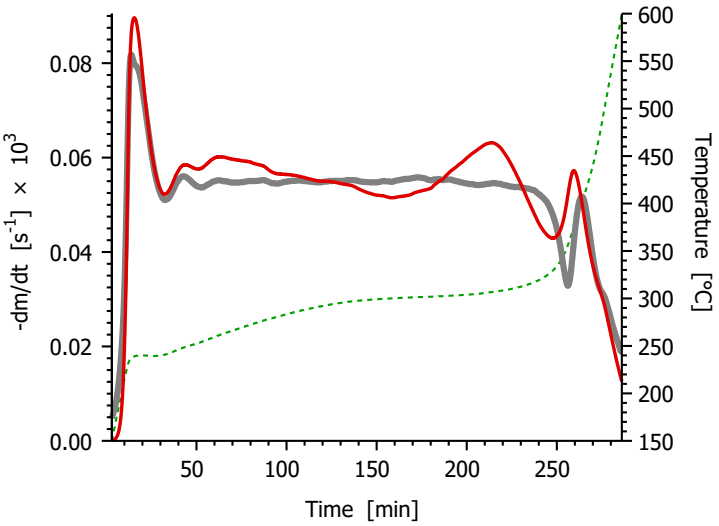
Birch, 20°C/min, 3mg
Relative deviation: 4.32%, Deviation: 0.53 µg/s
rms rel. dev. of 9 experiments: 5.17%
Model: x=2α-1
E(x) = 171.15
$\log_{10}$ Ã(x) = 11.984T_0(x) -1.459T_1(x) -.106T_2(x) -.502T_3(x) -.328T_4(x) -.121T_5(x)
c = 0.876



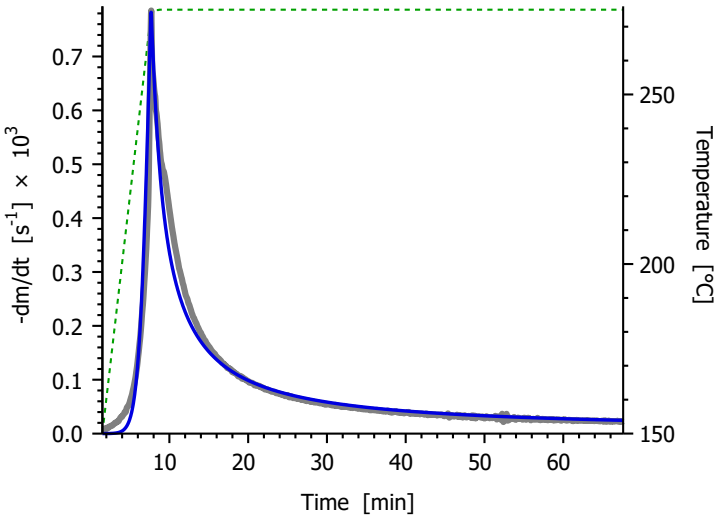
Birch, CRR T(t) (10°C/min), 10mg
Relative deviation: 11.09%, Deviation: 0.090 µg/s
rms rel. dev. of 9 experiments: 5.17%
Model: x=2α-1
E(x) = 171.15
$\log_{10}$ Ã(x) = 11.984T_0(x) -1.459T_1(x) -.106T_2(x) -.502T_3(x) -.328T_4(x) -.121T_5(x)
c = 0.876



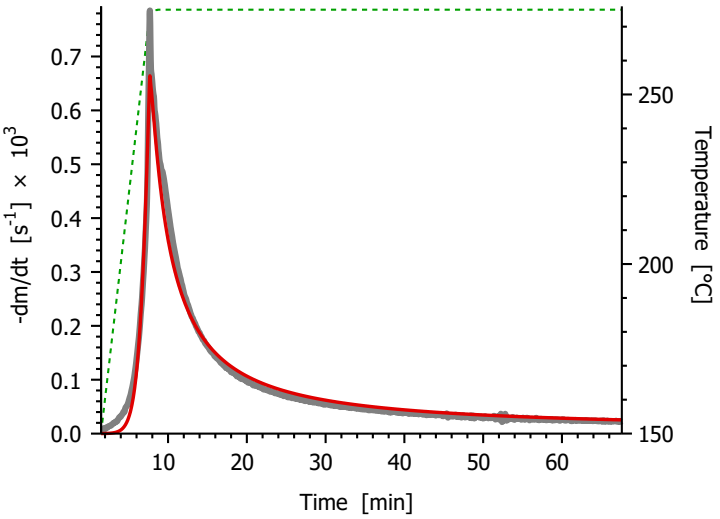
Birch, 20°C/min, 3mg
Relative deviation: 3.64%, Deviation: 0.45 µg/s
rms rel. dev. of 9 experiments: 3.43%
Model: x=2α-1
E(x) = 141.04T_0(x) -21.68T_1(x) -32.9T_2(x) -16.01T_3(x)
$\log_{10}$ Ã(x) = 9.341T_0(x) -2.942T_1(x) -2.892T_2(x) -1.733T_3(x) -.233T_4(x) -.071T_5(x)
c = 0.906



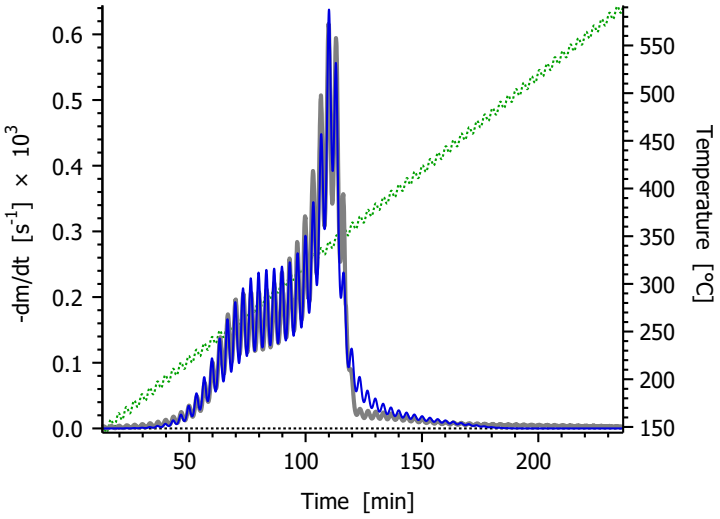
Birch, CRR T(t) (10°C/min), 10mg
Relative deviation: 6.09%, Deviation: 0.049 µg/s
rms rel. dev. of 9 experiments: 3.43%
Model: x=2α-1
E(x) = 141.04T_0(x) -21.68T_1(x) -32.9T_2(x) -16.01T_3(x)
$\log_{10}$ Ã(x) = 9.341T_0(x) -2.942T_1(x) -2.892T_2(x) -1.733T_3(x) -.233T_4(x) -.071T_5(x)
c = 0.906



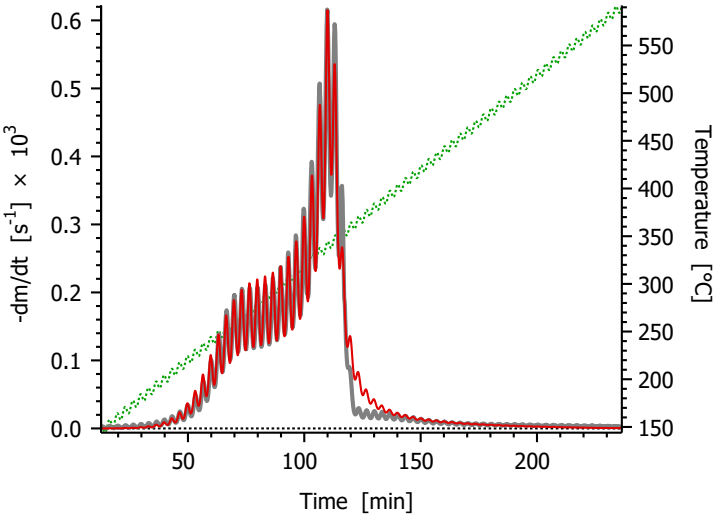
Birch, isothermal: 20°C/min till 275°C (60min), 4mg
Relative deviation: 2.89%, Deviation: 0.088 µg/s
rms rel. dev. of 9 experiments: 5.17%
Model: x=2α-1
E(x) = 171.15
$\log_{10}$ Ã(x) = 11.984T_0(x) -1.459T_1(x) -.106T_2(x) -.502T_3(x) -.328T_4(x) -.121T_5(x)
c = 0.876



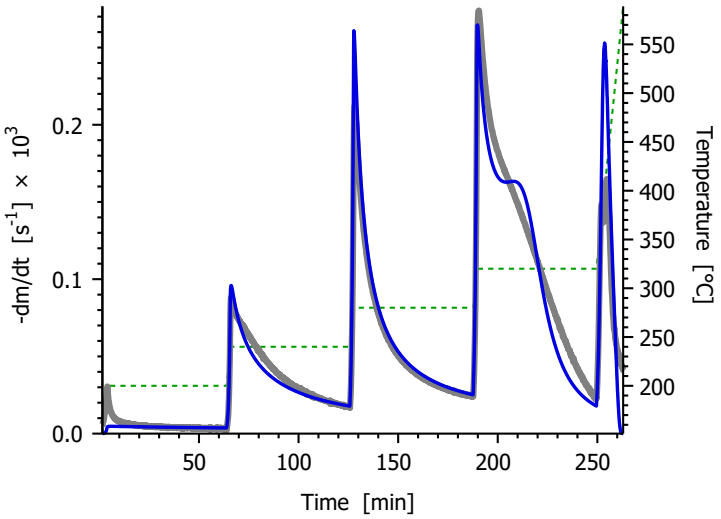
Birch, isothermal: 20°C/min till 275°C (60min), 4mg
Relative deviation: 1.97%, Deviation: 0.060 µg/s
rms rel. dev. of 9 experiments: 3.43%
Model: x=2α-1
E(x) = 141.04T_0(x) -21.68T_1(x) -32.9T_2(x) -16.01T_3(x)
$\log_{10}$ Ã(x) = 9.341T_0(x) -2.942T_1(x) -2.892T_2(x) -1.733T_3(x) -.233T_4(x) -.071T_5(x)
c = 0.906



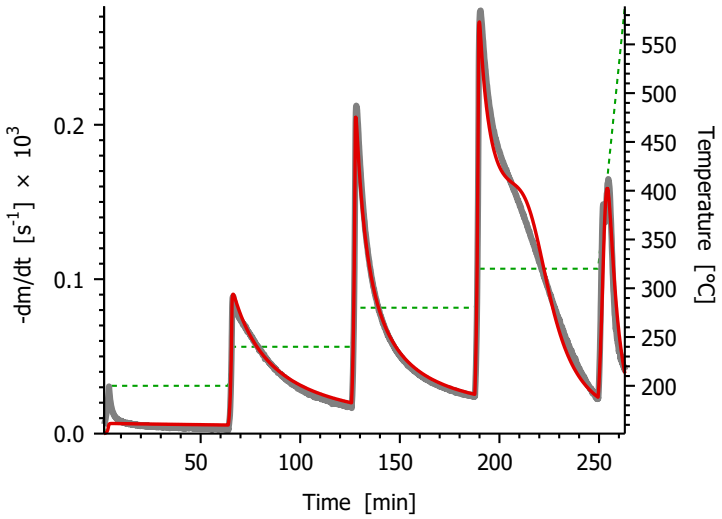
Birch, modulated T(t) (2°C/min), 10mg
Relative deviation: 2.81%, Deviation: 0.16 µg/s
rms rel. dev. of 9 experiments: 5.17%
Model: x=2α-1
E(x) = 171.15
$\log_{10}$ Ã(x) = 11.984T_0(x) -1.459T_1(x) -.106T_2(x) -.502T_3(x) -.328T_4(x) -.121T_5(x)
c = 0.876



Birch, modulated T(t) (2°C/min), 10mg
Relative deviation: 2.31%, Deviation: 0.13 µg/s
rms rel. dev. of 9 experiments: 3.43%
Model: x=2α-1
E(x) = 141.04T_0(x) -21.68T_1(x) -32.9T_2(x) -16.01T_3(x)
$\log_{10}$ Ã(x) = 9.341T_0(x) -2.942T_1(x) -2.892T_2(x) -1.733T_3(x) -.233T_4(x) -.071T_5(x)
c = 0.906



Birch, stepwise T(t) 200-320°C, 5mg
Relative deviation: 5.23%, Deviation: 0.075 µg/s
rms rel. dev. of 9 experiments: 5.17%
Model: x=2α-1
E(x) = 171.15
$\log_{10}$ Ã(x) = 11.984T_0(x) -1.459T_1(x) -.106T_2(x) -.502T_3(x)
-.328T_4(x) -.121T_5(x)
c = 0.876



Birch, stepwise T(t) 200-320°C, 5mg
Relative deviation: 2.51%, Deviation: 0.036 µg/s
rms rel. dev. of 9 experiments: 3.43%
Model: x=2α-1
E(x) = 141.04T_0(x) -21.68T_1(x) -32.9T_2(x) -16.01T_3(x)
$\log_{10}$ Ã(x) = 9.341T_0(x) -2.942T_1(x) -2.892T_2(x) -1.733T_3(x)
-.233T_4(x) -.071T_5(x)
c = 0.906

S5.2. Spruce

Model with constant E:

Input file: "S_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 168.22096$

$\log_{10}\tilde{A}(x)= 11.535869 -.420241x +1.585322x^2 +.849588x^3 -2.744856x^4 -3.429088x^5$

Expressed by Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 11.299209T_0(x) -1.92623T_1(x) -.579767T_2(x) -.859193T_3(x) -.343107T_4(x) -.214318T_5(x)$

Model with third order E(α):

Input file: "S_3,5_oneC.PAR"

$x=2\alpha-1$

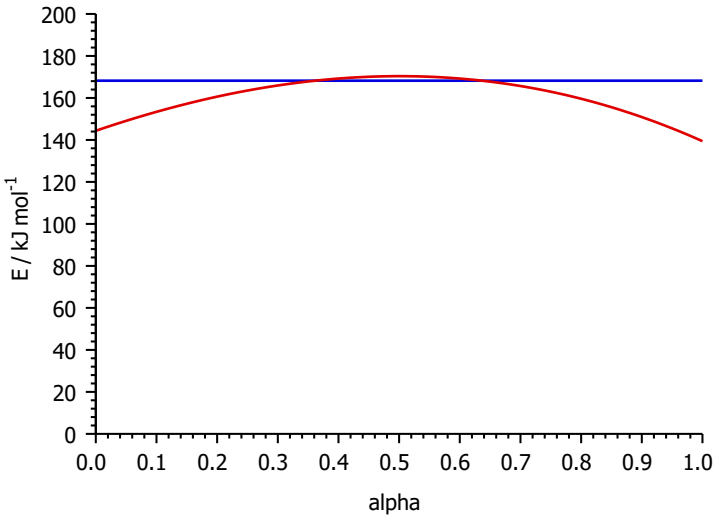
$E(x)= 170.37188 +.090612x -28.48678x^2 -2.571172x^3$

$\log_{10}\tilde{A}(x)= 11.715329 -.385387x -.952078x^2 +.50058x^3 -2.814936x^4 -3.108848x^5$

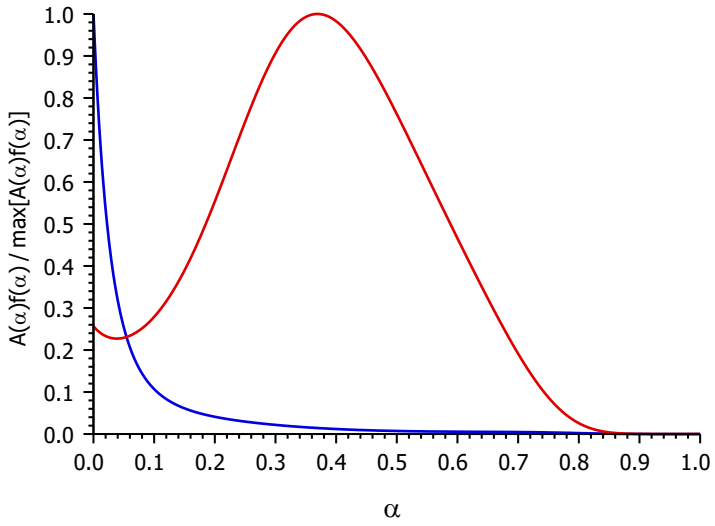
Expressed by Chebyshev polynomials of the first kind:

$E(x)= 156.12849T_0(x) -1.837767T_1(x) -14.24339T_2(x) -.642793T_3(x)$

$\log_{10}\tilde{A}(x)= 10.183689T_0(x) -1.952982T_1(x) -1.883507T_2(x) -.84637T_3(x) -.351867T_4(x) -.194303T_5(x)$



E(α) = polynomial of (2α-1)



Plot of A(α)f(α) / max[A(α)f(α)]

Parameter file: S_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 13.38$ $E(0)= 168.2$ $\log_{10}\tilde{A}(1)= 7.38$ $E(1)= 168.2$

mean $\log_{10}\tilde{A}= 11.52$ mean $E= 168.2$

Parameter file: S_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 10.94$ $E(0)= 144.4$ $\log_{10}\tilde{A}(1)= 4.95$ $E(1)= 139.4$

mean $\log_{10}\tilde{A}= 10.83$ mean $E= 160.9$

Parameter file: S_0,5_oneC.PAR

$A(0)f(0)= 2.377E+13$ $E(0)= 168.2$ $A(1)f(1)= 0.00$ $E(1)= 168.2$

mean $A(\alpha)f(\alpha)= 1.136E+12$ mean $E= 168.2$

max $A(\alpha)f(\alpha)= 2.377E+13$ at $\alpha= 0.000$ and $E= 168.2$

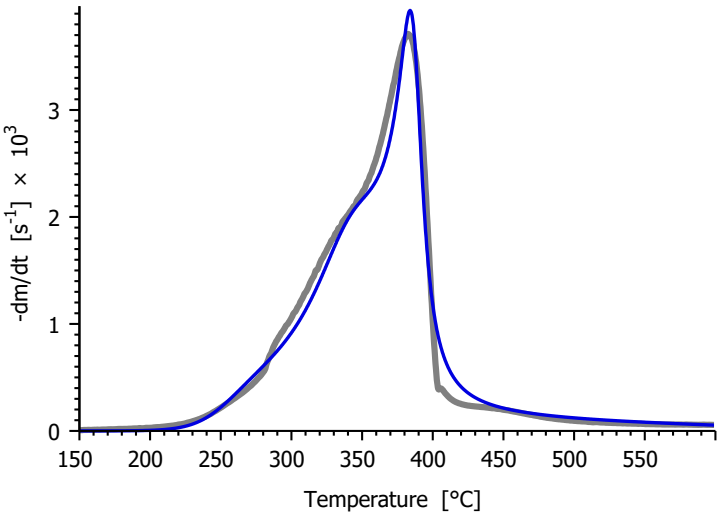
Parameter file: S_3,5_oneC.PAR

$A(0)f(0)= 8.749E+10$ $E(0)= 144.4$ $A(1)f(1)= 0.00$ $E(1)= 139.4$

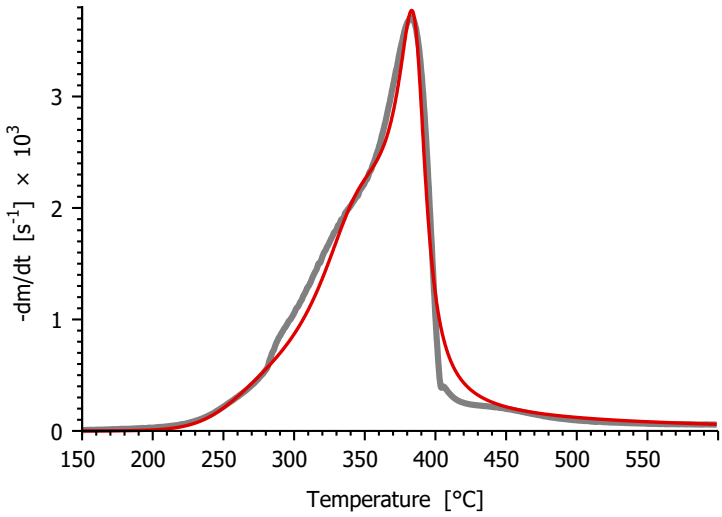
mean $A(\alpha)f(\alpha)= 1.459E+11$ mean $E= 160.9$

max $A(\alpha)f(\alpha)= 3.408E+11$ at $\alpha= 0.369$ and $E= 168.4$

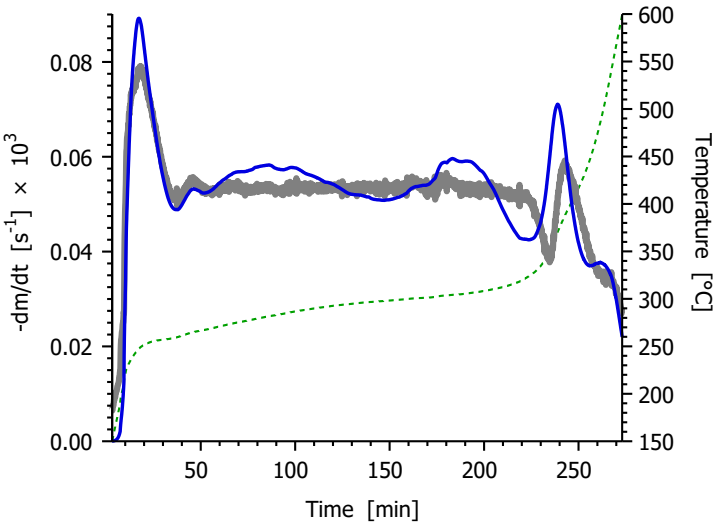
Figures illustrating the fit quality *(cf. Figure 6 in reference [S5])*



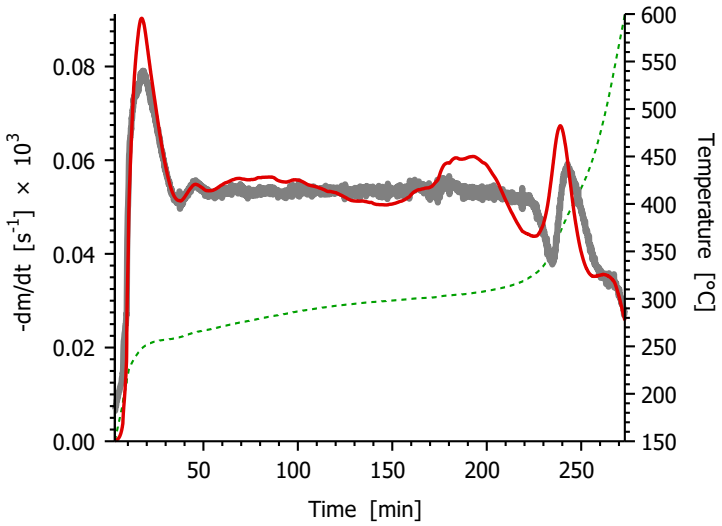
Spruce, 20°C/min, 3mg
Relative deviation: 3.18%, Deviation: 0.38 µg/s
rms rel. dev. of 9 experiments: 3.51%
Model: x=2α-1
E(x) = 168.22
$\log_{10}$ Ã(x) = 11.299T_0(x) -1.926T_1(x) -.58T_2(x) -.859T_3(x) -.343T_4(x) -.214T_5(x)
c = 0.856



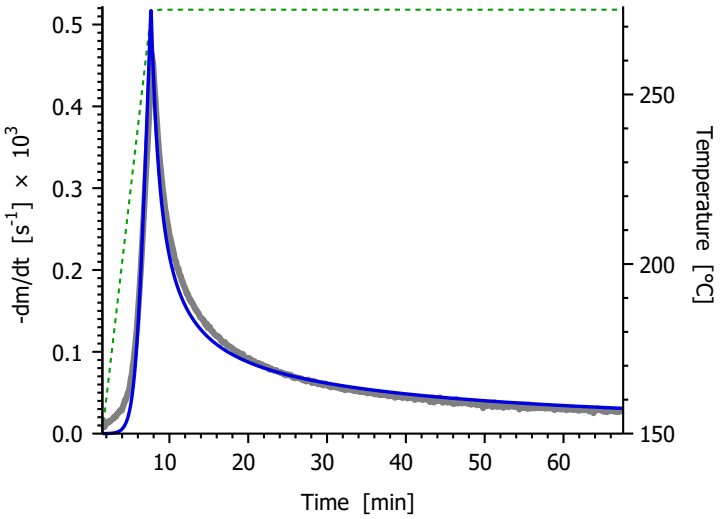
Spruce, 20°C/min, 3mg
Relative deviation: 3.14%, Deviation: 0.38 µg/s
rms rel. dev. of 9 experiments: 3.30%
Model: x=2α-1
E(x) = 156.13T_0(x) -1.84T_1(x) -14.24T_2(x) -.64T_3(x)
$\log_{10}$ Ã(x) = 10.184T_0(x) -1.953T_1(x) -1.884T_2(x) -.846T_3(x) -.352T_4(x) -.194T_5(x)
c = 0.866



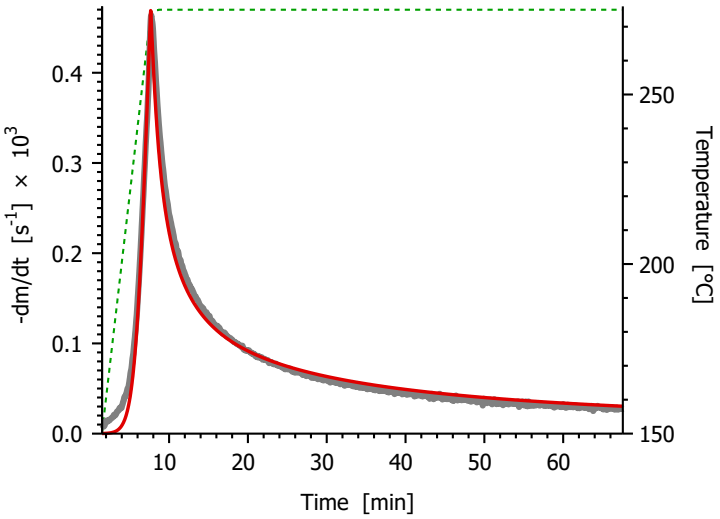
Spruce, CRR T(t) (10°C/min), 9mg
Relative deviation: 7.28%, Deviation: 0.053 µg/s
rms rel. dev. of 9 experiments: 3.51%
Model: x=2α-1
E(x) = 168.22
$\log_{10}$ Ã(x) = 11.299T_0(x) -1.926T_1(x) -.58T_2(x) -.859T_3(x) -.343T_4(x) -.214T_5(x)
c = 0.856



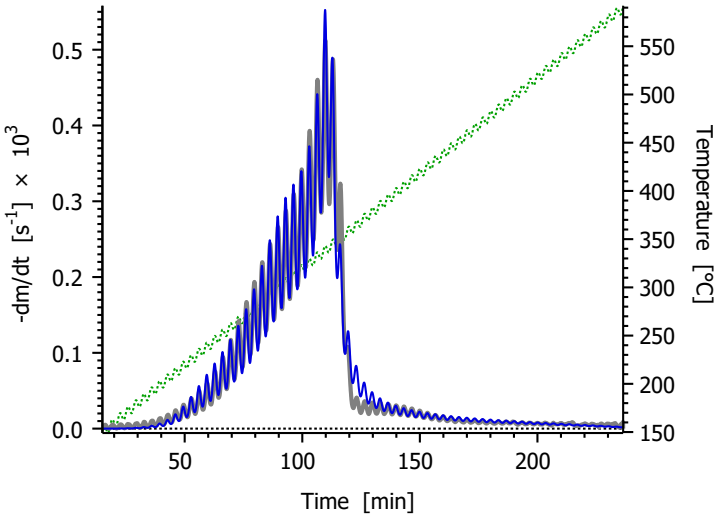
Spruce, CRR T(t) (10°C/min), 9mg
Relative deviation: 6.62%, Deviation: 0.048 µg/s
rms rel. dev. of 9 experiments: 3.30%
Model: x=2α-1
E(x) = 156.13T_0(x) -1.84T_1(x) -14.24T_2(x) -.64T_3(x)
$\log_{10}$ Ã(x) = 10.184T_0(x) -1.953T_1(x) -1.884T_2(x) -.846T_3(x) -.352T_4(x) -.194T_5(x)
c = 0.866



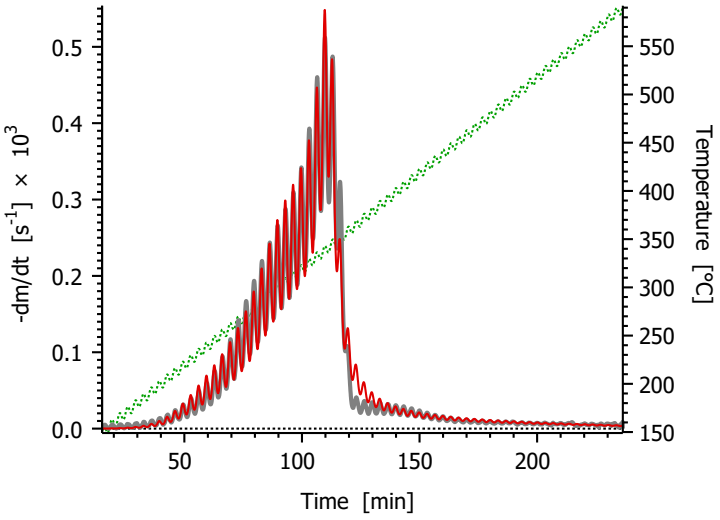
Spruce, isothermal: 20°C/min till 275°C (60min), 3mg
Relative deviation: 2.56%, Deviation: 0.037 µg/s
rms rel. dev. of 9 experiments: 3.51%
Model: x=2α-1
E(x) = 168.22
$\log_{10} \tilde{A}(x) = 11.299T_0(x) -1.926T_1(x) -.58T_2(x) -.859T_3(x) -.343T_4(x) -.214T_5(x)$
c = 0.856



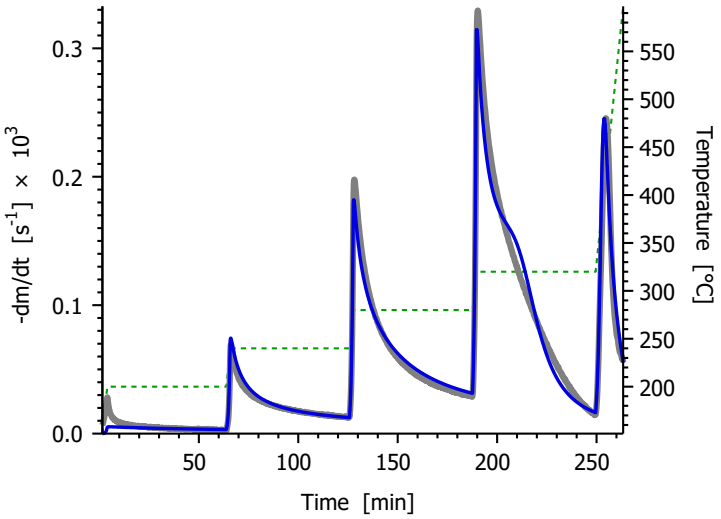
Spruce, isothermal: 20°C/min till 275°C (60min), 3mg
3mg 2012-02-19
Relative deviation: 1.95%, Deviation: 0.028 µg/s
rms rel. dev. of 9 experiments: 3.30%
Model: x=2α-1
E(x) = 156.13T_0(x) -1.84T_1(x) -14.24T_2(x) -.64T_3(x)
$\log_{10} \tilde{A}(x) = 10.184T_0(x) -1.953T_1(x) -1.884T_2(x) -.846T_3(x) -.352T_4(x) -.194T_5(x)$
c = 0.866



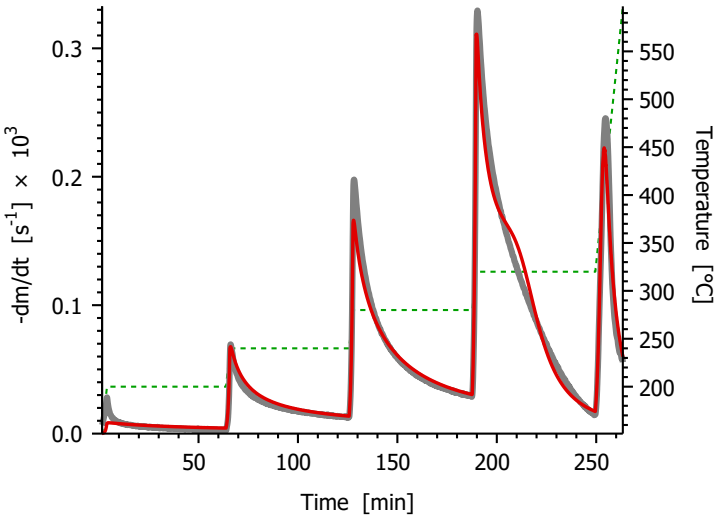
Spruce, modulated T(t) (2°C/min), 3mg
Relative deviation: 2.71%, Deviation: 0.046 µg/s
rms rel. dev. of 9 experiments: 3.51%
Model: x=2α-1
E(x) = 168.22
$\log_{10} \tilde{A}(x) = 11.299T_0(x) -1.926T_1(x) -.58T_2(x) -.859T_3(x) -.343T_4(x) -.214T_5(x)$
c = 0.856



Spruce, modulated T(t) (2°C/min), 3mg
Relative deviation: 2.59%, Deviation: 0.044 µg/s
rms rel. dev. of 9 experiments: 3.30%
Model: x=2α-1
E(x) = 156.13T_0(x) -1.84T_1(x) -14.24T_2(x) -.64T_3(x)
$\log_{10} \tilde{A}(x) = 10.184T_0(x) -1.953T_1(x) -1.884T_2(x) -.846T_3(x) -.352T_4(x) -.194T_5(x)$
c = 0.866



Spruce, stepwise T(t) 200-320°C, 4mg
Relative deviation: 2.64%, Deviation: 0.033 µg/s
rms rel. dev. of 9 experiments: 3.51%
Model: x=2α-1
E(x) = 168.22
$\log_{10}$ Ã(x) = 11.299T_0(x) -1.926T_1(x) -.58T_2(x) -.859T_3(x) -.343T_4(x) -.214T_5(x)
c = 0.856



Spruce, stepwise T(t) 200-320°C, 4mg
Relative deviation: 2.66%, Deviation: 0.033 µg/s
rms rel. dev. of 9 experiments: 3.30%
Model: x=2α-1
E(x) = 156.13T_0(x) -1.84T_1(x) -14.24T_2(x) -.64T_3(x)
$\log_{10}$ Ã(x) = 10.184T_0(x) -1.953T_1(x) -1.884T_2(x) -.846T_3(x) -.352T_4(x) -.194T_5(x)
c = 0.866

S6. Bark and Wood

Source of the data:

[S6] 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

Spruce (Norway spruce) and its bark were examined. The samples were obtained from a forest in South Norway. Eight TGA experiments were available for each sample: three with linear heating (2.5, 10 and 40 °C/min), two with stepwise heating, and isothermal experiments at 225, 275 and 325°C. (The isothermal experiments were evaluated together with the heat-up sections, as shown in the next pages.) The figure below shows the corresponding temperature programs. It is a redrawn/rearranged version of Figure 1 of the cited paper.

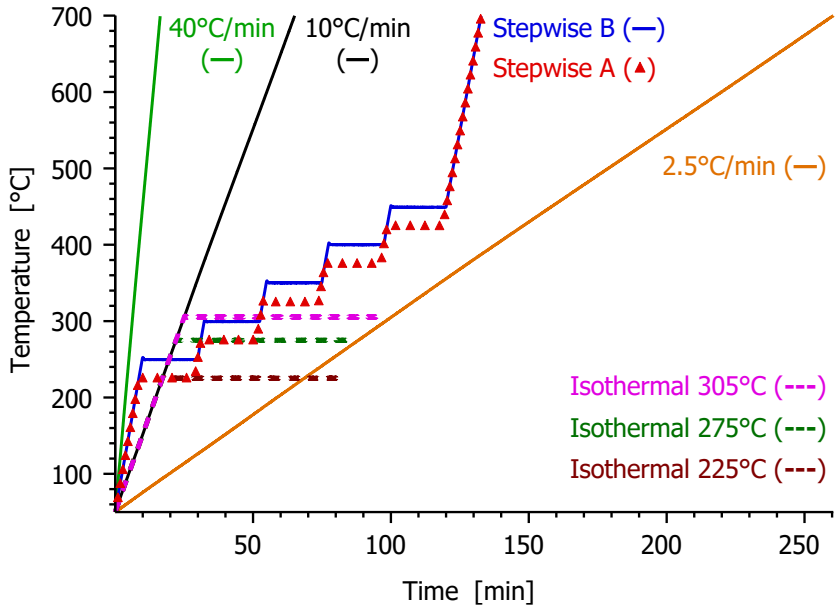


Figure S6.1: Temperature programs used for the TGA experiments of this section.

S6.1. Bark

Model with constant E:

Input file: "B_0,5_oneC.PAR"

$x=2\alpha-1$

E= 183.7358

$\log_{10}\tilde{A}(x)= 12.815827 -.505444x +.87104x^2 -3.110812x^3 -5.027752x^4 -3.535776x^5$

Expressed with Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 11.36594T_0(x) -5.048413T_1(x) -2.078356T_2(x) -1.882633T_3(x) -.628469T_4(x) -.220986T_5(x)$

Model with third order E(α):

Input file: "B_3,5_oneC.PAR"

$x=2\alpha-1$

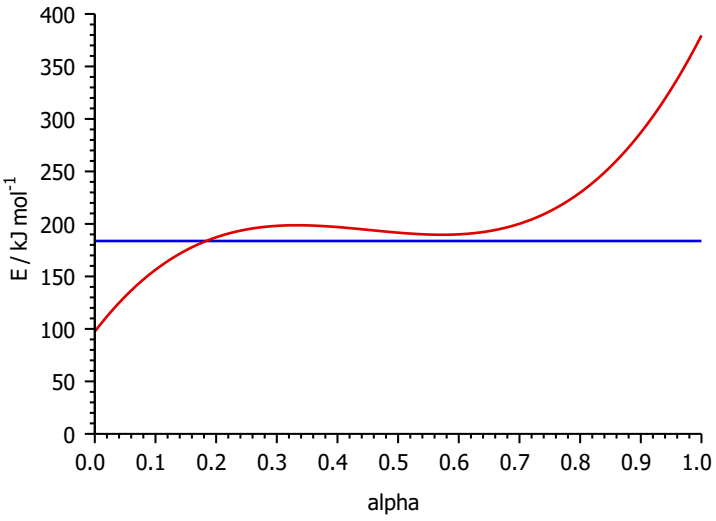
$E(x)= 191.660298 -23.91577x +46.847964x^2 +164.984172x^3$

$\log_{10}\tilde{A}(x)= 13.514137 -2.5125887x +5.545716x^2 +10.0581952x^3 -6.413064x^4 -1.645296x^5$

Expressed with Chebyshev polynomials of the first kind:

$E(x)= 215.08428T_0(x) +99.822359T_1(x) +23.423982T_2(x) +41.246043T_3(x)$

$\log_{10}\tilde{A}(x)= 13.882096T_0(x) +4.0027477T_1(x) -.433674T_2(x) +2.0003938T_3(x) -.801633T_4(x) -.102831T_5(x)$



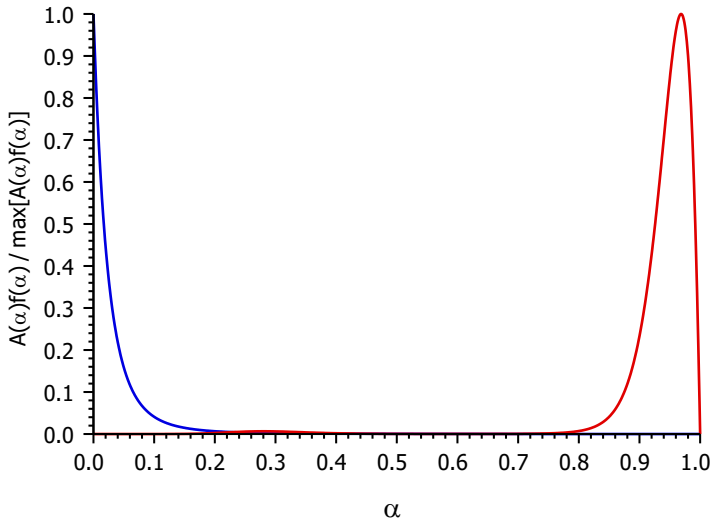
E(α) = polynomial of (2α-1)

Parameter file: B_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 15.81 E(0)= 183.7 $\log_{10}\tilde{A}(1)$= 1.51 E(1)= 183.7
mean $\log_{10}\tilde{A}$= 12.10 mean E= 183.7

Parameter file: B_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)$= 6.75 E(0)= 97.4 $\log_{10}\tilde{A}(1)$= 18.55 E(1)= 379.6
mean $\log_{10}\tilde{A}$= 14.08 mean E= 207.3



Plot of A(α)f(α) / max[A(α)f(α)]

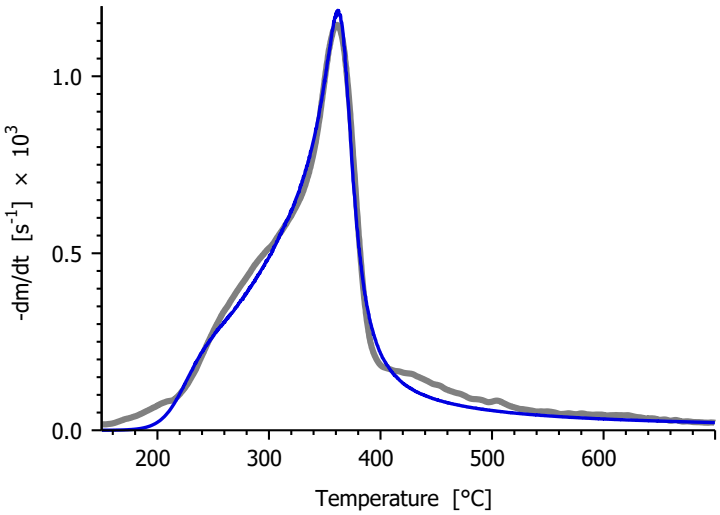
Parameter file: B_0,5_oneC.PAR

A(0)f(0)= 6.474E+15 E(0)= 183.7 A(1)f(1)= 0.00 E(1)= 183.7
mean A(α)f(α)= 1.841E+14 mean E= 183.7
max A(α)f(α)= 6.474E+15 at α= 0.000 and E= 183.7

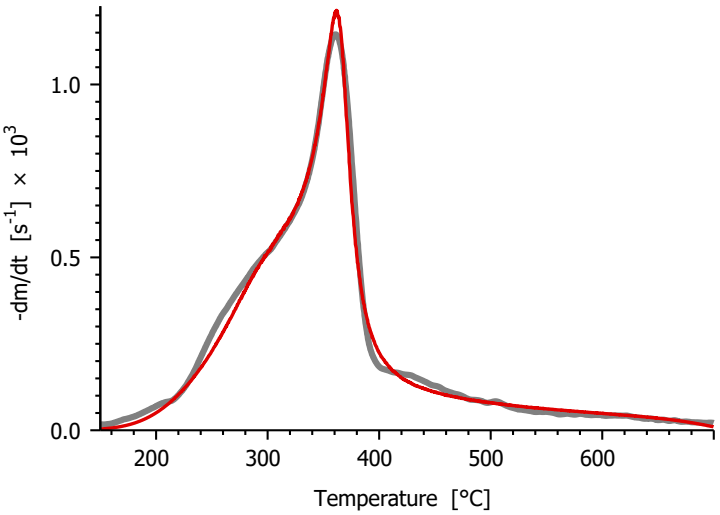
Parameter file: B_3,5_oneC.PAR

A(0)f(0)= 5.578E+06 E(0)= 97.4 A(1)f(1)= 0.00 E(1)= 379.6
mean A(α)f(α)= 3.402E+15 mean E= 207.3
max A(α)f(α)= 4.676E+16 at α= 0.969 and E= 346.2

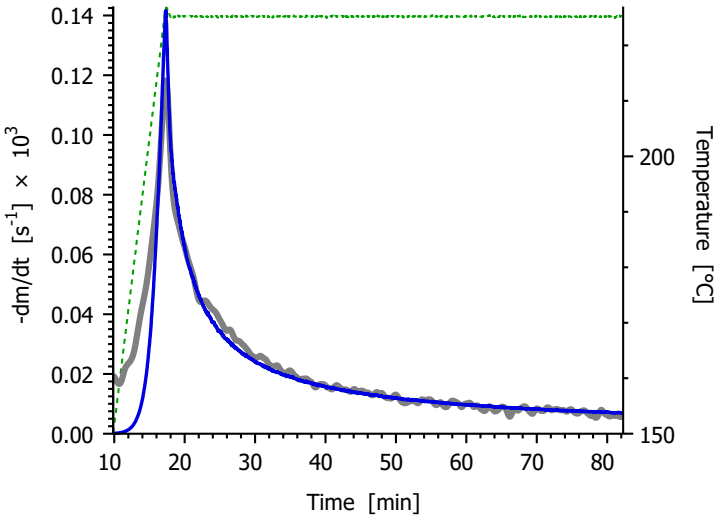
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S6])*



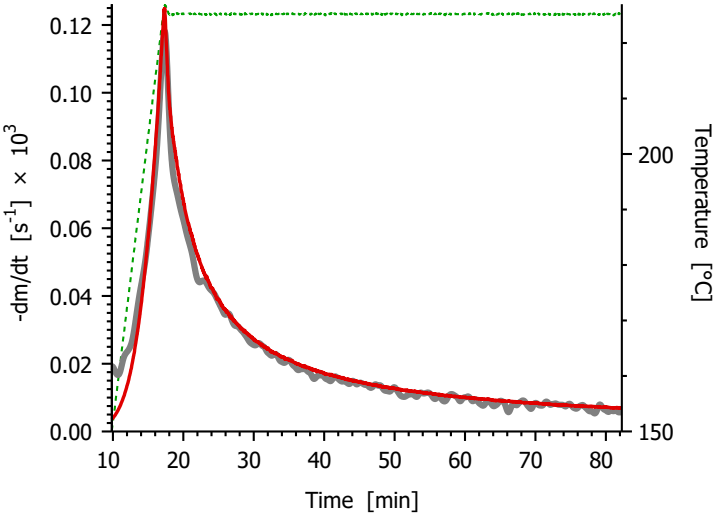
Bark, 10°C/min, 2mg
Relative deviation: 2.33%, Deviation: 0.058 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x)
-.628T_4(x) -.221T_5(x)
c = 0.723



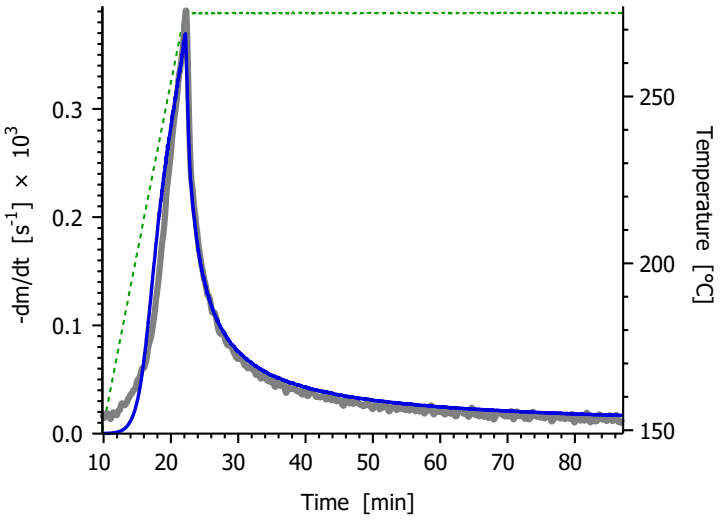
Bark, 10°C/min, 2mg
Relative deviation: 2.05%, Deviation: 0.051 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x)
-.802T_4(x) -.103T_5(x)
c = 0.702



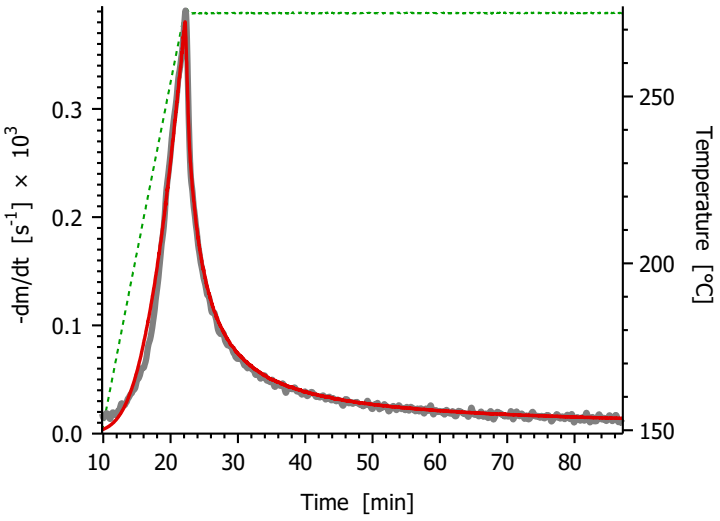
Bark, 65min at 225°C (10°C/min), 4mg
Relative deviation: 6.25%, Deviation: 0.029 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x)
-.628T_4(x) -.221T_5(x)
c = 0.723



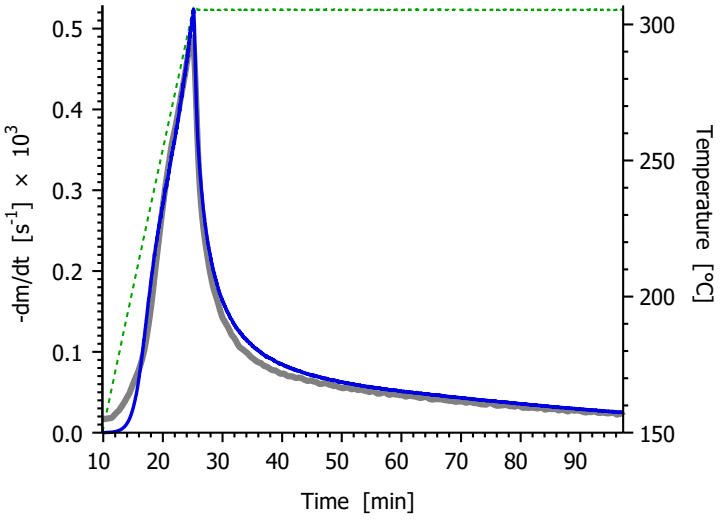
Bark, 65min at 225°C (10°C/min), 4mg
Relative deviation: 2.77%, Deviation: 0.013 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x)
-.802T_4(x) -.103T_5(x)
c = 0.702



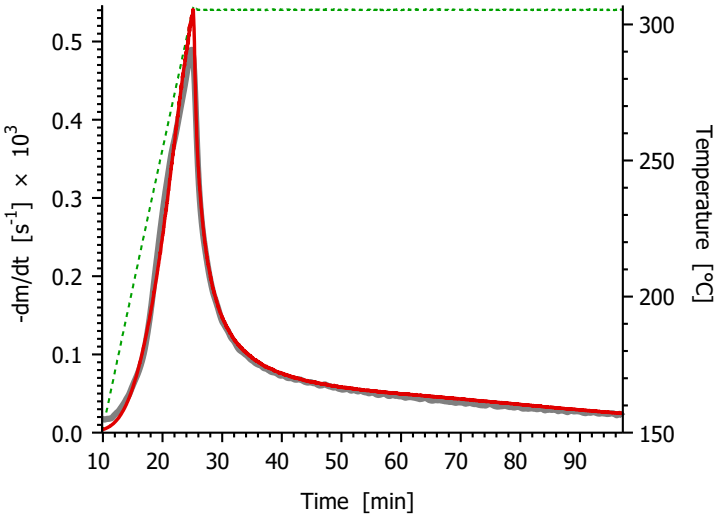
Bark, 65min at 275°C (10°C/min), 4mg
Relative deviation: 3.13%, Deviation: 0.049 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x) -.628T_4(x) -.221T_5(x)
c = 0.723



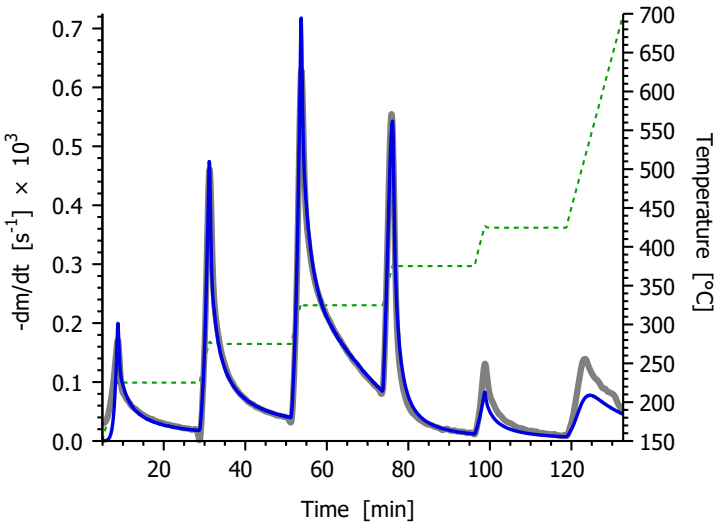
Bark, 65min at 275°C (10°C/min), 4mg
Relative deviation: 1.57%, Deviation: 0.024 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x) -.802T_4(x) -.103T_5(x)
c = 0.702



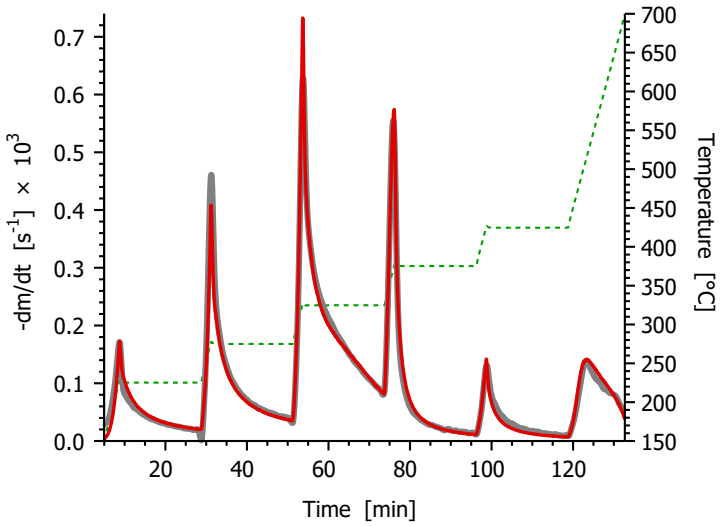
Bark, 65min at 305°C (10°C/min), 4mg
Relative deviation: 2.43%, Deviation: 0.044 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x) -.628T_4(x) -.221T_5(x)
c = 0.723



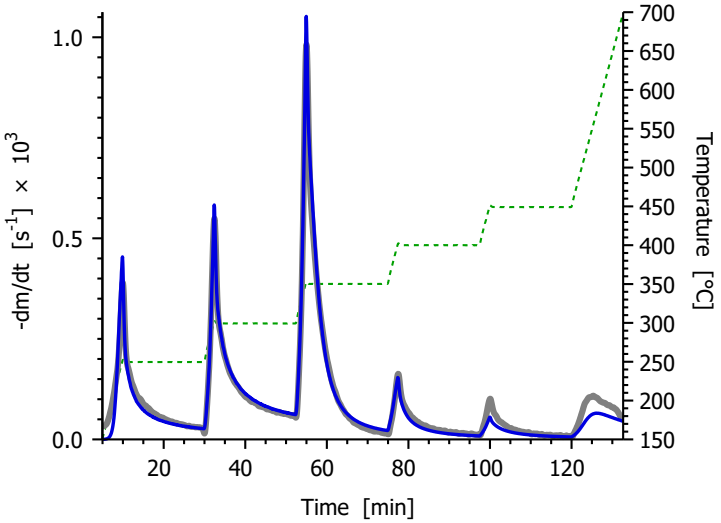
Bark, 65min at 305°C (10°C/min), 4mg
Relative deviation: 1.76%, Deviation: 0.032 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x) -.802T_4(x) -.103T_5(x)
c = 0.702



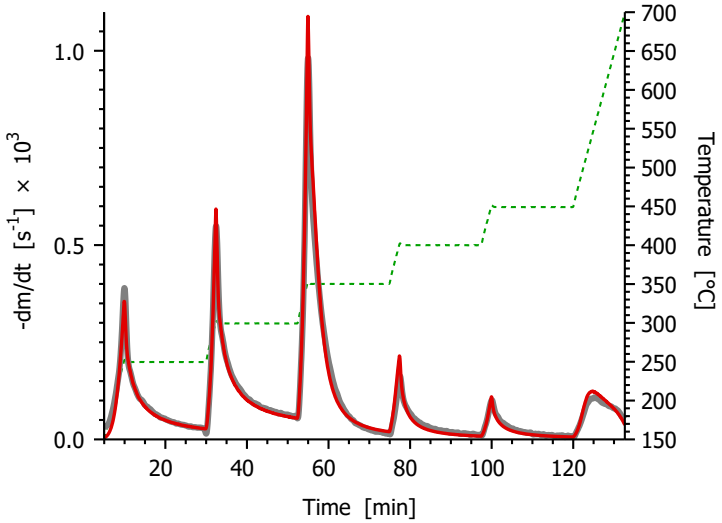
Bark, stepwise T(t) "A" (20°C/min), 4mg
Relative deviation: 2.88%, Deviation: 0.073 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x) -.628T_4(x) -.221T_5(x)
c = 0.723



Bark, stepwise T(t) "A" (20°C/min), 4mg
Relative deviation: 2.21%, Deviation: 0.056 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x) -.802T_4(x) -.103T_5(x)
c = 0.702



Bark, stepwise T(t) "B" (20°C/min), 4mg
Relative deviation: 1.86%, Deviation: 0.074 µg/s
rms rel. dev. of 8 experiments: 3.33%
Model: x=2α-1
E(x) = 183.74
$\log_{10}$ Ã(x) = 11.366T_0(x) -5.048T_1(x) -2.078T_2(x) -1.883T_3(x) -.628T_4(x) -.221T_5(x)
c = 0.723



Bark, stepwise T(t) "B" (20°C/min), 4mg
Relative deviation: 1.48%, Deviation: 0.059 µg/s
rms rel. dev. of 8 experiments: 2.18%
Model: x=2α-1
E(x) = 215.08T_0(x) +99.82T_1(x) +23.42T_2(x) +41.25T_3(x)
$\log_{10}$ Ã(x) = 13.882T_0(x) +4.003T_1(x) -.434T_2(x) +2.0T_3(x) -.802T_4(x) -.103T_5(x)
c = 0.702

S6.2. Wood

Model with constant E:

Input file: "W_0,5_oneC.PAR"

$x=2\alpha-1$

$E= 173.51359$

$\log_{10}\tilde{A}(x)= 11.638268 -.41031x +2.179856x^2 +.7517x^3 -6.469424x^4 -6.64784x^5$

Expressed with Chebyshev polynomials of the first kind:

$\log_{10}\tilde{A}(x)= 10.302162T_0(x) -4.001435T_1(x) -2.144784T_2(x) -1.889525T_3(x) -.808678T_4(x) -.41549T_5(x)$

Model with third order E(α):

Input file: "W_3,5_oneC.PAR"

$x=2\alpha-1$

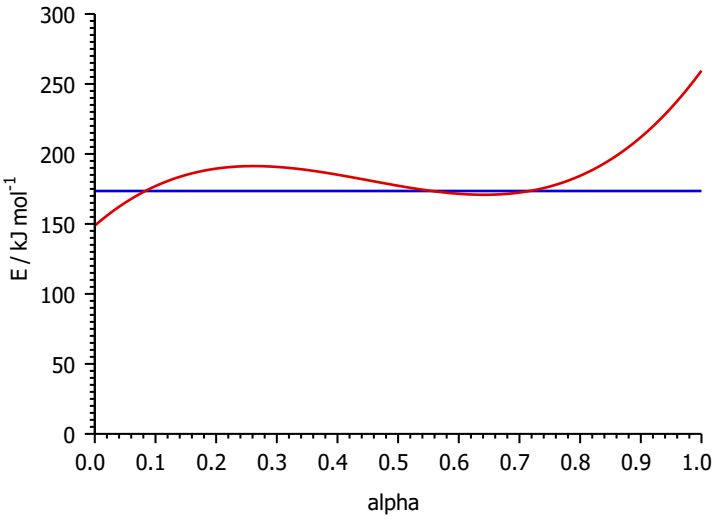
$E(x)= 177.269618 -37.801456x +26.878364x^2 +93.1628x^3$

$\log_{10}\tilde{A}(x)= 12.0739416 -3.7579116x +4.1196608x^2 +9.0435888x^3 -3.131296x^4 -3.355152x^5$

Expressed with Chebyshev polynomials of the first kind:

$E(x)= 190.7088T_0(x) +32.070644T_1(x) +13.439182T_2(x) +23.2907T_3(x)$

$\log_{10}\tilde{A}(x)= 12.959536T_0(x) +.92781T_1(x) +.4941824T_2(x) +1.2124122T_3(x) -.391412T_4(x) -.209697T_5(x)$



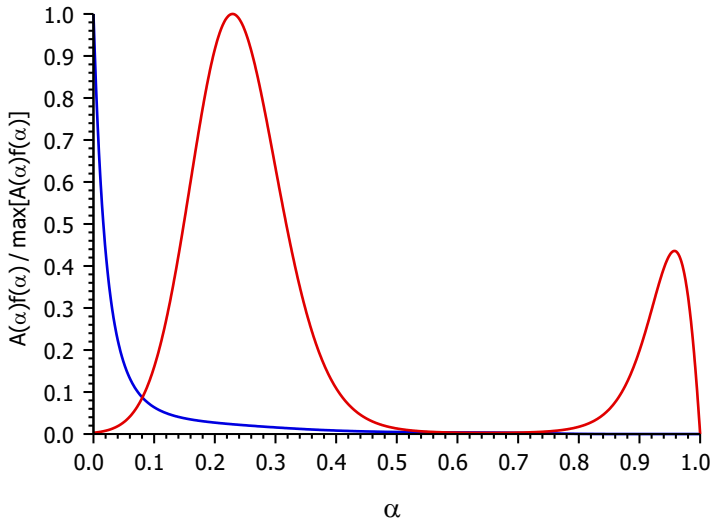
E(α) = polynomial of (2α-1)

Parameter file: W_0,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 13.66$ E(0)= 173.5 $\log_{10}\tilde{A}(1)= 1.04$ E(1)= 173.5
mean $\log_{10}\tilde{A}= 11.07$ mean E= 173.5

Parameter file: W_3,5_oneC.PAR

$\log_{10}\tilde{A}(0)= 11.13$ E(0)= 148.8 $\log_{10}\tilde{A}(1)= 14.99$ E(1)= 259.5
mean $\log_{10}\tilde{A}= 12.82$ mean E= 186.2



Plot of A(α)f(α) / max[A(α)f(α)]

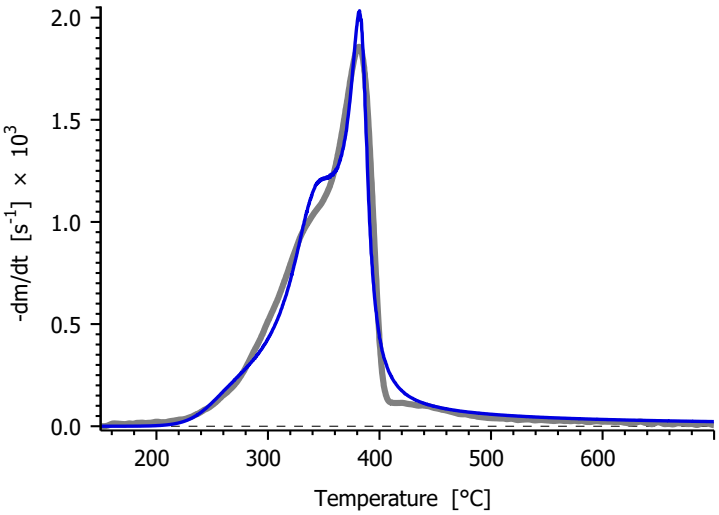
Parameter file: W_0,5_oneC.PAR

A(0)f(0)= 4.520E+13 E(0)= 173.5 A(1)f(1)= 0.00 E(1)= 173.5
mean A(α)f(α)= 1.608E+12 mean E= 173.5
max A(α)f(α)= 4.520E+13 at α= 0.000 and E= 173.5

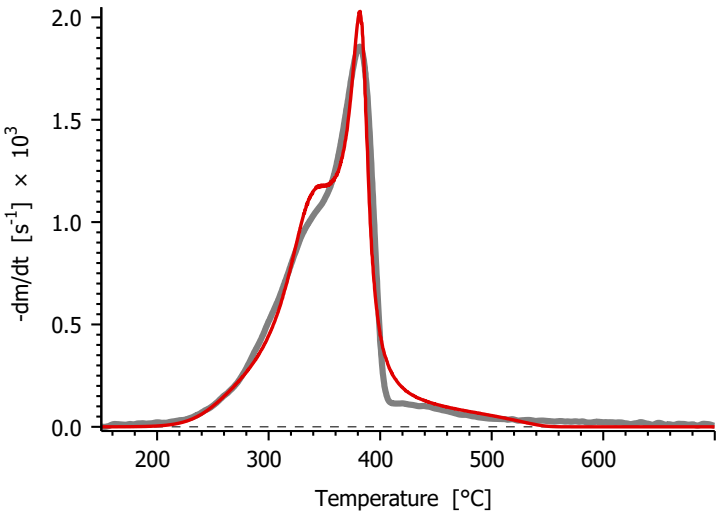
Parameter file: W_3,5_oneC.PAR

A(0)f(0)= 1.355E+11 E(0)= 148.8 A(1)f(1)= 0.00 E(1)= 259.5
mean A(α)f(α)= 1.011E+13 mean E= 186.2
max A(α)f(α)= 4.516E+13 at α= 0.229 and E= 190.8

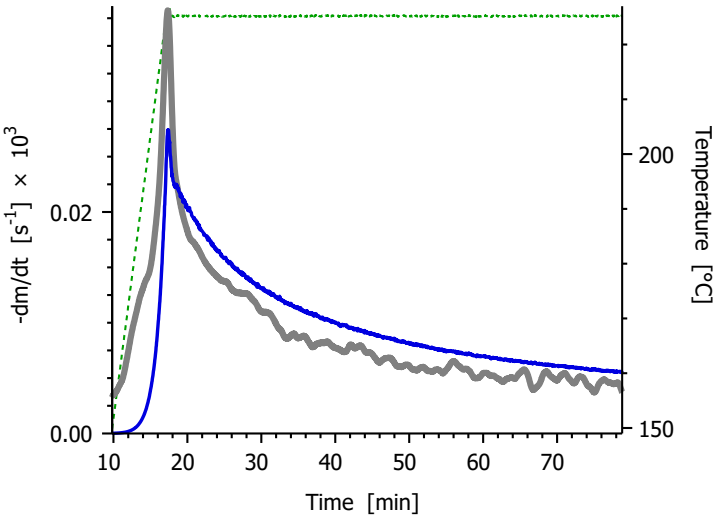
Figures illustrating the fit quality *(cf. Figure S1 in the Supporting Information of reference [S6])*



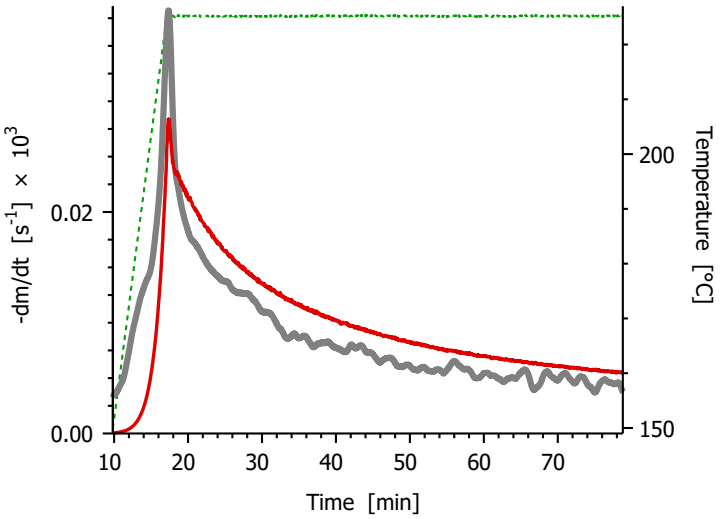
Wood, 10°C/min, 2mg
Relative deviation: 3.29%, Deviation: 0.12 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x)
-.809T_4(x) -.415T_5(x)
c = 0.912



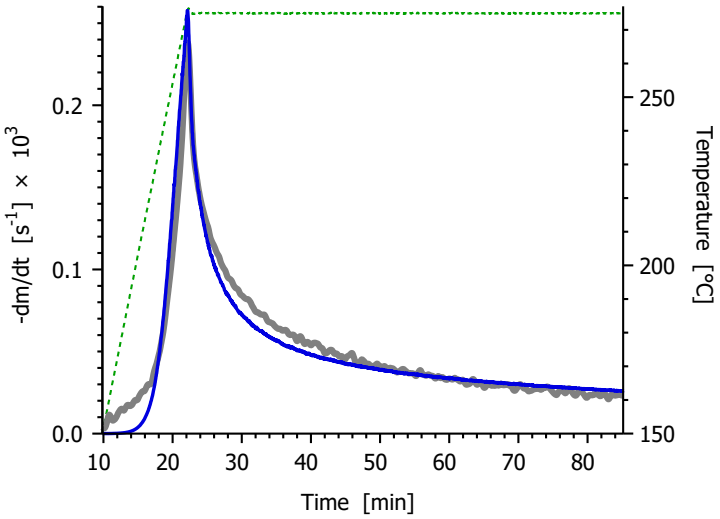
Wood, 10°C/min, 2mg
Relative deviation: 3.33%, Deviation: 0.12 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x)
-.391T_4(x) -.21T_5(x)
c = 0.835



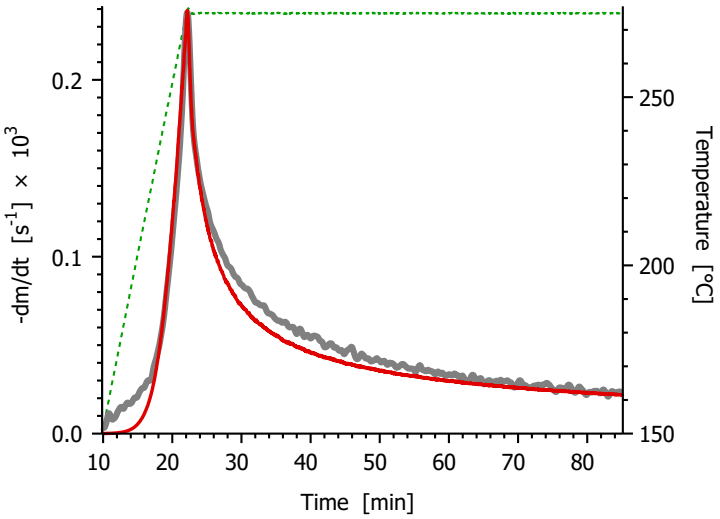
Wood, 65min at 225°C (10°C/min), 4mg
Relative deviation: 9.83%, Deviation: 0.015 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x)
-.809T_4(x) -.415T_5(x)
c = 0.912



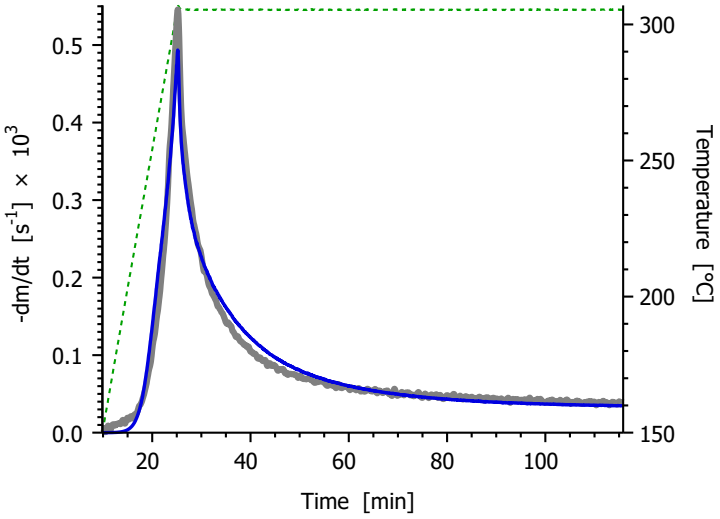
Wood, 65min at 225°C (10°C/min), 4mg
Relative deviation: 9.35%, Deviation: 0.015 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x)
-.391T_4(x) -.21T_5(x)
c = 0.835



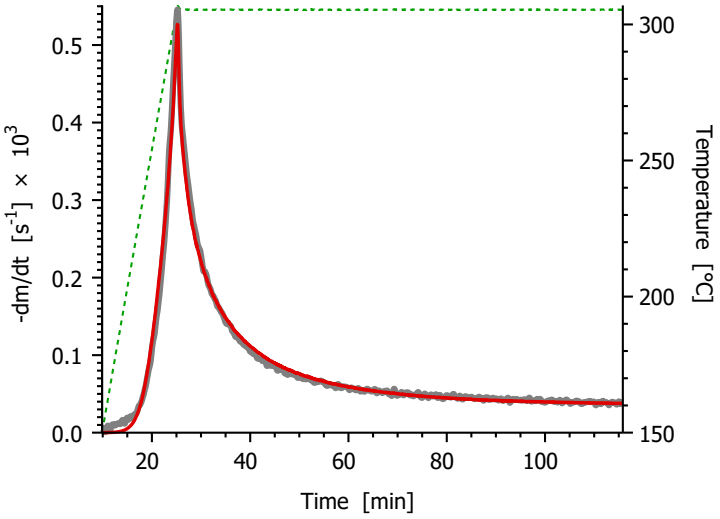
Wood, 65min at 275°C (10°C/min), 4mg
Relative deviation: 3.76%, Deviation: 0.030 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x) -.809T_4(x) -.415T_5(x)
c = 0.912



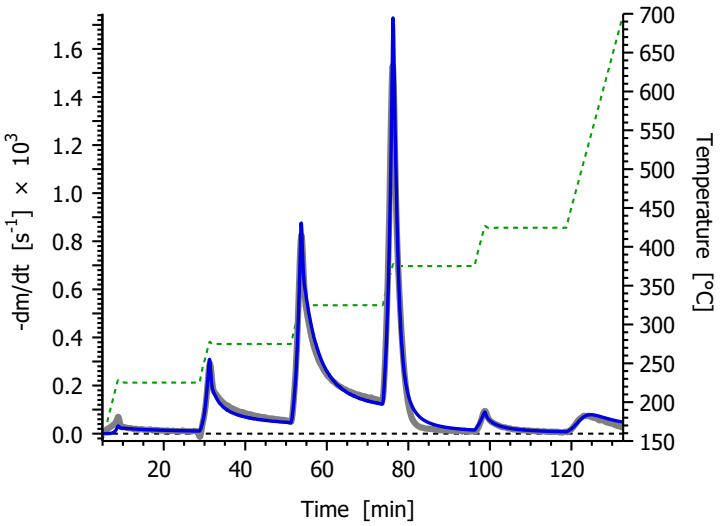
Wood, 65min at 275°C (10°C/min), 4mg
Relative deviation: 3.14%, Deviation: 0.025 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x) -.391T_4(x) -.21T_5(x)
c = 0.835



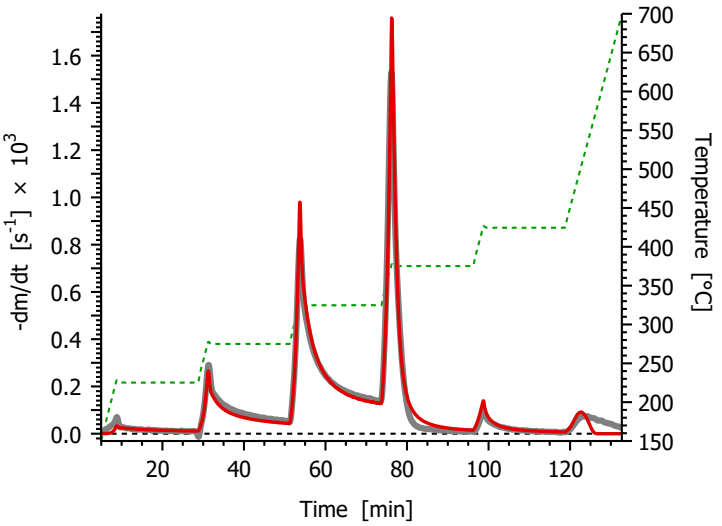
Wood, 90min at 305°C (10°C/min), 4mg
Relative deviation: 2.42%, Deviation: 0.052 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x) -.809T_4(x) -.415T_5(x)
c = 0.912



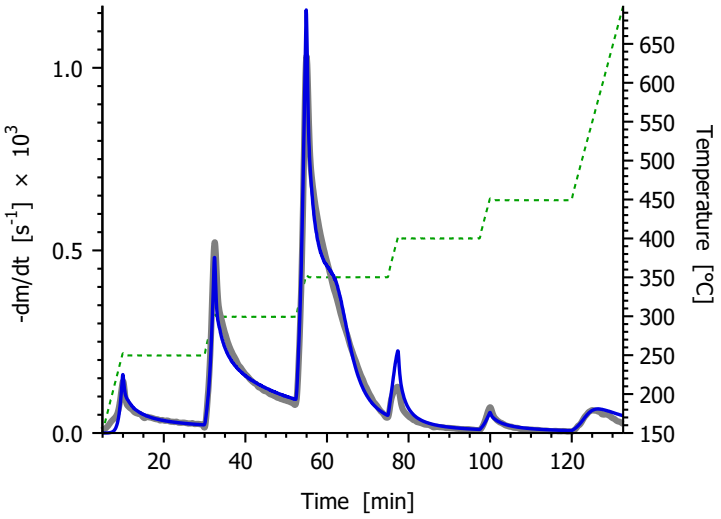
Wood, 90min at 305°C (10°C/min), 4mg
Relative deviation: 1.29%, Deviation: 0.028 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x) -.391T_4(x) -.21T_5(x)
c = 0.835



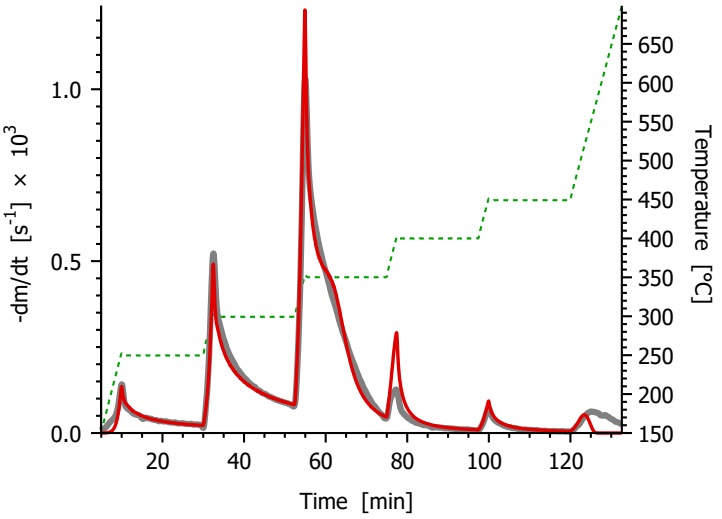
Wood, stepwise T(t) "A" (20°C/min), 4mg
Relative deviation: 1.65%, Deviation: 0.097 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x)
-.809T_4(x) -.415T_5(x)
c = 0.912



Wood, stepwise T(t) "A" (20°C/min), 4mg
Relative deviation: 1.86%, Deviation: 0.11 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x)
-.391T_4(x) -.21T_5(x)
c = 0.835



Wood, stepwise T(t) "B" (20°C/min), 4mg
Relative deviation: 2.14%, Deviation: 0.096 µg/s
rms rel. dev. of 8 experiments: 4.43%
Model: x=2α-1
E(x) = 173.51
$\log_{10}$ Ã(x) = 10.302T_0(x) -4.001T_1(x) -2.145T_2(x) -1.89T_3(x)
-.809T_4(x) -.415T_5(x)
c = 0.912



Wood, stepwise T(t) "B" (20°C/min), 4mg
Relative deviation: 2.85%, Deviation: 0.13 µg/s
rms rel. dev. of 8 experiments: 4.26%
Model: x=2α-1
E(x) = 190.71T_0(x) +32.07T_1(x) +13.44T_2(x) +23.29T_3(x)
$\log_{10}$ Ã(x) = 12.96T_0(x) +.928T_1(x) +.494T_2(x) +1.212T_3(x)
-.391T_4(x) -.21T_5(x)
c = 0.835