

Supplementary Content for Article

Várhegyi, G.; Czégény, Zs.; Jakab, E.; McAdam, K.; Liu, C.: Tobacco pyrolysis. Kinetic evaluation of thermogravimetric – mass spectrometric experiments.

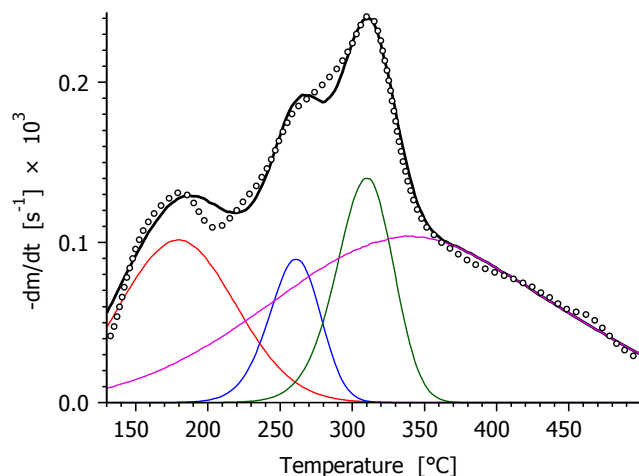
J. Anal. Appl. Pyrolysis **2009**, 86, 310-322. doi: [10.1016/j.jaap.2009.08.008](https://doi.org/10.1016/j.jaap.2009.08.008)

Scope of this document: This work was based on the reaction kinetic evaluation of 10 TG-MS experiments measured at different temperature programs. Altogether 10 DTG curves and 110 MS intensity curves were evaluated. Due to space limitations, only the 10°C/min experiments were shown in the figures of the article.

This Supplementary Content shows the full versions of Figures 2 – 5 displaying 120 plots in total. The plots were generated by the kinetic evaluation software and were upgraded by automated software tools for the requirements of the present document.

The graphics include textual information that was also computer-generated. The first line beneath each plot describes the given experiment. Here G_0 stands for the initial sample mass. Another line displays the quality of the fit calculated for the given plot (fit_1) and for the series of experiments evaluated together (fit_{10} , fit_{20} , or fit_{50}), as described in the article. The rest of the lines below each panel list the model parameters. Note that the parameter values have the same color as the corresponding partial curve (calculated peak) in the plot.

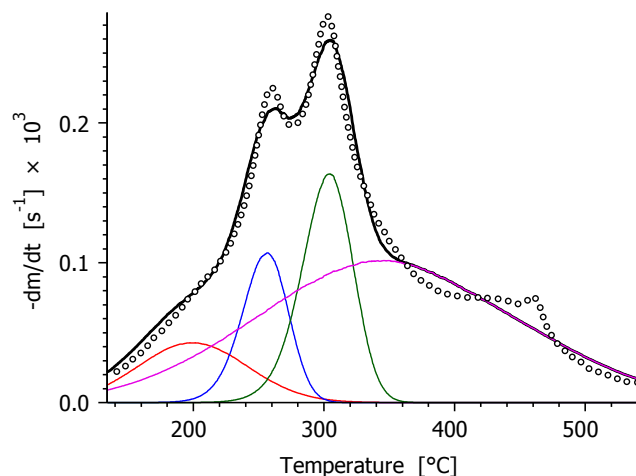
Further information. Please address any question with this document to the corresponding author. Email: varhegyi.gabor@t-online.hu or gvarhegyi@gmail.com



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

$\text{fit}_1 = 2.48\%$; $\text{fit}_{10} = 2.45\%$

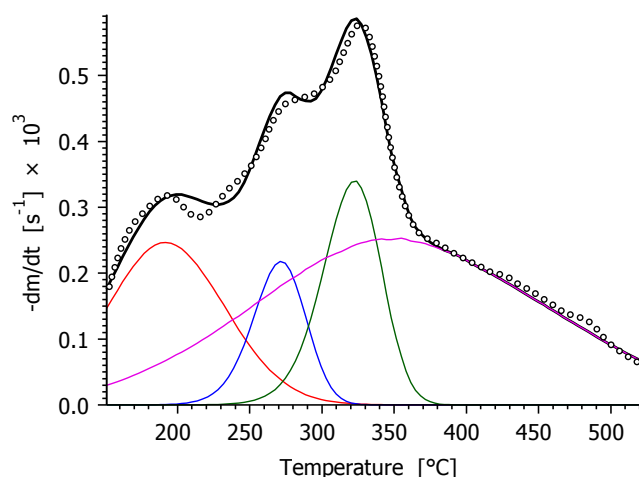
1: $E_0=117.9$ $\log_{10} A=11.11$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.40$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=15.93$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.77$ $\sigma(E)=40.2$
 σ_j : 14.5 5.9 10.4 38.0



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

$\text{fit}_1 = 3.14\%$; $\text{fit}_{10} = 2.45\%$

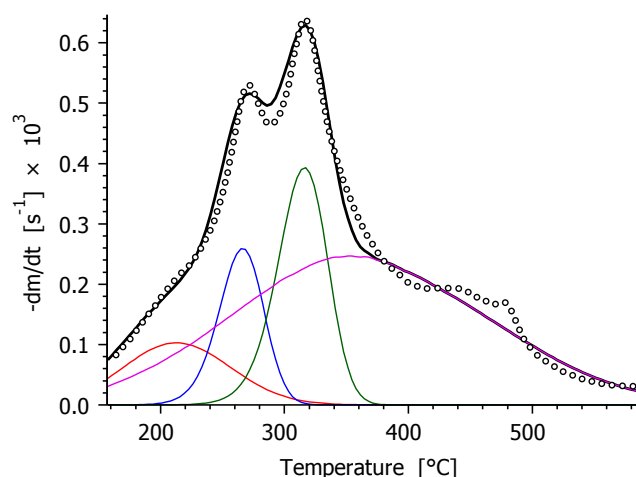
1: $E_0=117.9$ $\log_{10} A=10.47$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.60$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=16.13$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.59$ $\sigma(E)=40.2$
 σ_j : 6.4 6.9 11.8 37.6



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

$\text{fit}_1 = 2.08\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=11.11$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.40$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=15.93$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.77$ $\sigma(E)=40.2$
 σ_j : 14.5 5.9 10.4 38.0

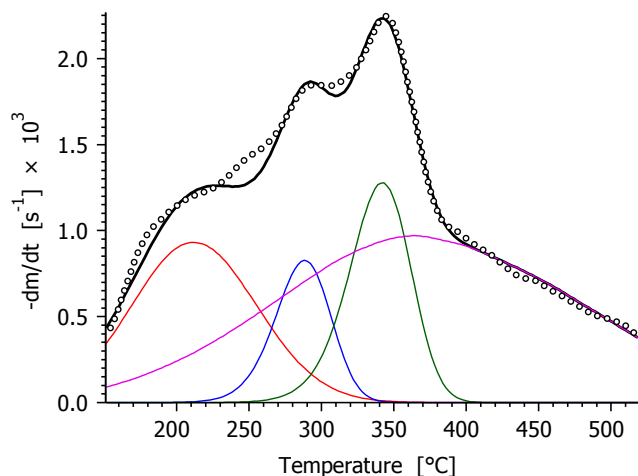


Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

$\text{fit}_1 = 3.25\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=10.47$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.60$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=16.13$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.59$ $\sigma(E)=40.2$
 σ_j : 6.4 6.9 11.8 37.6

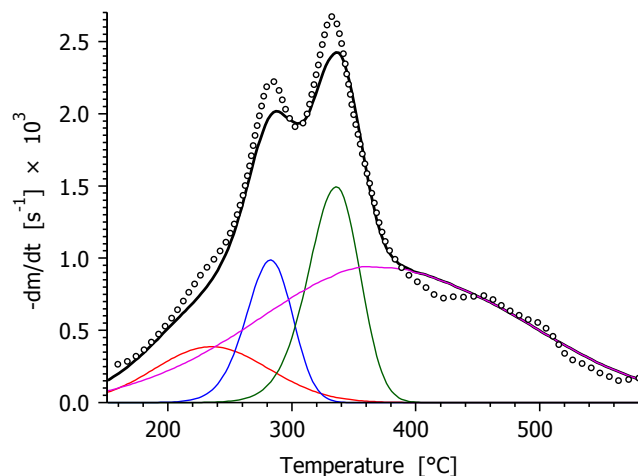
Fig. 2. Evaluation of ten DTG curves assuming identical $E_{0,j}$ and σ_j parameters for both samples. The experimental data ($\circ \circ \circ$), their simulated counterparts (—) and the calculated partial curves (—) are shown. The stepwise temperature programs ($- - -$) are also displayed when appropriate.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

$\text{fit}_1 = 2.14\%$; $\text{fit}_{10} = 2.45\%$

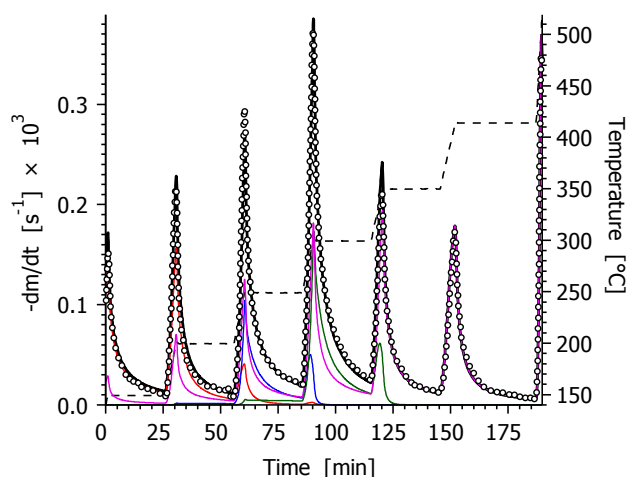
1: $E_0=117.9$ $\log_{10} A=11.11$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.40$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=15.93$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.77$ $\sigma(E)=40.2$
 ζ : 14.5 5.9 10.4 38.0



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

$\text{fit}_1 = 3.28\%$; $\text{fit}_{10} = 2.45\%$

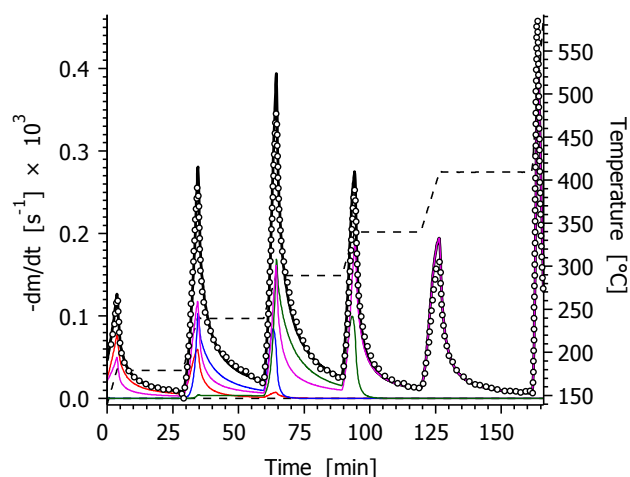
1: $E_0=117.9$ $\log_{10} A=10.47$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.60$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=16.13$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.59$ $\sigma(E)=40.2$
 ζ : 6.4 6.9 11.8 37.6



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

$\text{fit}_1 = 1.92\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=11.11$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.40$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=15.93$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.77$ $\sigma(E)=40.2$
 ζ : 14.5 5.9 10.4 38.0

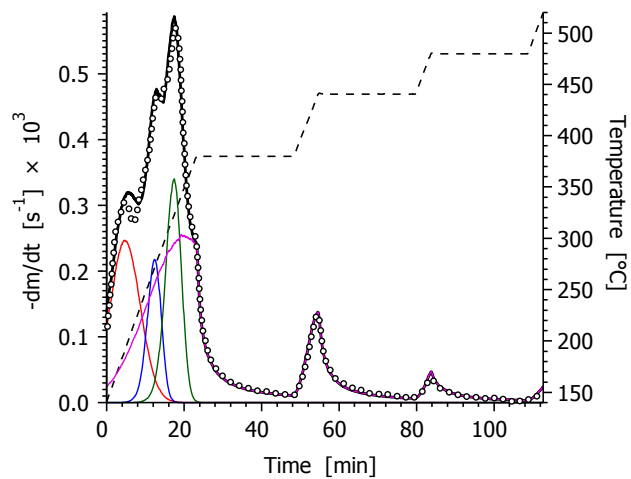


Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

$\text{fit}_1 = 2.41\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=10.47$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.60$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=16.13$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.59$ $\sigma(E)=40.2$
 ζ : 6.4 6.9 11.8 37.6

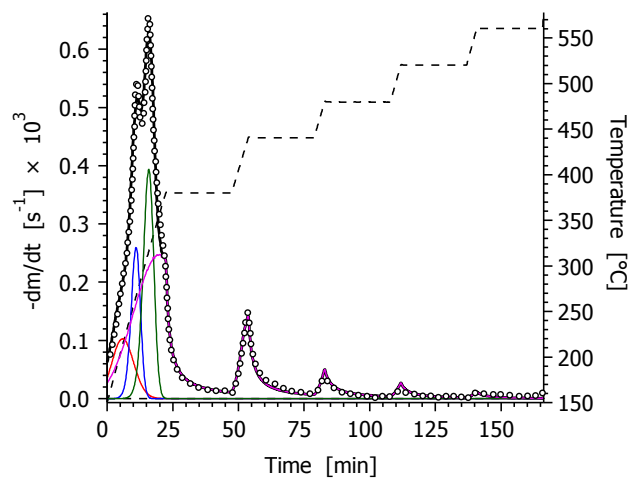
Fig. 2. (Continued.)



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

$\text{fit}_1 = 1.61\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=11.11$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.40$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=15.93$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.77$ $\sigma(E)=40.2$
 ζ : 14.5 5.9 10.4 38.0

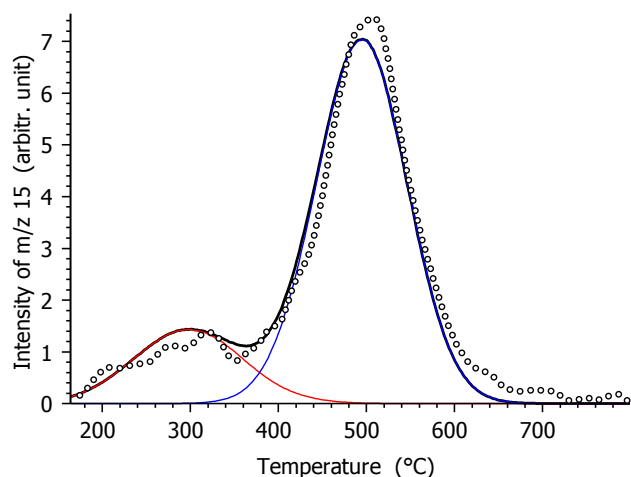


Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

$\text{fit}_1 = 1.33\%$; $\text{fit}_{10} = 2.45\%$

1: $E_0=117.9$ $\log_{10} A=10.47$ $\sigma(E)=9.9$
 2: $E_0=202.1$ $\log_{10} A=17.60$ $\sigma(E)=4.8$
 3: $E_0=204.8$ $\log_{10} A=16.13$ $\sigma(E)=4.7$
 4: $E_0=252.3$ $\log_{10} A=18.59$ $\sigma(E)=40.2$
 ζ : 6.4 6.9 11.8 37.6

Fig. 2. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

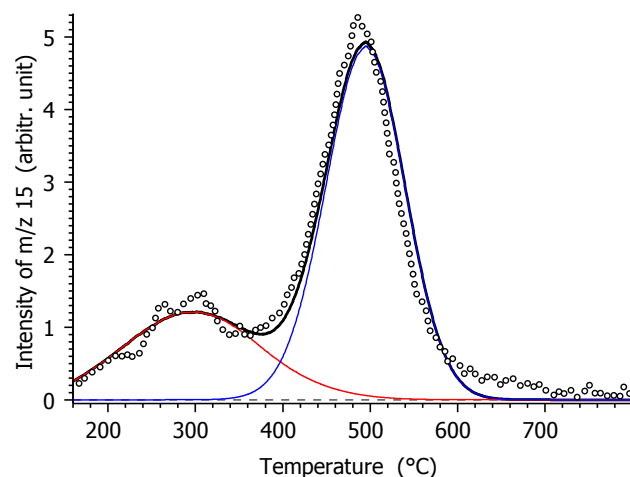
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 4.58\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=22.8$ scalefactor=1.34

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=16.5$

scalefactor* c_j : 3283. 13666.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

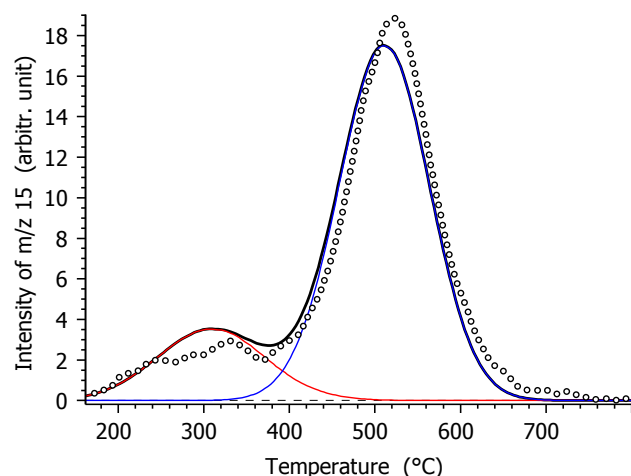
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 4.47\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=29.4$ scalefactor=1.18

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=14.1$

scalefactor* c_j : 3536. 8285.



Virginia blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

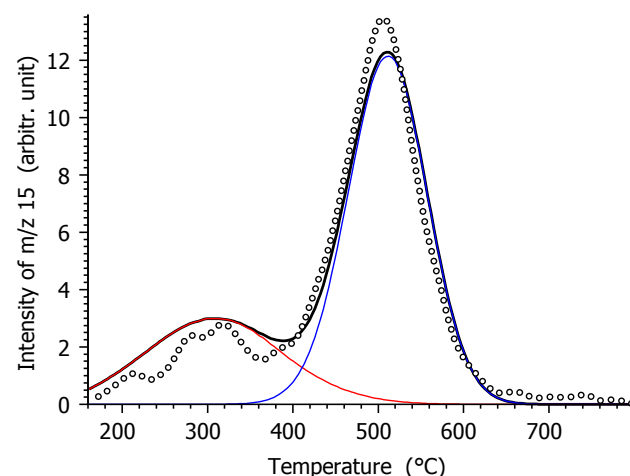
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 5.40\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=22.8$ scalefactor=1.35

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=16.5$

scalefactor* c_j : 3314. 13793.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

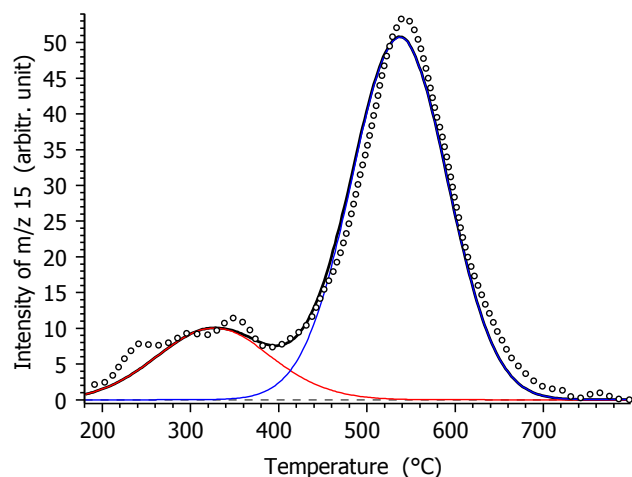
$\text{fit}_1 = 4.67\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=29.4$ scalefactor=1.19

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=14.1$

scalefactor* c_j : 3589. 8410.

Fig. 3. Simultaneous evaluation of fifty MS intensity curves as described in Section 4.2. The experimental data ($\circ\circ\circ$), their simulated counterparts (—) and the calculated partial curves (—) are shown. The stepwise temperature programs (-- --) are also displayed when appropriate.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

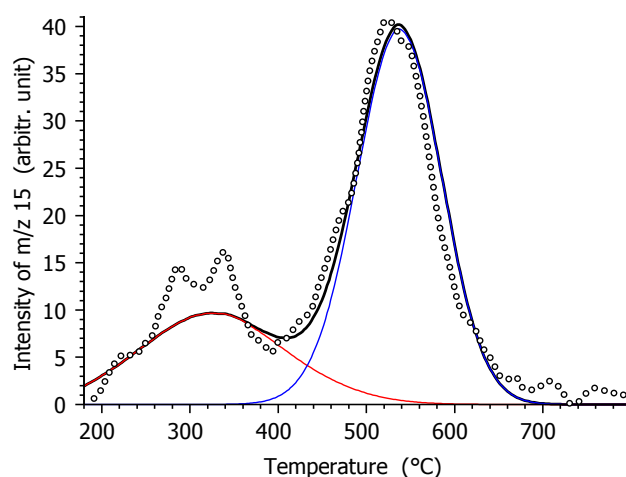
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 4.10\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=22.8$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=16.5$

$\text{scalefactor} \cdot c_j$: 2455. 10219.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

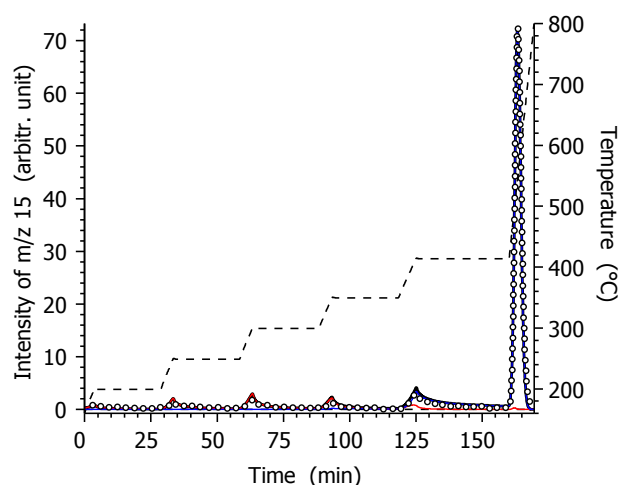
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 6.34\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=29.4$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=14.1$

$\text{scalefactor} \cdot c_j$: 3007. 7045.



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

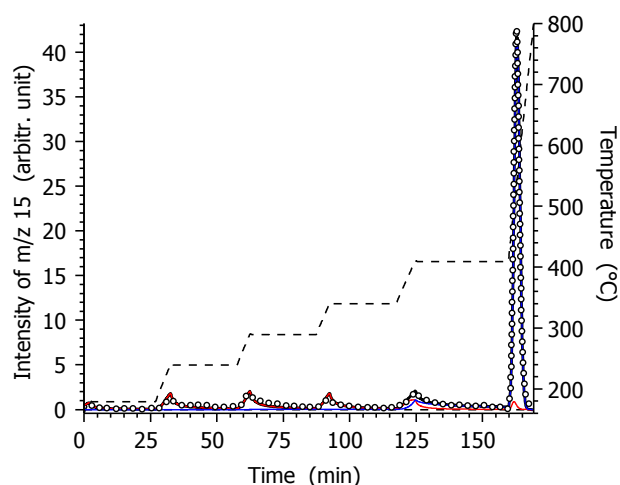
DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

$\text{fit}_1 = 1.36\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=22.8$ $\text{scalefactor}=1.51$

2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=16.5$

$\text{scalefactor} \cdot c_j$: 3700. 15403.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]

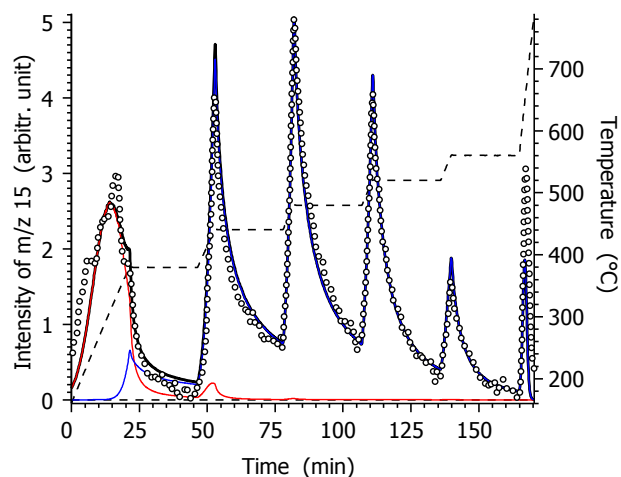
$\text{fit}_1 = 0.83\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=29.4$ $\text{scalefactor}=1.09$

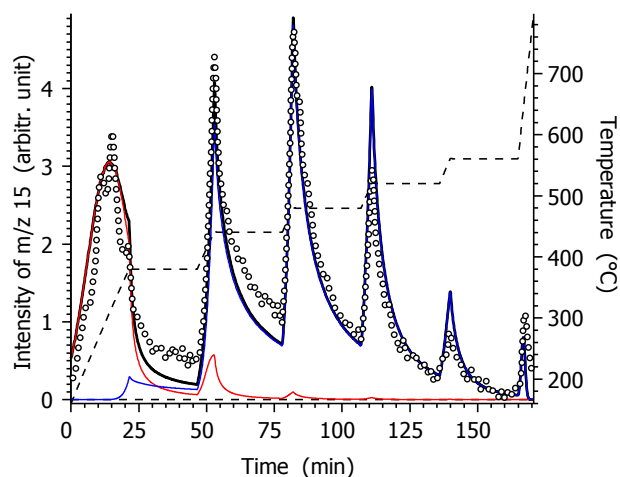
2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=14.1$

$\text{scalefactor} \cdot c_j$: 3283. 7692.

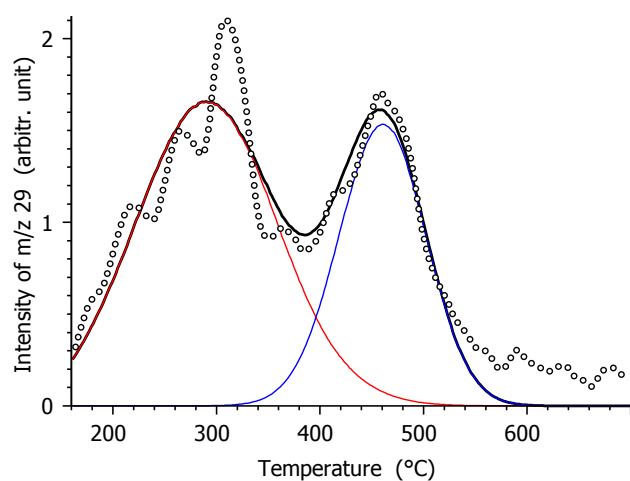
Fig. 3. (Continued.)



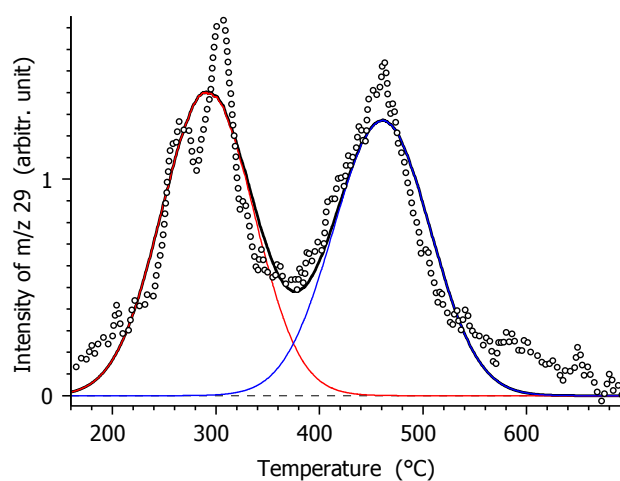
Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T
 DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]
 $\text{fit}_1 = 5.82\%$; $\text{fit}_{50} = 6.18\%$
 1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=22.8$ $\text{scalefactor}=0.993$
 2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=16.5$
 $\text{scalefactor} \cdot c_j$: 2438. 10150.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T
 DAEM kinetics of intensity $m/z\ 15$ [CH_3^+ (mainly from CH_4)]
 $\text{fit}_1 = 6.86\%$; $\text{fit}_{50} = 6.18\%$
 1: $E_0=211.5$ $\log_{10} A=16.78$ $\sigma(E)=29.4$ $\text{scalefactor}=1.22$
 2: $E_0=265.7$ $\log_{10} A=15.47$ $\sigma(E)=14.1$
 $\text{scalefactor} \cdot c_j$: 3655. 8564.

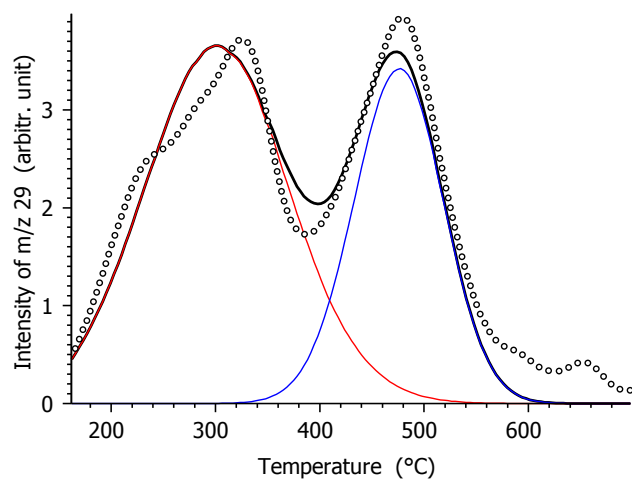


Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$
 DAEM kinetics of intensity $m/z\ 29$ (CHO^+ , C_2H_5^+)
 $\text{fit}_1 = 8.51\%$; $\text{fit}_{50} = 6.18\%$
 1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=25.5$ $\text{scalefactor}=1.47$
 2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=13.5$
 $\text{scalefactor} \cdot c_j$: 4157. 2466.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$
 DAEM kinetics of intensity $m/z\ 29$ (CHO^+ , C_2H_5^+)
 $\text{fit}_1 = 8.42\%$; $\text{fit}_{50} = 6.18\%$
 1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=16.1$ $\text{scalefactor}=1.20$
 2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=15.3$
 $\text{scalefactor} \cdot c_j$: 2299. 2267.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

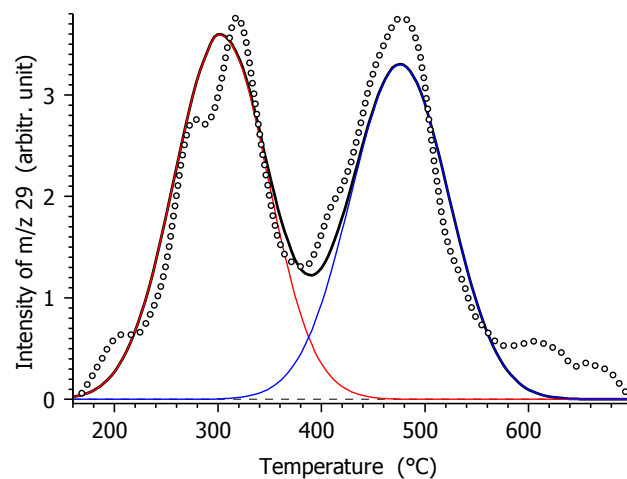
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 7.69\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=25.5$ $\text{scalefactor}=1.32$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 3750. 2224.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

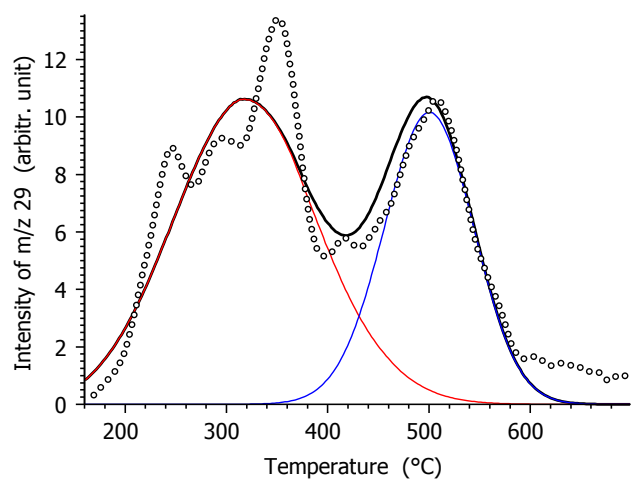
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 8.79\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=16.1$ $\text{scalefactor}=1.26$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=15.3$

$\text{scalefactor} \cdot c_j$: 2415. 2381.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

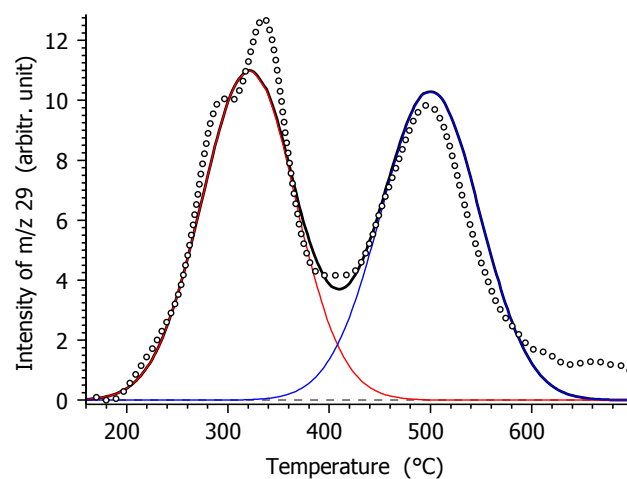
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 9.44\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=25.5$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 2835. 1682.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

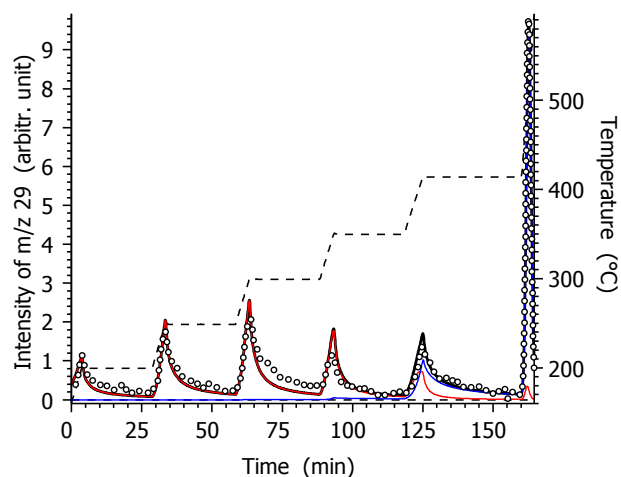
$\text{fit}_1 = 6.65\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=16.1$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=15.3$

$\text{scalefactor} \cdot c_j$: 1918. 1891.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

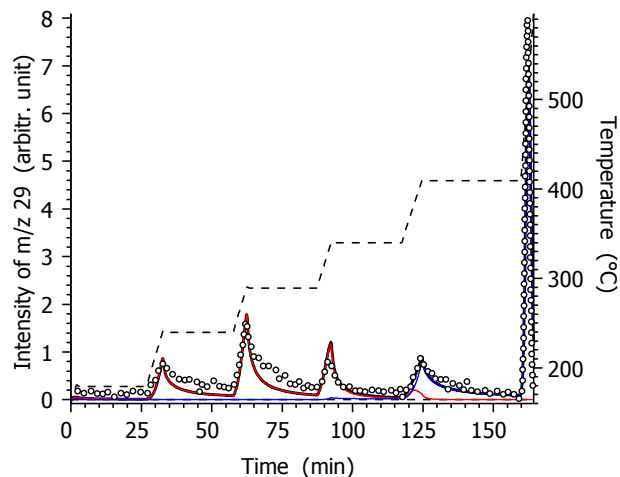
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 1.91\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=25.5$ $\text{scalefactor}=1.20$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 3402. 2018.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

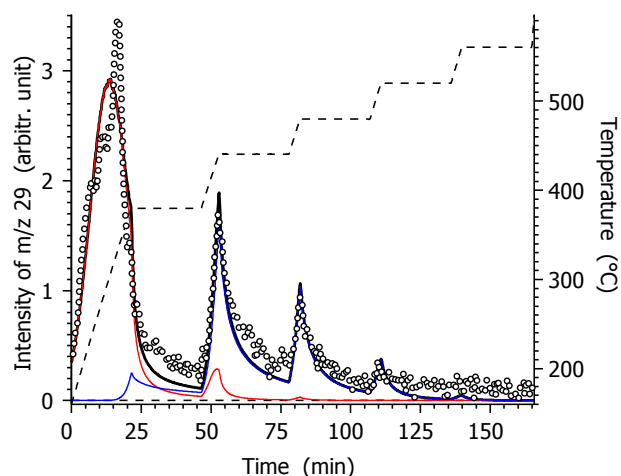
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 3.02\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=16.1$ $\text{scalefactor}=0.833$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=15.3$

$\text{scalefactor} \cdot c_j$: 1597. 1575.



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

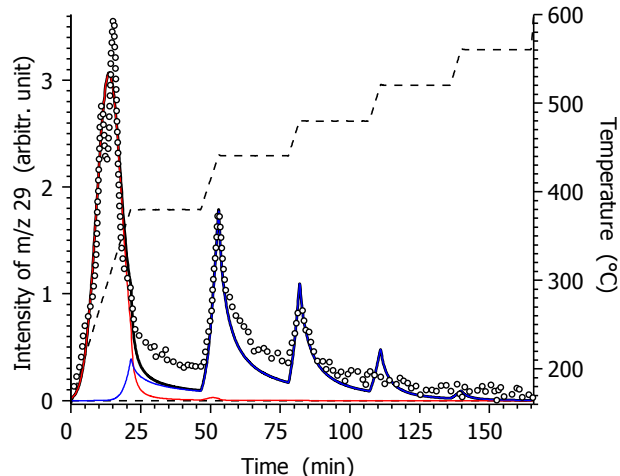
DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

$\text{fit}_1 = 5.44\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=25.5$ $\text{scalefactor}=1.05$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 2983. 1769.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 29 (CHO^+ , C_2H_5^+)

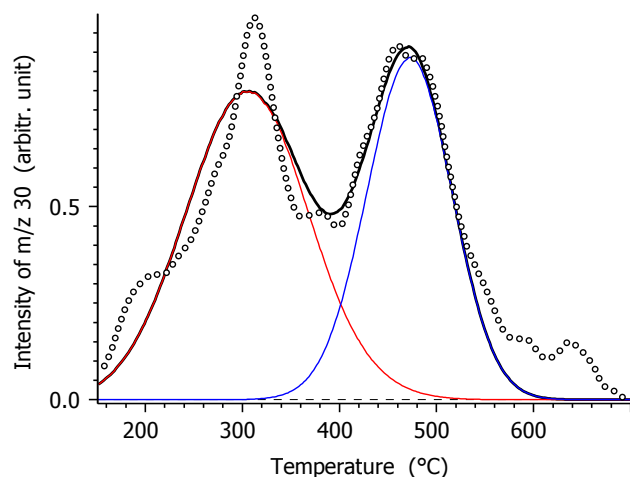
$\text{fit}_1 = 5.31\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.03$ $\sigma(E)=16.1$ $\text{scalefactor}=1.07$

2: $E_0=265.7$ $\log_{10} A=16.33$ $\sigma(E)=15.3$

$\text{scalefactor} \cdot c_j$: 2060. 2031.

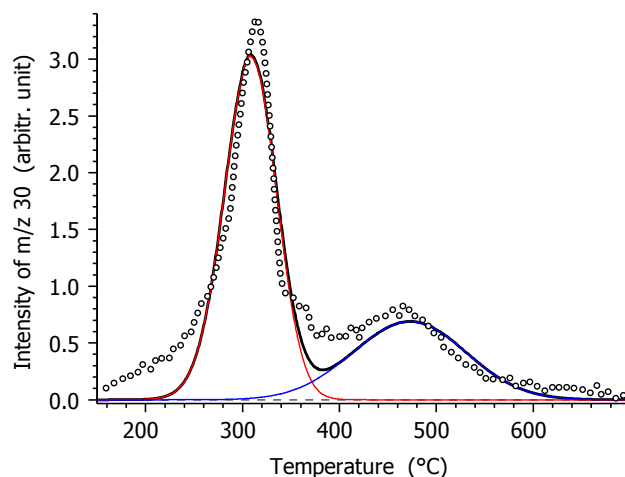
Fig. 3. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 8.80\%$; $\text{fit}_{50} = 6.18\%$

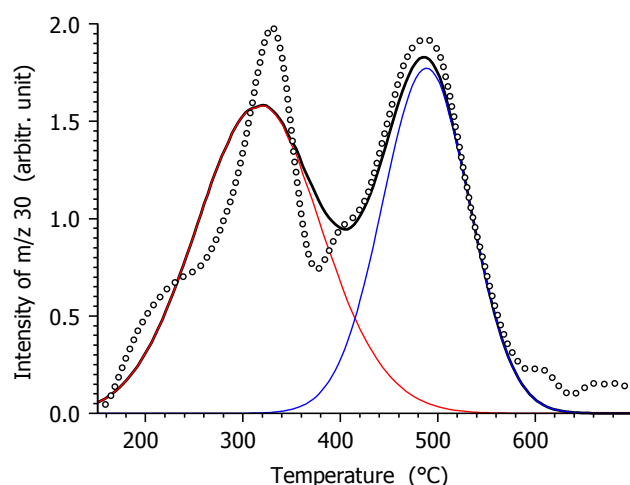
1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=23.1$ scalefactor=1.59
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=14.0$
 scalefactor* c_j : 1883. 1482.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 6.15\%$; $\text{fit}_{50} = 6.18\%$

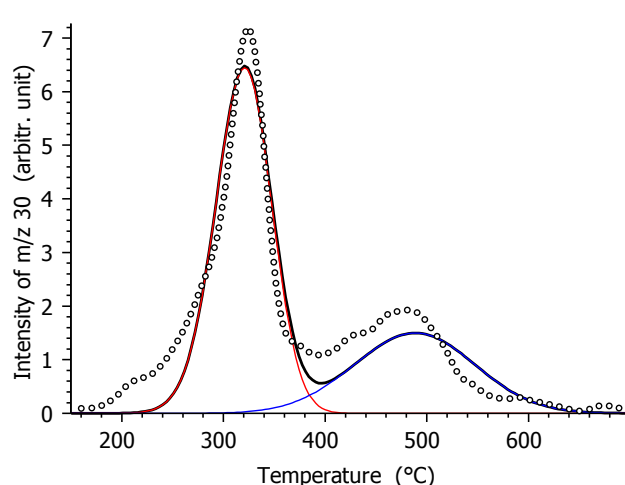
1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=8.3$ scalefactor=1.36
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=19.6$
 scalefactor* c_j : 3020. 1526.



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 8.85\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=23.1$ scalefactor=1.29
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=14.0$
 scalefactor* c_j : 1527. 1201.

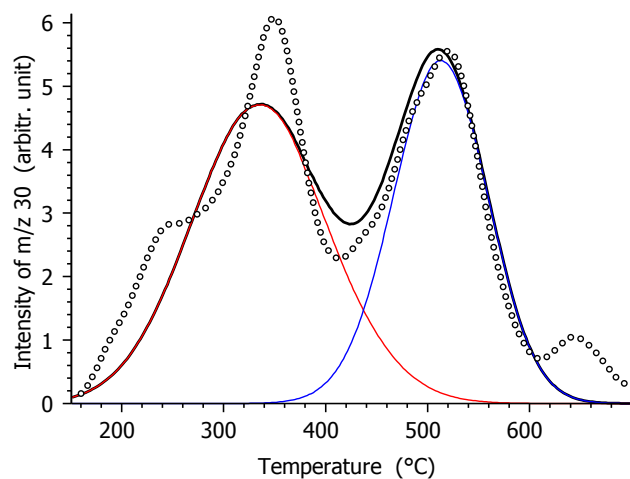


Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 6.22\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=8.3$ scalefactor=1.19
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=19.6$
 scalefactor* c_j : 2654. 1341.

Fig. 3. (Continued.)



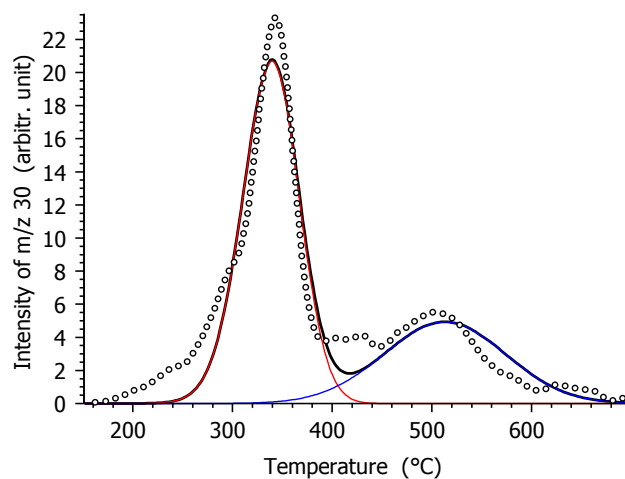
Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 9.88\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=23.1$ scalefactor=1

2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=14.0$

scalefactor* c_j : 1188. 934.



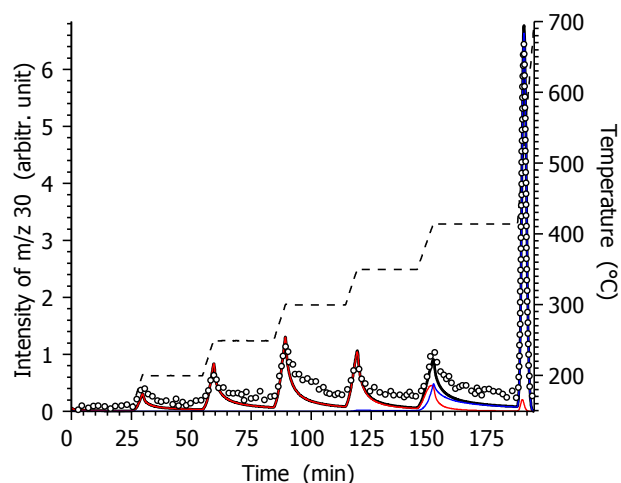
Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 5.85\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=8.3$ scalefactor=1

2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=19.6$

scalefactor* c_j : 2223. 1123.



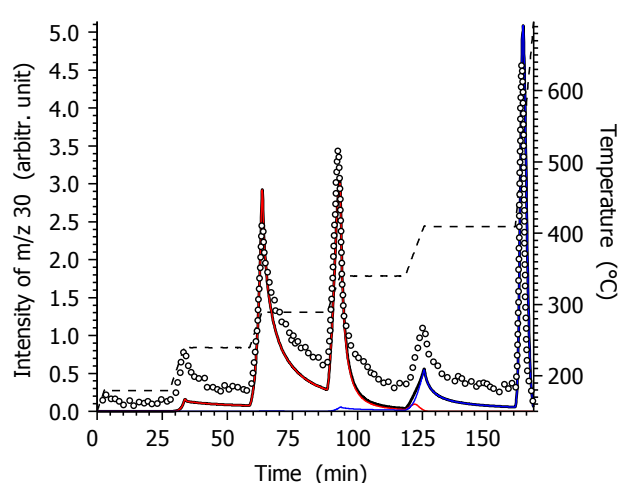
Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 2.98\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=23.1$ scalefactor=1.43

2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=14.0$

scalefactor* c_j : 1701. 1338.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

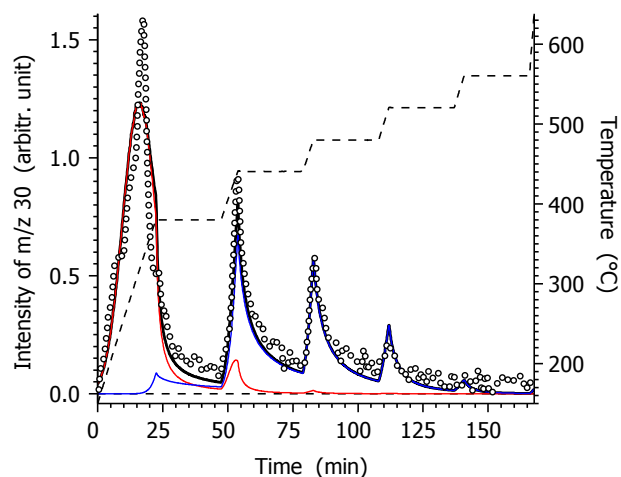
DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 7.97\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=8.3$ scalefactor=1.14

2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=19.6$

scalefactor* c_j : 2527. 1277.

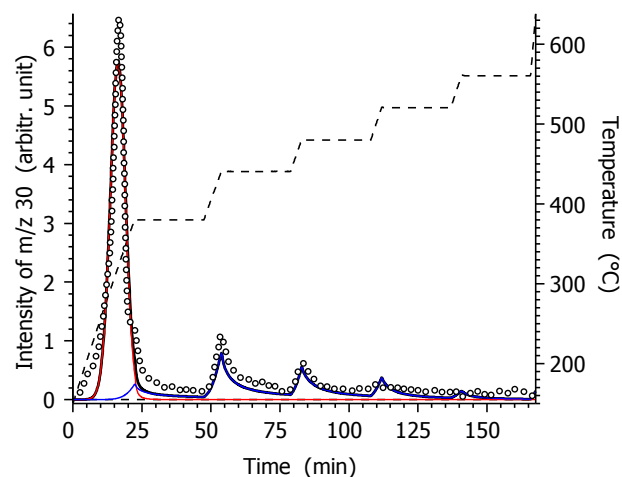
Fig. 3. (Continued.)



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 5.55\%$; $\text{fit}_{50} = 6.18\%$

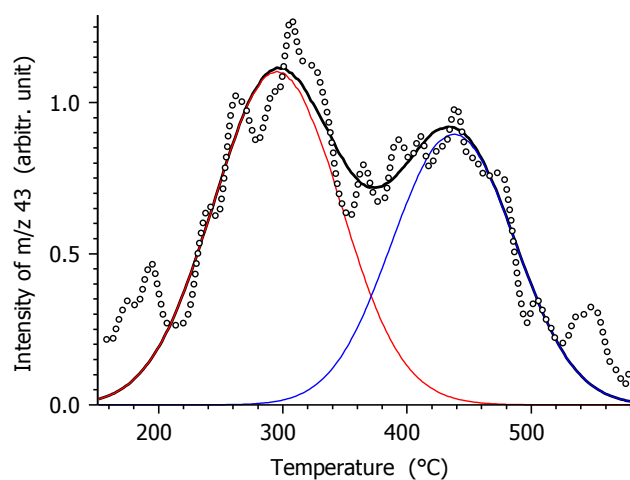
1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=23.1$ scalefactor=1.00
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=14.0$
 scalefactor* c_j : 1188. 935.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity $m/z\ 30\ [\text{CH}_2\text{O}^+]$ (with lower amounts of NO^+)
 $\text{fit}_1 = 3.57\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.52$ $\sigma(E)=8.3$ scalefactor=1.06
 2: $E_0=265.7$ $\log_{10} A=16.03$ $\sigma(E)=19.6$
 scalefactor* c_j : 2366. 1196.

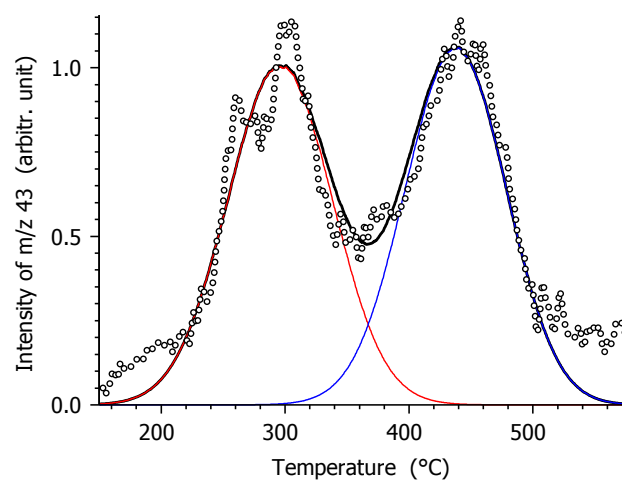


Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

$\text{fit}_1 = 9.78\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=18.6$ scalefactor=1.30
 2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=16.8$
 scalefactor* c_j : 2075. 1696.



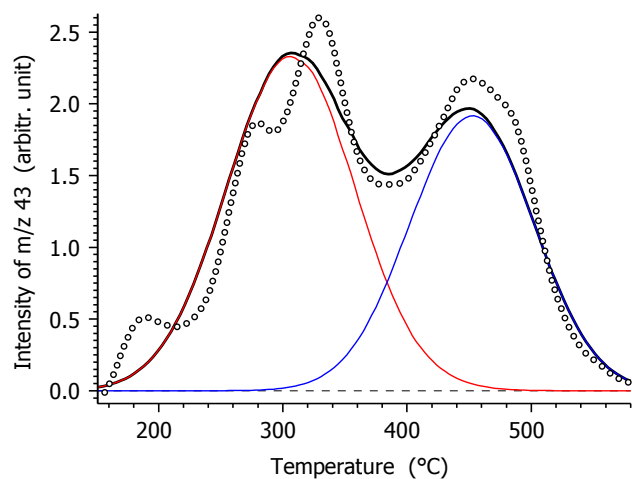
Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

$\text{fit}_1 = 9.11\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=15.0$ scalefactor=1.13
 2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=13.5$
 scalefactor* c_j : 1566. 1672.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

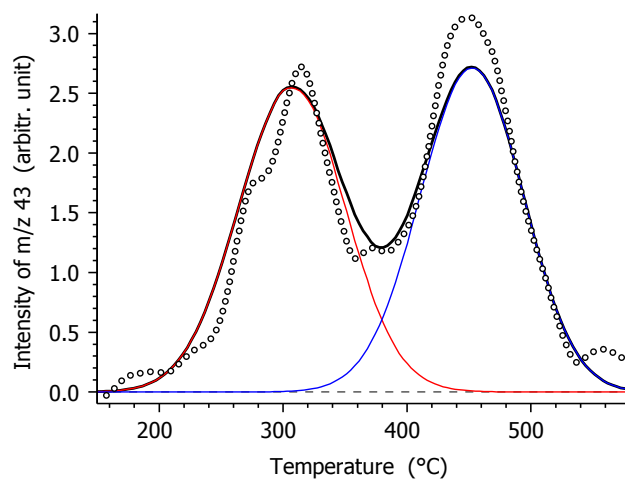
DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

$\text{fit}_1 = 8.17\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=18.6$ $\text{scalefactor}=1.12$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=16.8$

$\text{scalefactor} \cdot c_j$: 1798. 1470.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

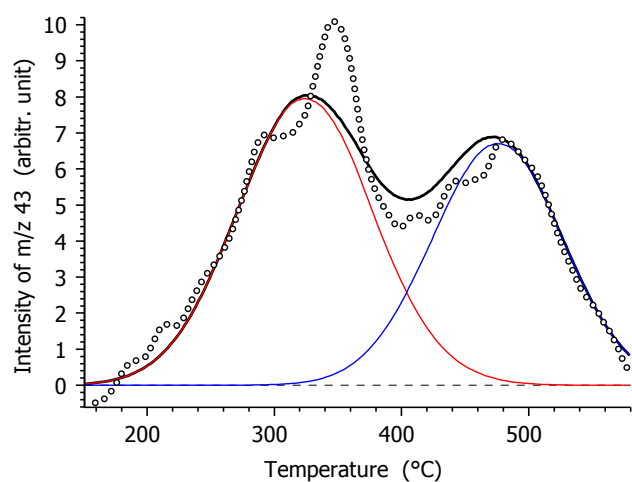
DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

$\text{fit}_1 = 7.45\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=15.0$ $\text{scalefactor}=1.17$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 1631. 1741.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

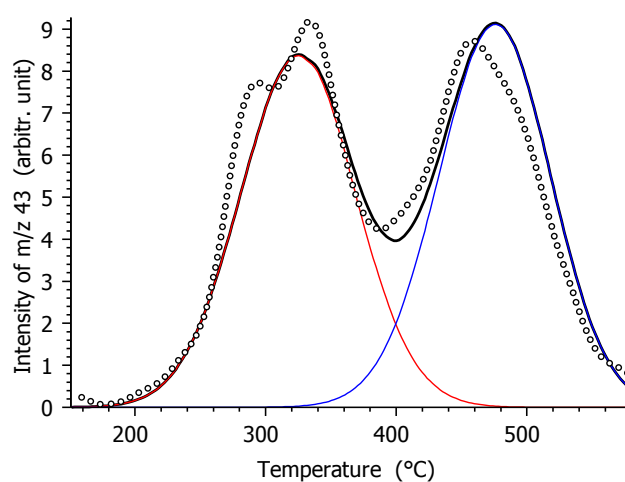
DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

$\text{fit}_1 = 7.31\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=18.6$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=16.8$

$\text{scalefactor} \cdot c_j$: 1598. 1306.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 43\ (\text{C}_2\text{H}_3\text{O}^+)$

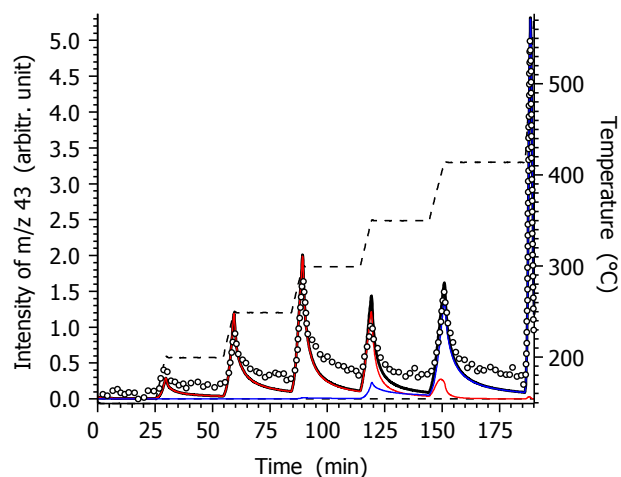
$\text{fit}_1 = 7.62\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=15.0$ $\text{scalefactor}=1$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=13.5$

$\text{scalefactor} \cdot c_j$: 1391. 1485.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

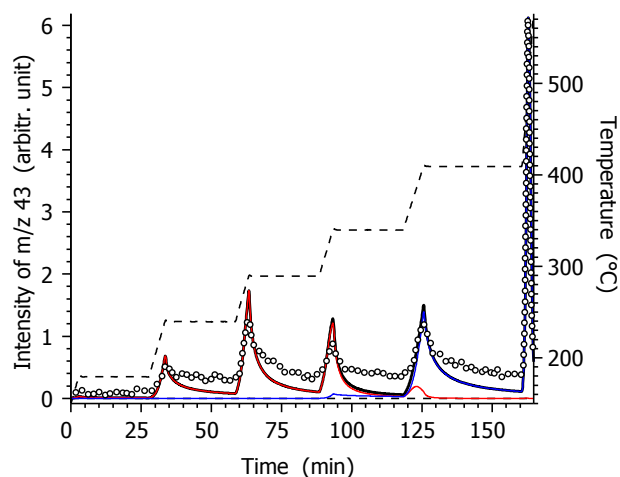
DAEM kinetics of intensity $m/z\ 43$ ($C_2H_3O^+$)

$fit_1 = 3.82\%$; $fit_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=18.6$ $scalefactor=1.25$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=16.8$

$scalefactor \cdot c_j$: 2003. 1637.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

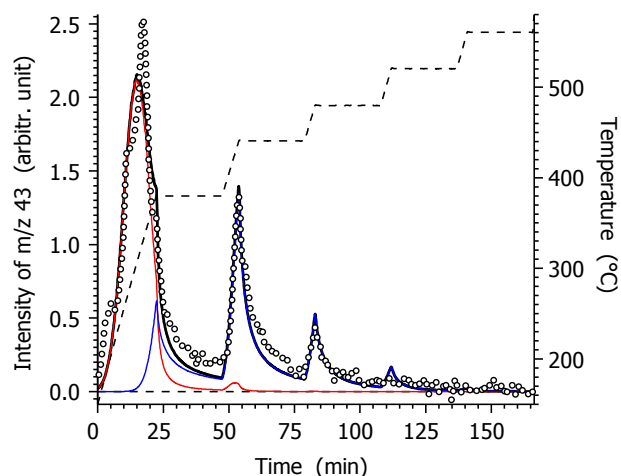
DAEM kinetics of intensity $m/z\ 43$ ($C_2H_3O^+$)

$fit_1 = 3.68\%$; $fit_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=15.0$ $scalefactor=1.10$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=13.5$

$scalefactor \cdot c_j$: 1526. 1629.



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

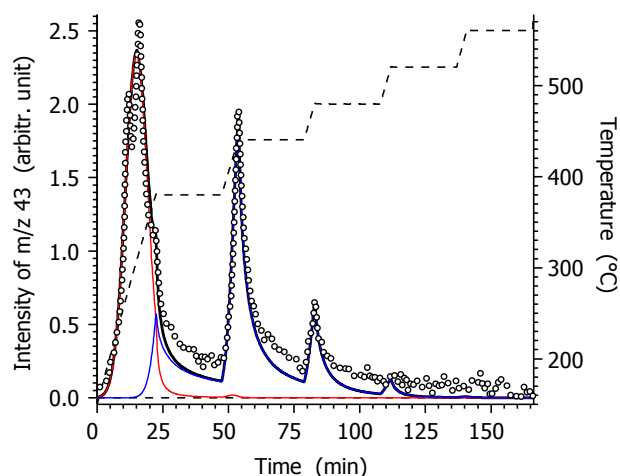
DAEM kinetics of intensity $m/z\ 43$ ($C_2H_3O^+$)

$fit_1 = 4.53\%$; $fit_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=18.6$ $scalefactor=1.02$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=16.8$

$scalefactor \cdot c_j$: 1630. 1332.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity $m/z\ 43$ ($C_2H_3O^+$)

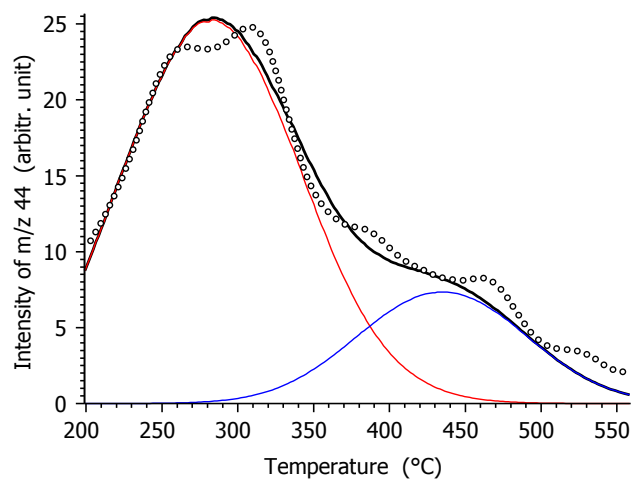
$fit_1 = 4.83\%$; $fit_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=16.89$ $\sigma(E)=15.0$ $scalefactor=1.08$

2: $E_0=265.7$ $\log_{10} A=16.95$ $\sigma(E)=13.5$

$scalefactor \cdot c_j$: 1500. 1601.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

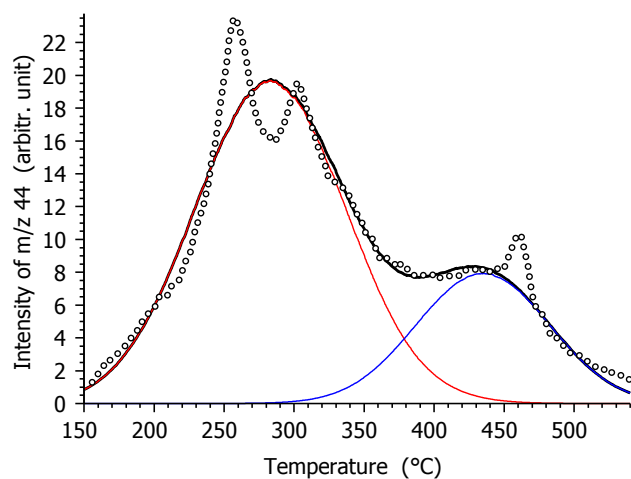
DAEM kinetics of intensity **m/z 44 (CO_2)**

fit₁ = 4.18%; fit₅₀ = 6.18%

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=22.2$ scalefactor=1.35

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=19.3$

scalefactor* c_j : 54509. 15662.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

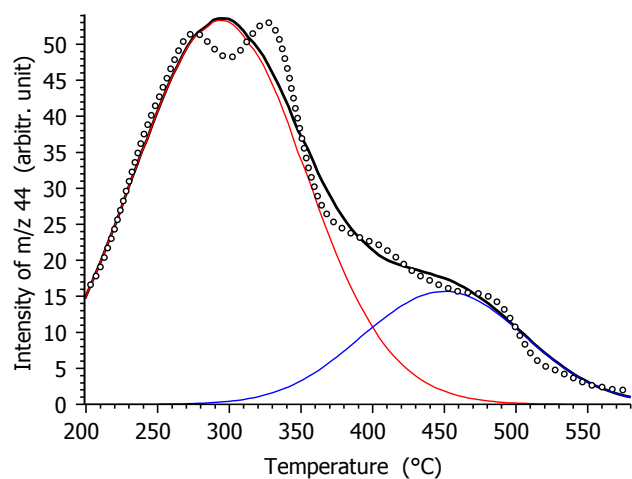
DAEM kinetics of intensity **m/z 44 (CO_2)**

fit₁ = 6.22%; fit₅₀ = 6.18%

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=20.1$ scalefactor=1.04

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=16.3$

scalefactor* c_j : 38687. 14547.



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

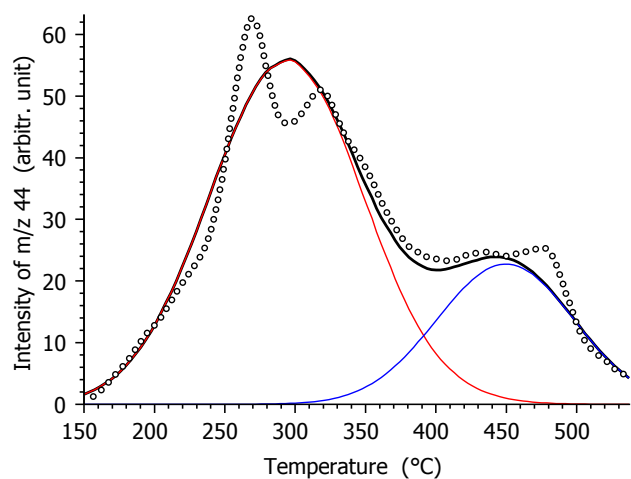
DAEM kinetics of intensity **m/z 44 (CO_2)**

fit₁ = 4.09%; fit₅₀ = 6.18%

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=22.2$ scalefactor=1.17

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=19.3$

scalefactor* c_j : 47094. 13531.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity **m/z 44 (CO_2)**

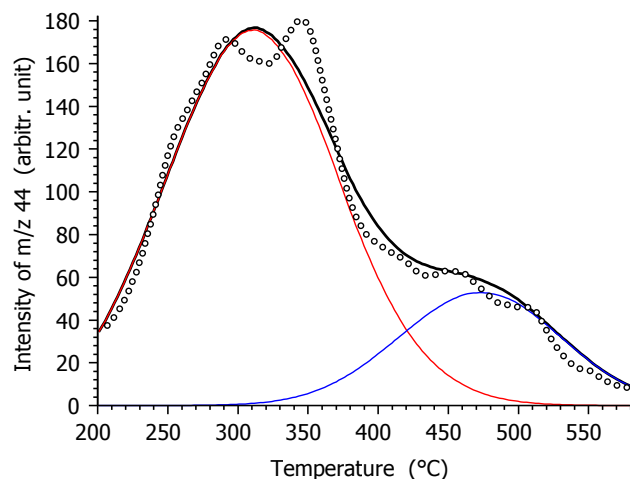
fit₁ = 6.25%; fit₅₀ = 6.18%

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=20.1$ scalefactor=1.21

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=16.3$

scalefactor* c_j : 45090. 16954.

Fig. 3. (Continued.)



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

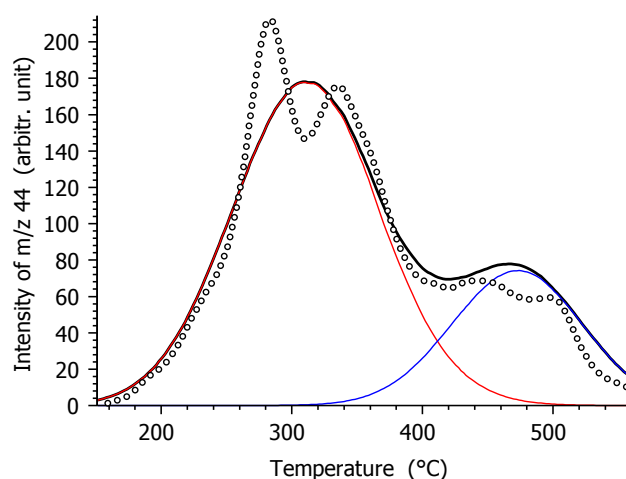
DAEM kinetics of intensity **m/z 44 (CO_2)**

$\text{fit}_1 = 4.95\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=22.2$ scalefactor=1

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=19.3$

scalefactor* c_j : 40301. 11580.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

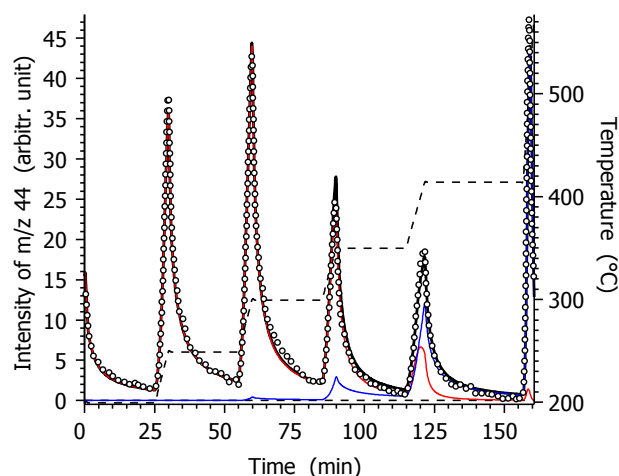
DAEM kinetics of intensity **m/z 44 (CO_2)**

$\text{fit}_1 = 7.28\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=20.1$ scalefactor=1

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=16.3$

scalefactor* c_j : 37340. 14040.



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

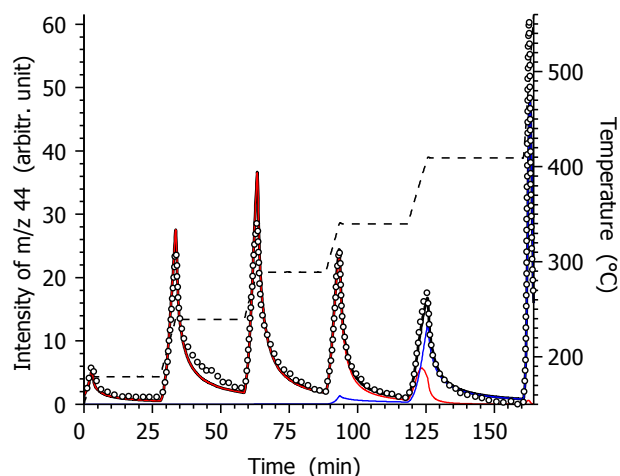
DAEM kinetics of intensity **m/z 44 (CO_2)**

$\text{fit}_1 = 2.42\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=22.2$ scalefactor=1.25

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=19.3$

scalefactor* c_j : 50407. 14483.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity **m/z 44 (CO_2)**

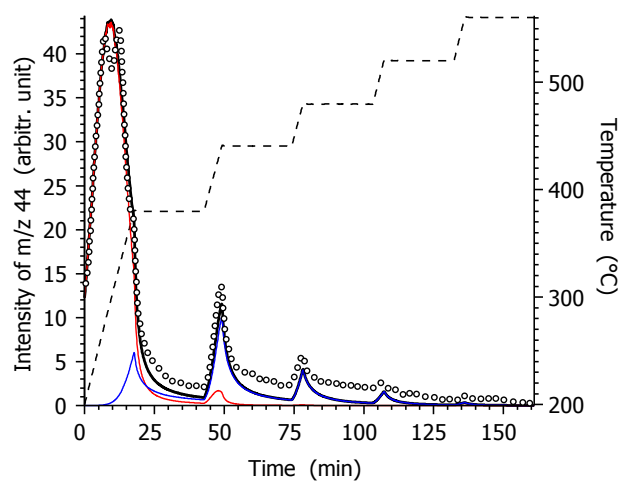
$\text{fit}_1 = 2.78\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=20.1$ scalefactor=1.02

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=16.3$

scalefactor* c_j : 38055. 14309.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

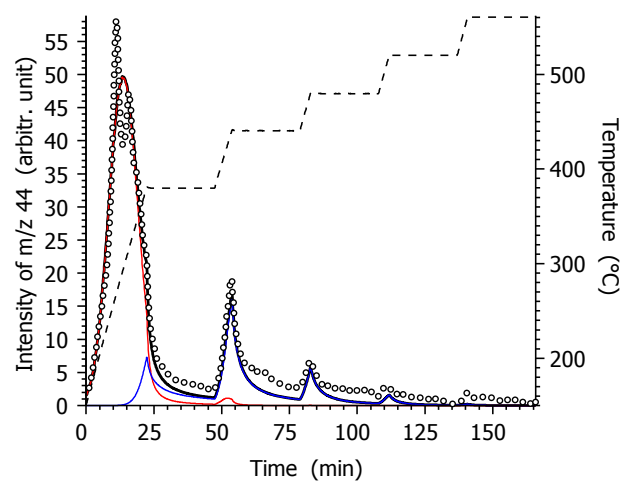
DAEM kinetics of intensity m/z 44 (CO_2)

$\text{fit}_1 = 3.63\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=22.2$ $\text{scalefactor}=0.955$

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=19.3$

$\text{scalefactor} \cdot C_i$: 38486. 11058.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 44 (CO_2)

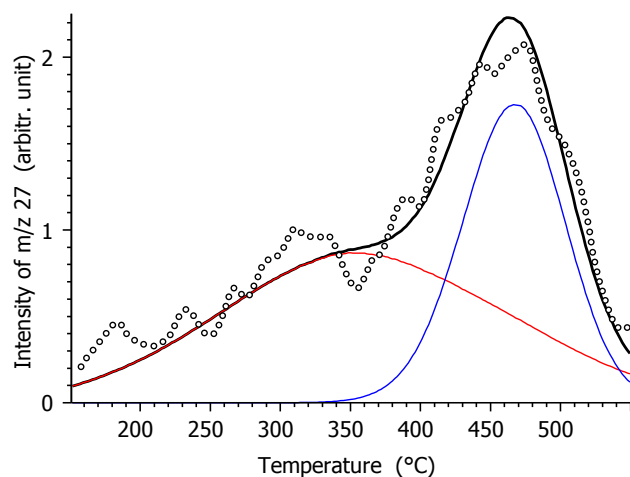
$\text{fit}_1 = 3.77\%$; $\text{fit}_{50} = 6.18\%$

1: $E_0=211.5$ $\log_{10} A=17.34$ $\sigma(E)=20.1$ $\text{scalefactor}=1.07$

2: $E_0=265.7$ $\log_{10} A=17.02$ $\sigma(E)=16.3$

$\text{scalefactor} \cdot C_i$: 40036. 15054.

Fig. 3. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

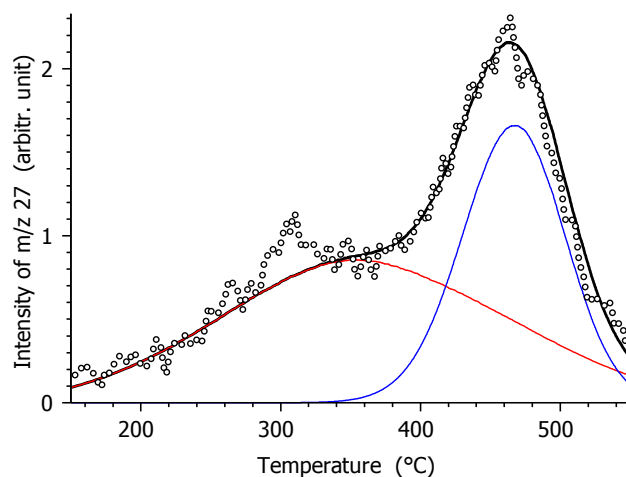
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 6.73\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.52$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 3317. 2423.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

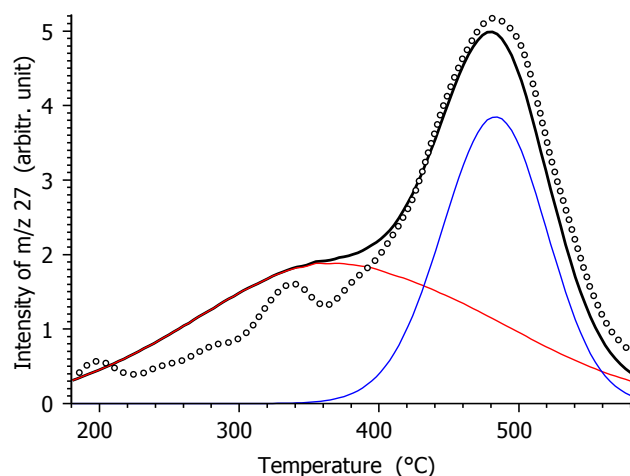
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 4.63\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.51$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 3268. 2328.



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

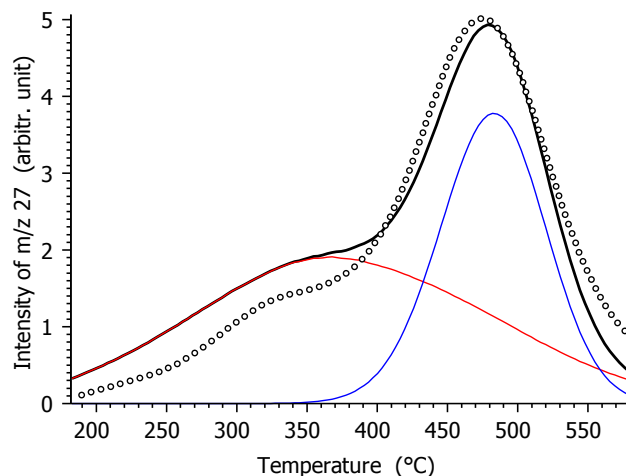
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 6.90\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.37$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 2994. 2187.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

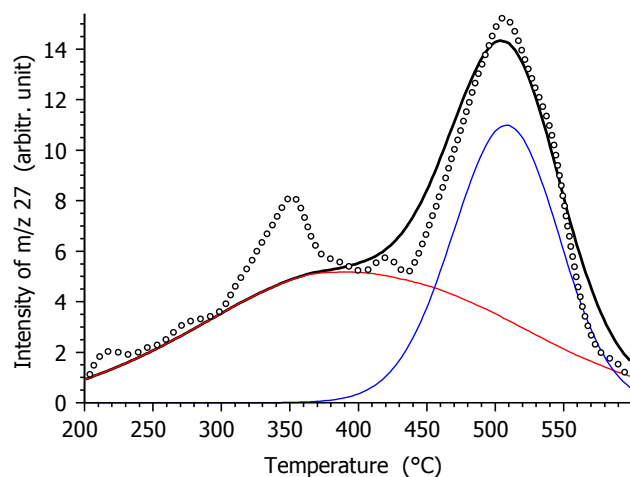
$\text{fit}_1 = 7.19\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.40$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 3020. 2151.

Fig. 4. Simultaneous evaluation of twenty MS intensity curves as described in Section 4.4. The experimental data ($\circ \circ \circ$), their simulated counterparts (—) and the calculated partial curves (—) are shown. The stepwise temperature programs (---) are also displayed when appropriate.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

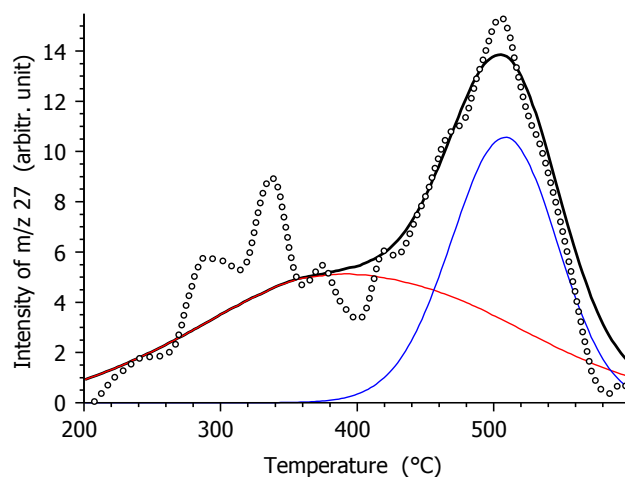
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 7.69\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 2184. 1595.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

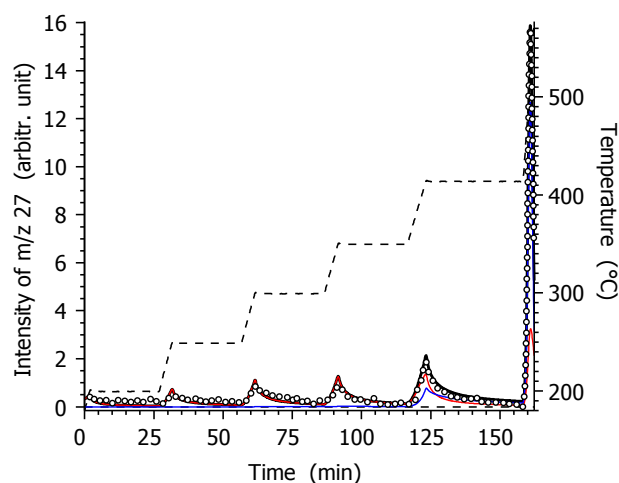
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 9.87\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 2159. 1537.



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

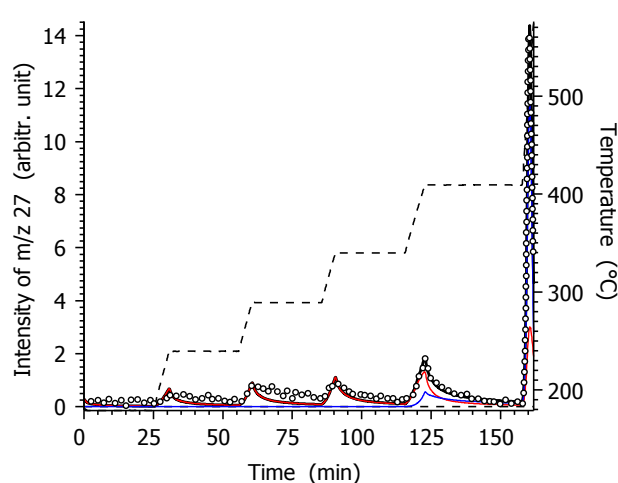
DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

$\text{fit}_1 = 1.11\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.43$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 3133. 2289.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity $m/z\ 27\ (\text{C}_2\text{H}_3^+)$

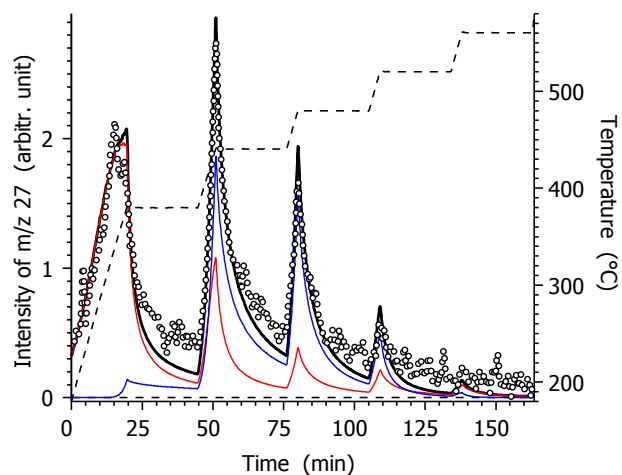
$\text{fit}_1 = 1.52\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ $\text{scalefactor}=1.28$

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

$\text{scalefactor} \cdot c_j$: 2765. 1970.

Fig. 4. (Continued.)



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

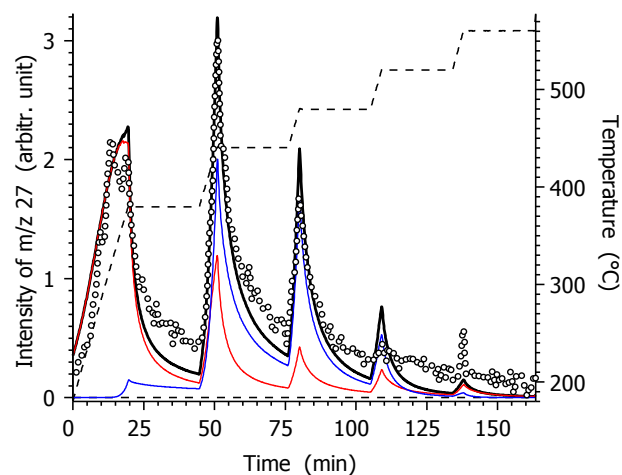
DAEM kinetics of intensity $m/z\ 27\ (C_2H_3^+)$

$fit_1 = 5.73\%$; $fit_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ scalefactor=1.43

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

scalefactor* c_j : 3112. 2274.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

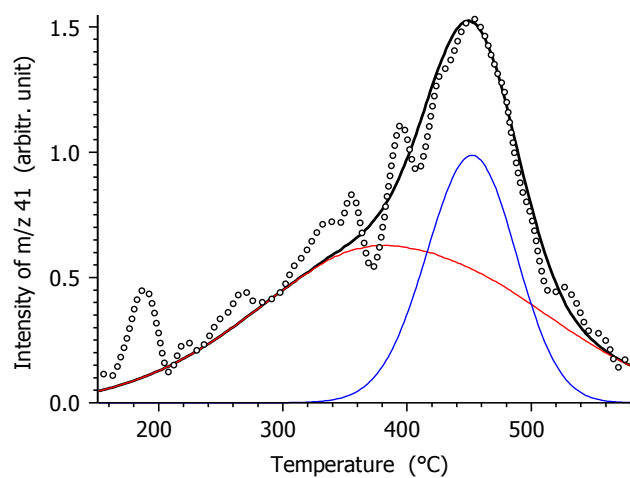
DAEM kinetics of intensity $m/z\ 27\ (C_2H_3^+)$

$fit_1 = 6.76\%$; $fit_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=14.29$ $\sigma(E)=32.9$ scalefactor=1.58

2: $E_0=260.9$ $\log_{10} A=15.83$ $\sigma(E)=10.9$

scalefactor* c_j : 3415. 2432.



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

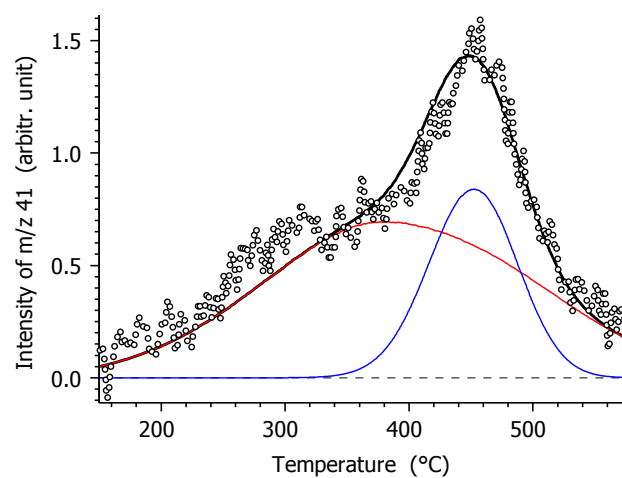
DAEM kinetics of intensity $m/z\ 41\ (C_2HO^+, C_3H_5^+)$

$fit_1 = 7.03\%$; $fit_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.52

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2597. 1368.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 41\ (C_2HO^+, C_3H_5^+)$

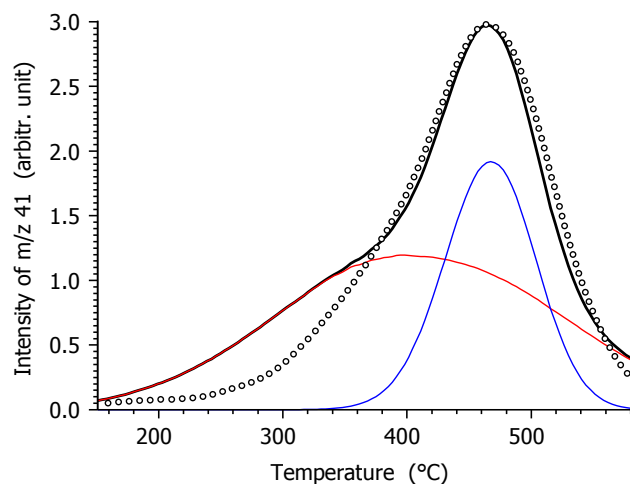
$fit_1 = 6.73\%$; $fit_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.28

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2869. 1163.

Fig. 4. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

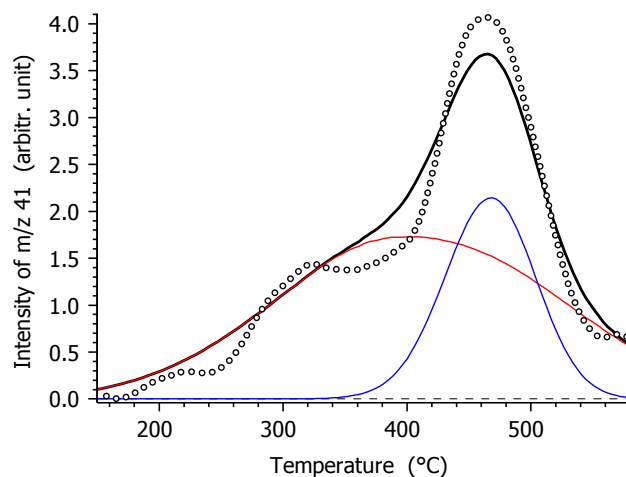
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 7.10\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.20

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2046. 1078.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

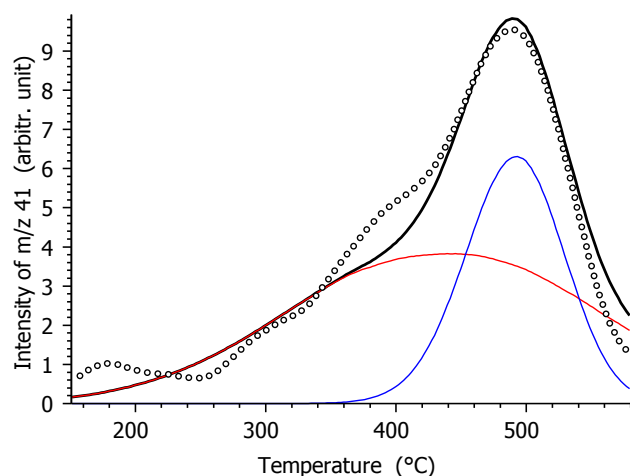
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 6.18\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.33

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2971. 1204.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

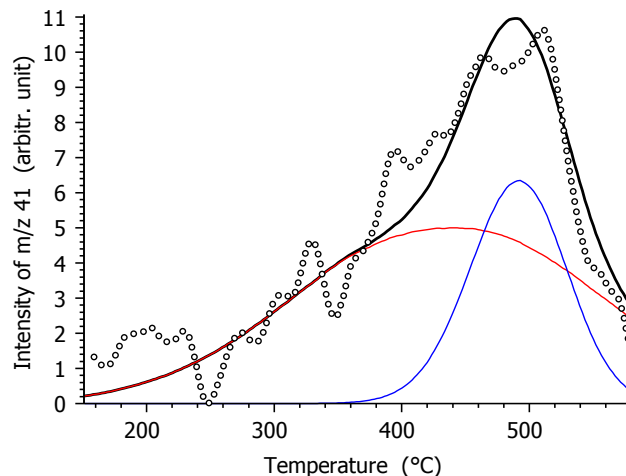
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 5.60\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 1712. 902.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

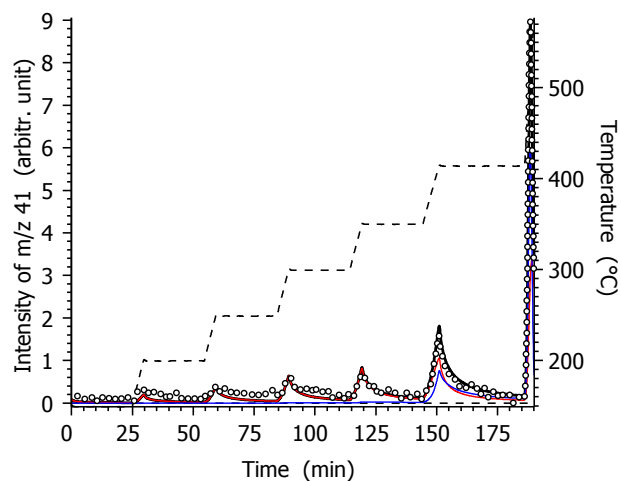
$\text{fit}_1 = 9.01\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2236. 907.

Fig. 4. (Continued.)



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

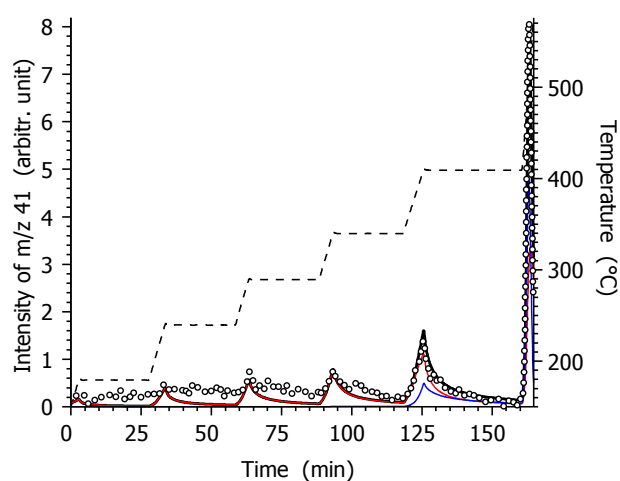
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 1.34\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.42

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2436. 1283.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

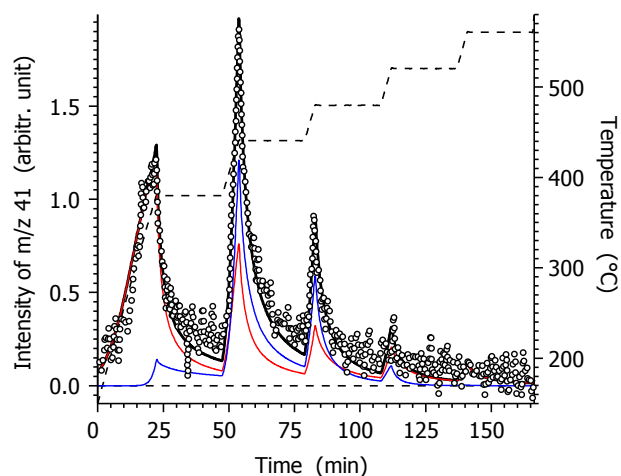
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 2.48\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.06

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2372. 961.



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

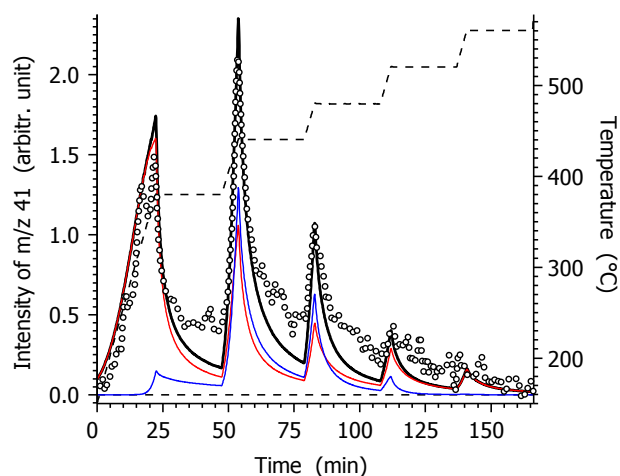
DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

$\text{fit}_1 = 4.80\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.18

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2019. 1064.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 41 (C_2HO^+ , C_3H_5^+)

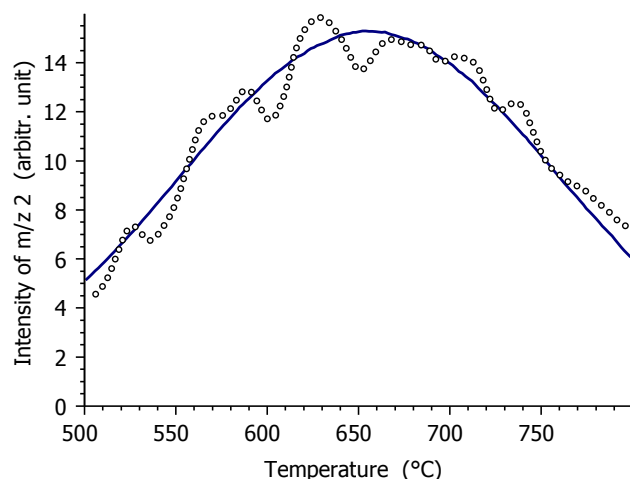
$\text{fit}_1 = 8.38\%$; $\text{fit}_{20} = 6.33\%$

1: $E_0=206.0$ $\log_{10} A=13.47$ $\sigma(E)=32.9$ scalefactor=1.25

2: $E_0=260.9$ $\log_{10} A=16.22$ $\sigma(E)=10.9$

scalefactor* c_j : 2786. 1130.

Fig. 4. (Continued.)

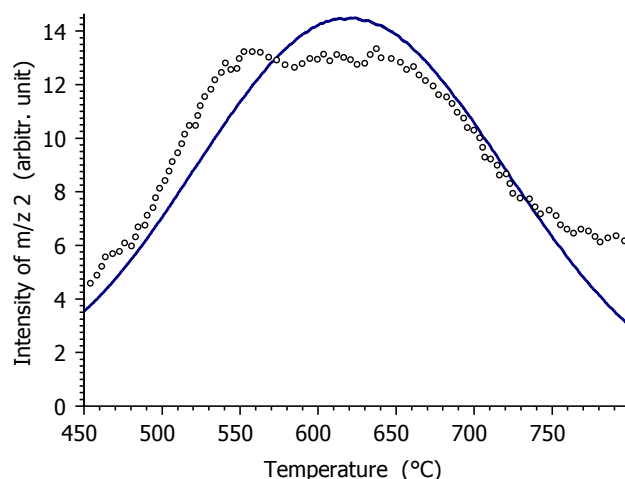


Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 2\ (\text{H}_2)$

$\text{fit}_1 = 4.86\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.07$ $\sigma(E)=29.7$ scalefactor=0.854
scalefactor* c_j : 58866.

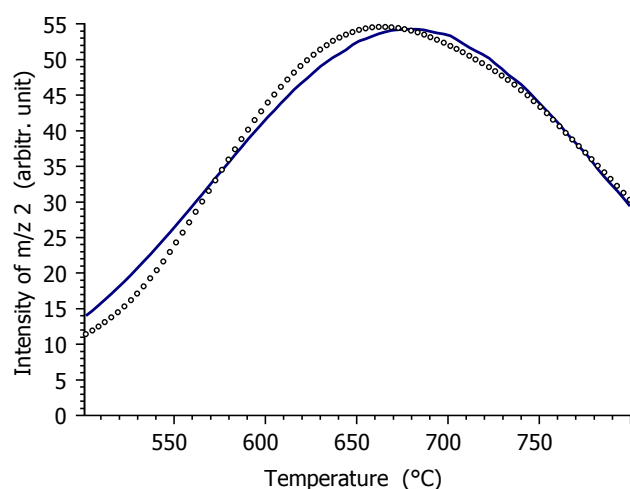


Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 2\ (\text{H}_2)$

$\text{fit}_1 = 9.68\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.72$ $\sigma(E)=29.7$ scalefactor=0.961
scalefactor* c_j : 53505.

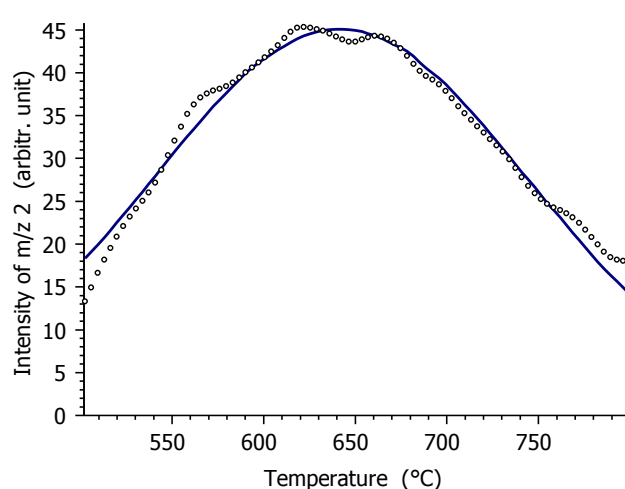


Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 2\ (\text{H}_2)$

$\text{fit}_1 = 3.32\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.07$ $\sigma(E)=29.7$ scalefactor=1.25
scalefactor* c_j : 86324.



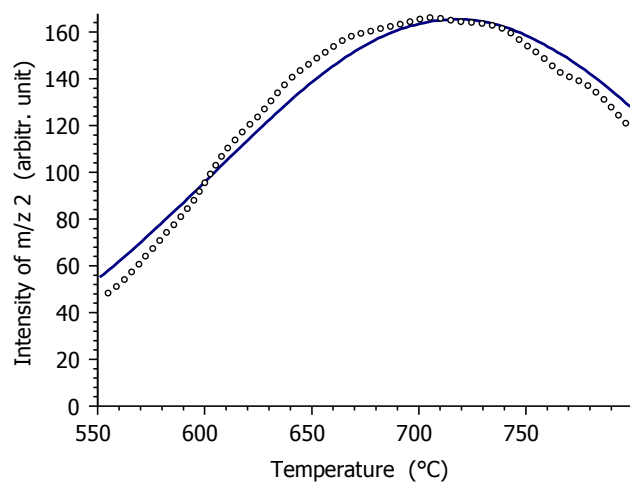
Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity $m/z\ 2\ (\text{H}_2)$

$\text{fit}_1 = 3.38\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.72$ $\sigma(E)=29.7$ scalefactor=1.23
scalefactor* c_j : 68380.

Fig. 5. Evaluation of groups of ten MS intensity curves as described in Section 4.5. The experimental data ($\circ \circ \circ$), their simulated counterparts (—) and the calculated partial curves (—) are shown. The stepwise temperature programs (---) are also displayed when appropriate.

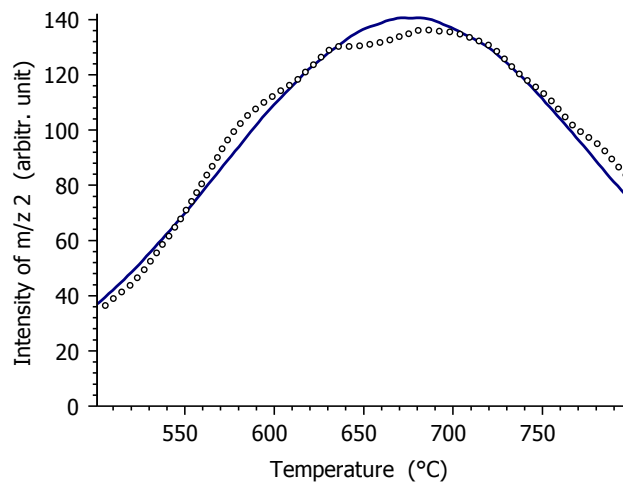


Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity **m/z 2 (H_2)**

$\text{fit}_1 = 3.66\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.07$ $\sigma(E)=29.7$ scalefactor=1
scalefactor* c_j : 68928.

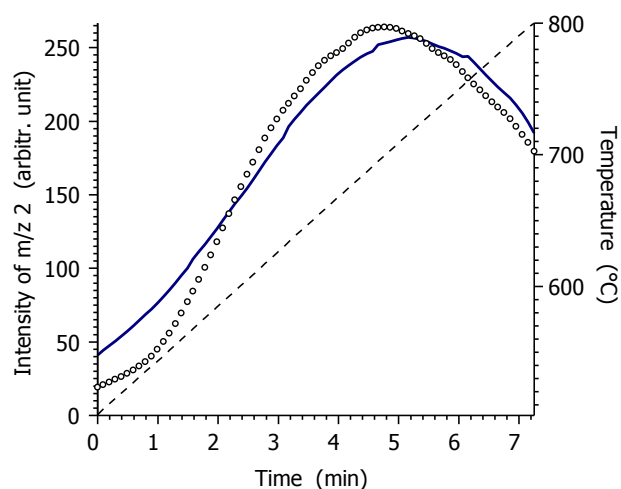


Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity **m/z 2 (H_2)**

$\text{fit}_1 = 3.09\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.72$ $\sigma(E)=29.7$ scalefactor=1
scalefactor* c_j : 55651.

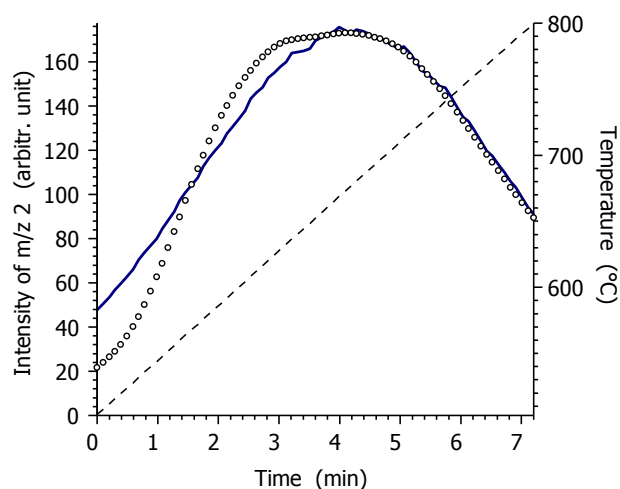


Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity **m/z 2 (H_2)**

$\text{fit}_1 = 6.63\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.07$ $\sigma(E)=29.7$ scalefactor=1.55
scalefactor* c_j : 106673.



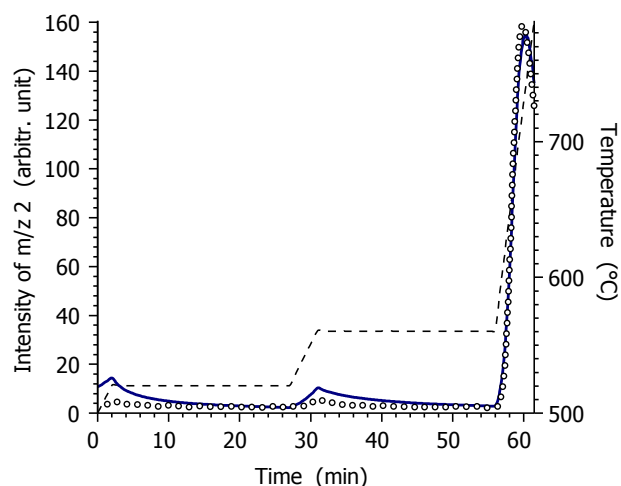
Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity **m/z 2 (H_2)**

$\text{fit}_1 = 6.67\%$; $\text{fit}_{10} = 5.13\%$

1: $E_0=265.1$ $\log_{10} A=12.72$ $\sigma(E)=29.7$ scalefactor=1.24
scalefactor* c_j : 68929.

Fig. 5. (Continued.)

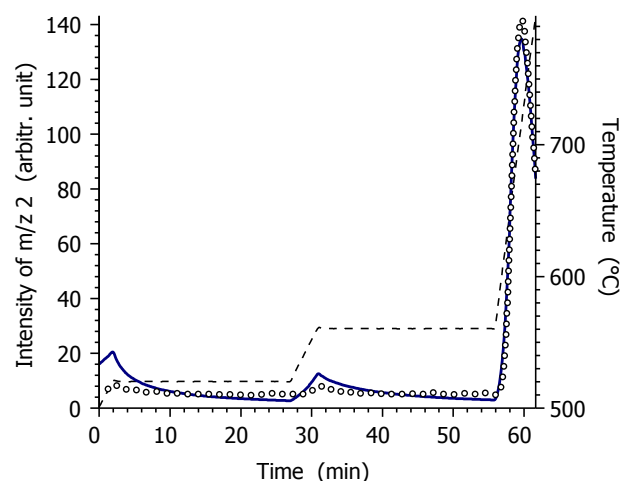


Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 2 (H_2)

fit₁ = 2.32%; fit₁₀ = 5.13%

1: $E_0=265.1$ $\log_{10} A=12.07$ $\sigma(E)=29.7$ scalefactor=1.00
scalefactor*c_j: 69150.

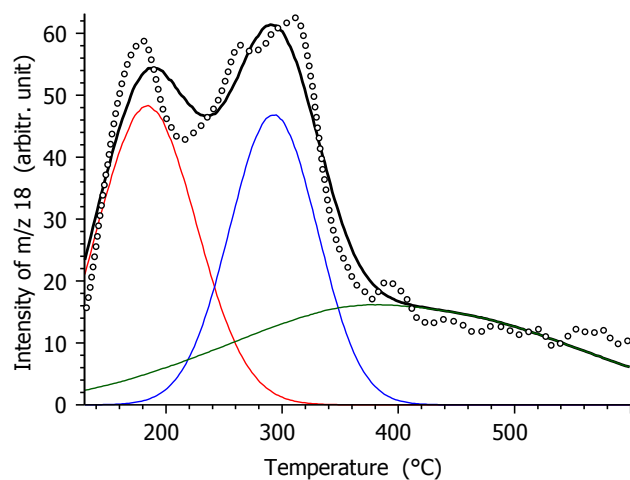


Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 2 (H_2)

fit₁ = 2.55%; fit₁₀ = 5.13%

1: $E_0=265.1$ $\log_{10} A=12.72$ $\sigma(E)=29.7$ scalefactor=1.13
scalefactor*c_j: 62804.

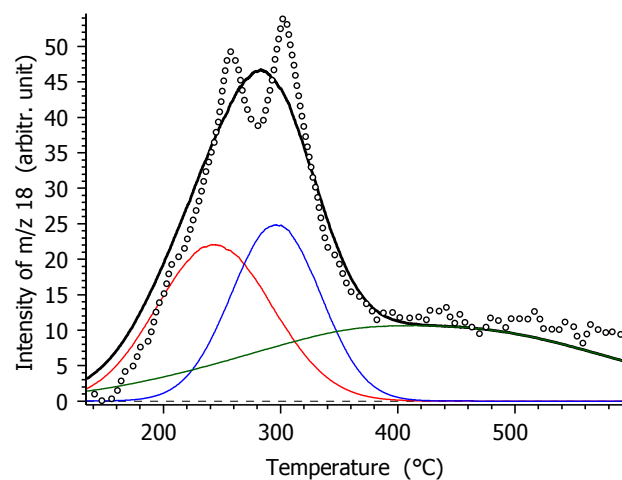


Virginia blend, $G_0=4.1\text{mg}$, Ar, 4°C/min

DAEM kinetics of intensity m/z 18 (H_2O)

fit₁ = 5.88%; fit₁₀ = 5.41%

1: $E_0=155.7$ $\log_{10} A=15.37$ $\sigma(E)=14.3$ scalefactor=1.33
2: $E_0=177.4$ $\log_{10} A=13.82$ $\sigma(E)=10.8$
3: $E_0=151.4$ $\log_{10} A=8.95$ $\sigma(E)=31.2$
scalefactor*c_j: 73013. 65247. 86071.



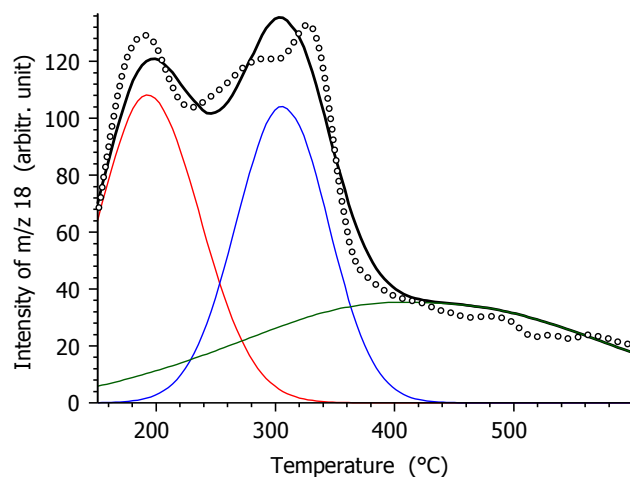
Burley blend, $G_0=4.0\text{mg}$, Ar, 4°C/min

DAEM kinetics of intensity m/z 18 (H_2O)

fit₁ = 6.73%; fit₁₀ = 5.41%

1: $E_0=155.7$ $\log_{10} A=13.17$ $\sigma(E)=14.3$ scalefactor=1.000
2: $E_0=177.4$ $\log_{10} A=13.71$ $\sigma(E)=10.8$
3: $E_0=151.4$ $\log_{10} A=8.55$ $\sigma(E)=31.2$
scalefactor*c_j: 39105. 34986. 59514.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 18 (H_2O)

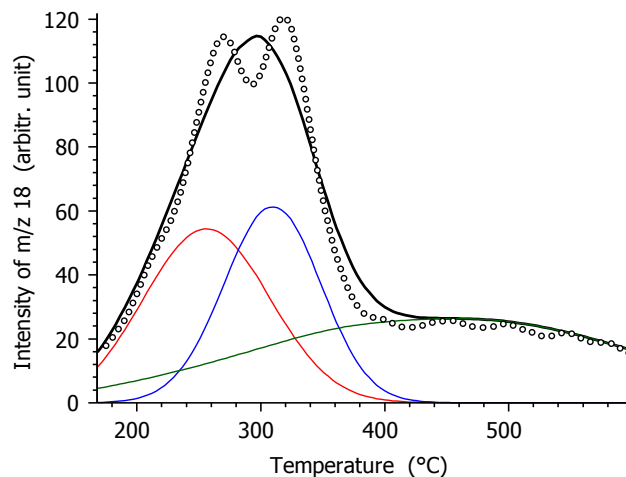
$\text{fit}_1 = 5.10\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=15.37$ $\sigma(E)=14.3$ scalefactor=1.22

2: $E_0=177.4$ $\log_{10} A=13.82$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.95$ $\sigma(E)=31.2$

scalefactor* c_j : 66980. 59856. 78959.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 18 (H_2O)

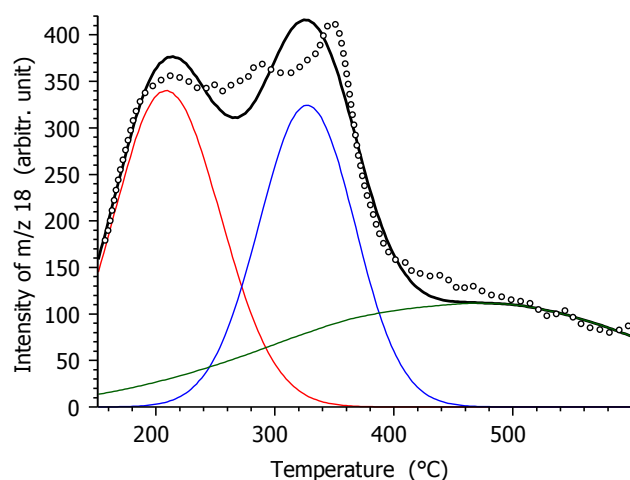
$\text{fit}_1 = 5.28\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=13.17$ $\sigma(E)=14.3$ scalefactor=1.02

2: $E_0=177.4$ $\log_{10} A=13.71$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.55$ $\sigma(E)=31.2$

scalefactor* c_j : 39856. 35658. 60657.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 18 (H_2O)

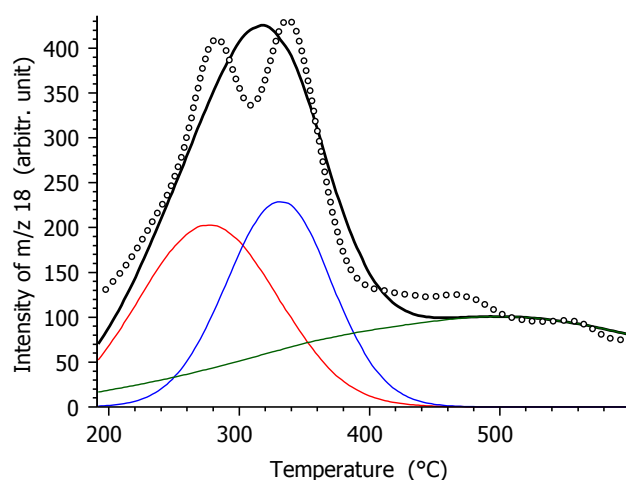
$\text{fit}_1 = 4.89\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=15.37$ $\sigma(E)=14.3$ scalefactor=1

2: $E_0=177.4$ $\log_{10} A=13.82$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.95$ $\sigma(E)=31.2$

scalefactor* c_j : 54991. 49142. 64826.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 18 (H_2O)

$\text{fit}_1 = 6.87\%$; $\text{fit}_{10} = 5.41\%$

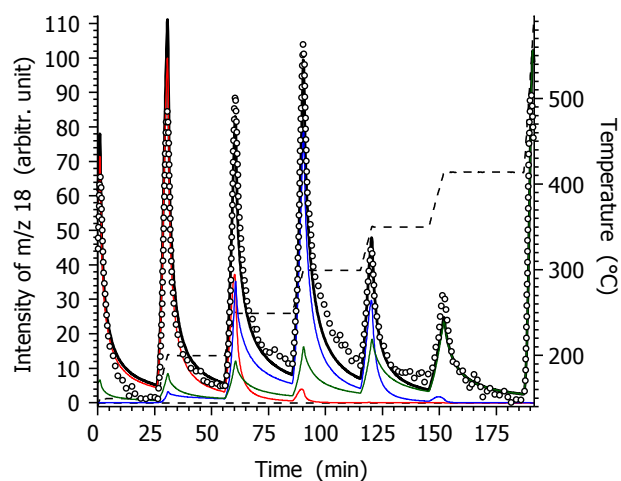
1: $E_0=155.7$ $\log_{10} A=13.17$ $\sigma(E)=14.3$ scalefactor=1

2: $E_0=177.4$ $\log_{10} A=13.71$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.55$ $\sigma(E)=31.2$

scalefactor* c_j : 39108. 34989. 59518.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity m/z 18 (H_2O)

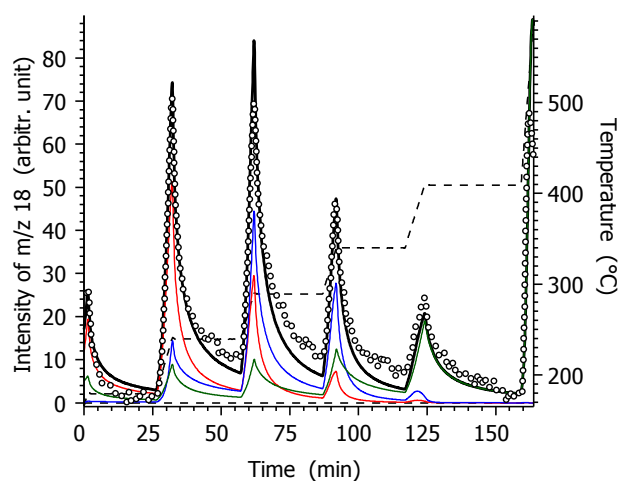
$\text{fit}_1 = 5.40\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=15.37$ $\sigma(E)=14.3$ scalefactor=1.39

2: $E_0=177.4$ $\log_{10} A=13.82$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.95$ $\sigma(E)=31.2$

scalefactor* c_j : 76365. 68242. 90023.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity m/z 18 (H_2O)

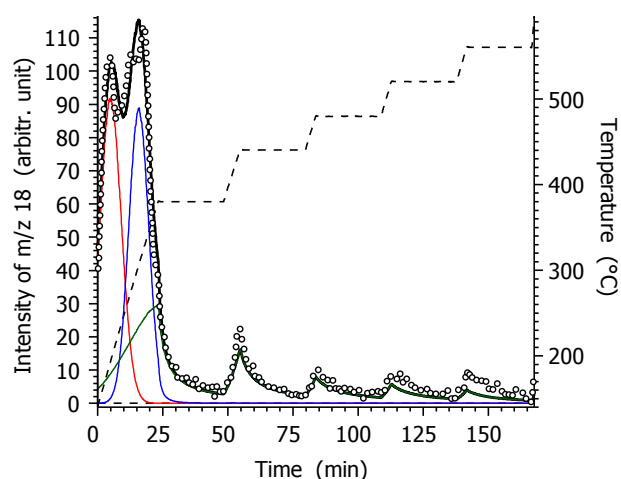
$\text{fit}_1 = 6.30\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=13.17$ $\sigma(E)=14.3$ scalefactor=1.17

2: $E_0=177.4$ $\log_{10} A=13.71$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.55$ $\sigma(E)=31.2$

scalefactor* c_j : 45945. 41106. 69924.



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 18 (H_2O)

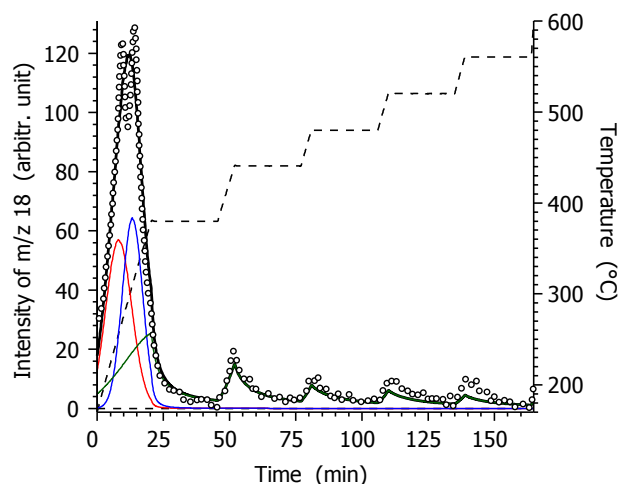
$\text{fit}_1 = 3.02\%$; $\text{fit}_{10} = 5.41\%$

1: $E_0=155.7$ $\log_{10} A=15.37$ $\sigma(E)=14.3$ scalefactor=1.03

2: $E_0=177.4$ $\log_{10} A=13.82$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.95$ $\sigma(E)=31.2$

scalefactor* c_j : 56772. 50733. 66925.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 18 (H_2O)

$\text{fit}_1 = 3.21\%$; $\text{fit}_{10} = 5.41\%$

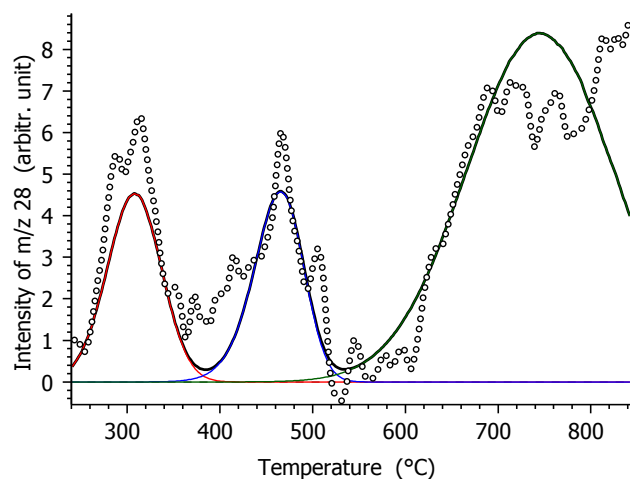
1: $E_0=155.7$ $\log_{10} A=13.17$ $\sigma(E)=14.3$ scalefactor=1.06

2: $E_0=177.4$ $\log_{10} A=13.71$ $\sigma(E)=10.8$

3: $E_0=151.4$ $\log_{10} A=8.55$ $\sigma(E)=31.2$

scalefactor* c_j : 41593. 37212. 63300.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

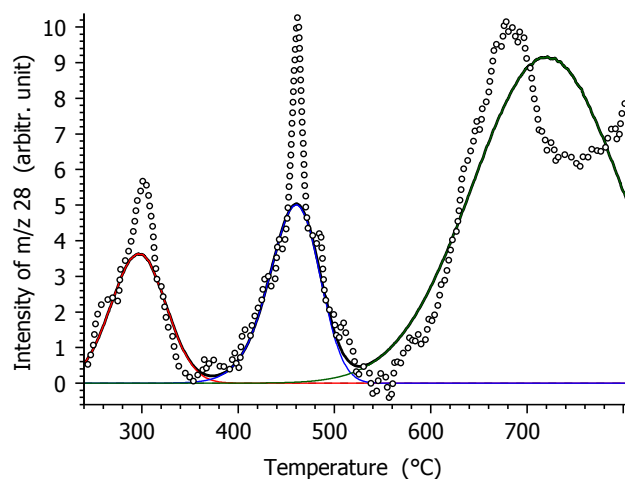
$\text{fit}_1=14.58\%$; $\text{fit}_{10}=8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.03$ $\sigma(E)=9.0$ scalefactor=0.921

2: $E_0=239.1$ $\log_{10} A=14.36$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=17.77$ $\sigma(E)=30.1$

scalefactor* c_j : 4912. 4716. 24552.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

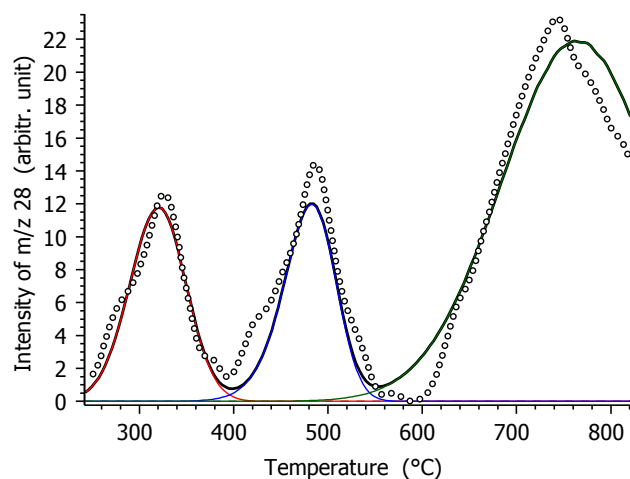
$\text{fit}_1=12.17\%$; $\text{fit}_{10}=8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.41$ $\sigma(E)=9.0$ scalefactor=0.882

2: $E_0=239.1$ $\log_{10} A=14.48$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=18.31$ $\sigma(E)=30.1$

scalefactor* c_j : 3835. 5123. 25995.



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

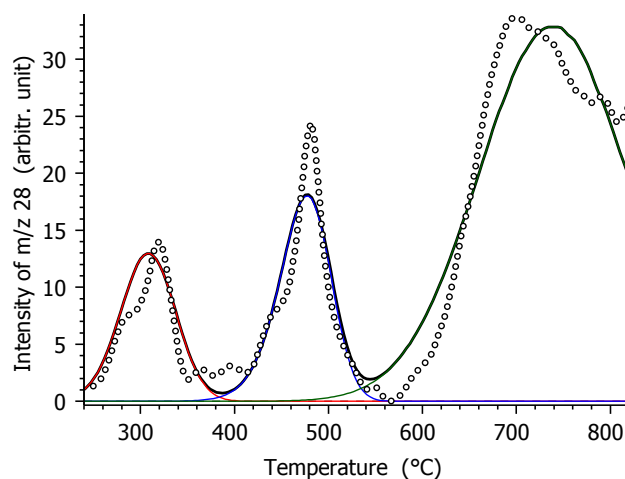
$\text{fit}_1=6.90\%$; $\text{fit}_{10}=8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.03$ $\sigma(E)=9.0$ scalefactor=0.984

2: $E_0=239.1$ $\log_{10} A=14.36$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=17.77$ $\sigma(E)=30.1$

scalefactor* c_j : 5250. 5040. 26239.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

$\text{fit}_1=8.16\%$; $\text{fit}_{10}=8.13\%$

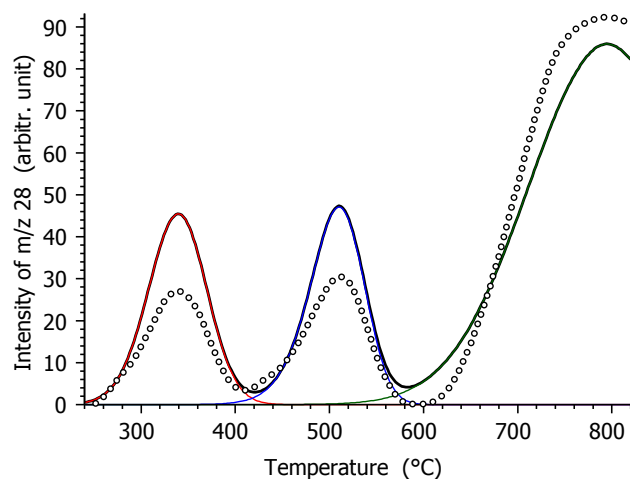
1: $E_0=206.1$ $\log_{10} A=16.41$ $\sigma(E)=9.0$ scalefactor=1.30

2: $E_0=239.1$ $\log_{10} A=14.48$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=18.31$ $\sigma(E)=30.1$

scalefactor* c_j : 5643. 7537. 38246.

Fig. 5. (Continued.)



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

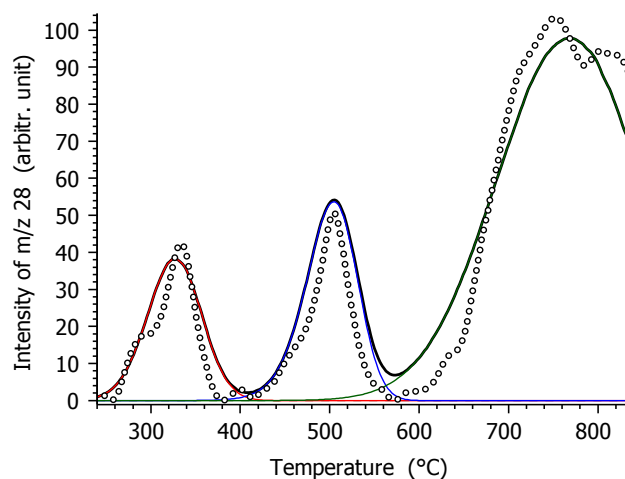
$\text{fit}_1 = 9.59\%$; $\text{fit}_{10} = 8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.03$ $\sigma(E)=9.0$ scalefactor=1

2: $E_0=239.1$ $\log_{10} A=14.36$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=17.77$ $\sigma(E)=30.1$

scalefactor* c_j : 5335. 5122. 26666.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

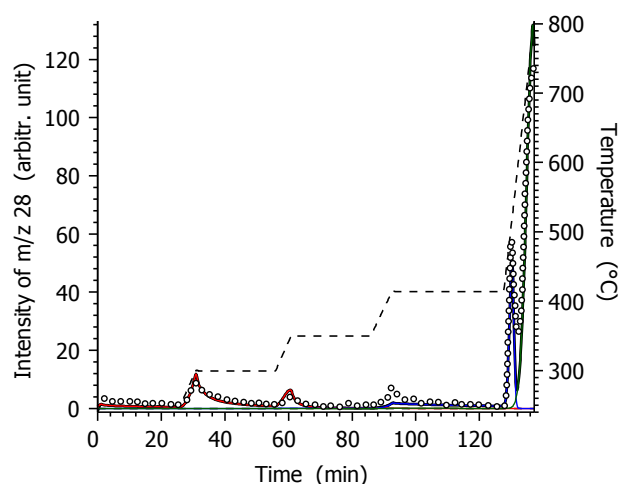
$\text{fit}_1 = 8.37\%$; $\text{fit}_{10} = 8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.41$ $\sigma(E)=9.0$ scalefactor=1

2: $E_0=239.1$ $\log_{10} A=14.48$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=18.31$ $\sigma(E)=30.1$

scalefactor* c_j : 4349. 5809. 29478.



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

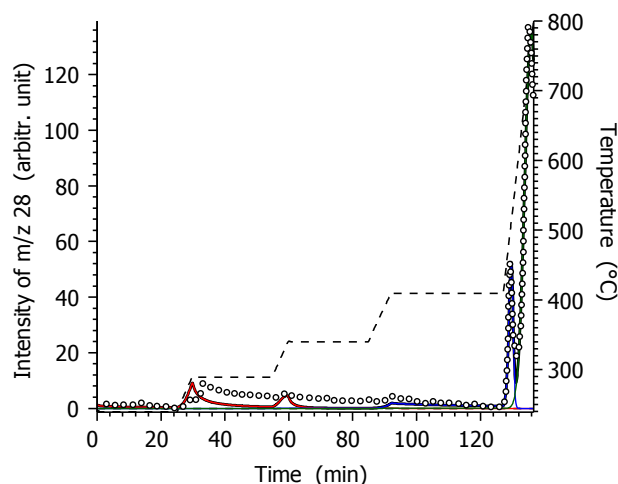
$\text{fit}_1 = 2.82\%$; $\text{fit}_{10} = 8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.03$ $\sigma(E)=9.0$ scalefactor=1.53

2: $E_0=239.1$ $\log_{10} A=14.36$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=17.77$ $\sigma(E)=30.1$

scalefactor* c_j : 8189. 7862. 40928.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

$\text{fit}_1 = 2.27\%$; $\text{fit}_{10} = 8.13\%$

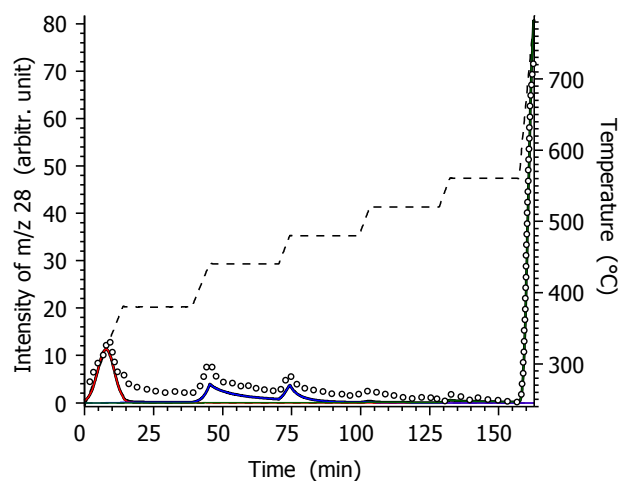
1: $E_0=206.1$ $\log_{10} A=16.41$ $\sigma(E)=9.0$ scalefactor=1.38

2: $E_0=239.1$ $\log_{10} A=14.48$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=18.31$ $\sigma(E)=30.1$

scalefactor* c_j : 6000. 8014. 40667.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

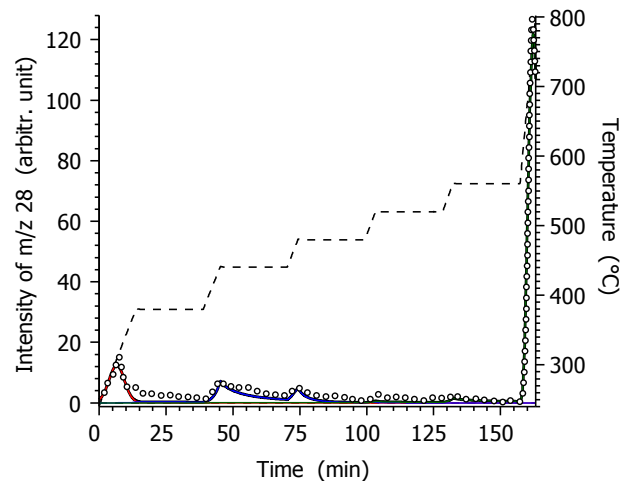
$\text{fit}_1 = 2.89\%$; $\text{fit}_{10} = 8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.03$ $\sigma(E)=9.0$ scalefactor=0.949

2: $E_0=239.1$ $\log_{10} A=14.36$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=17.77$ $\sigma(E)=30.1$

scalefactor* c_j : 5062. 4860. 25300.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity m/z 28 [CO (+ C_2H_4 and N_2)]

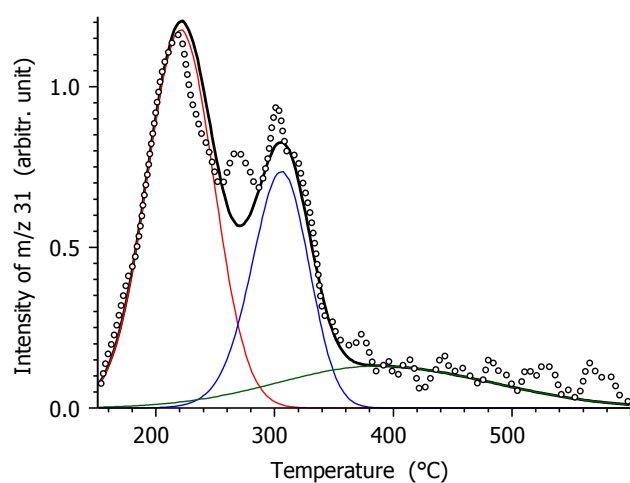
$\text{fit}_1 = 1.57\%$; $\text{fit}_{10} = 8.13\%$

1: $E_0=206.1$ $\log_{10} A=16.41$ $\sigma(E)=9.0$ scalefactor=1.24

2: $E_0=239.1$ $\log_{10} A=14.48$ $\sigma(E)=5.6$

3: $E_0=400$ $\log_{10} A=18.31$ $\sigma(E)=30.1$

scalefactor* c_j : 5372. 7176. 36412.



Virginia blend, $G_0=4.1\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

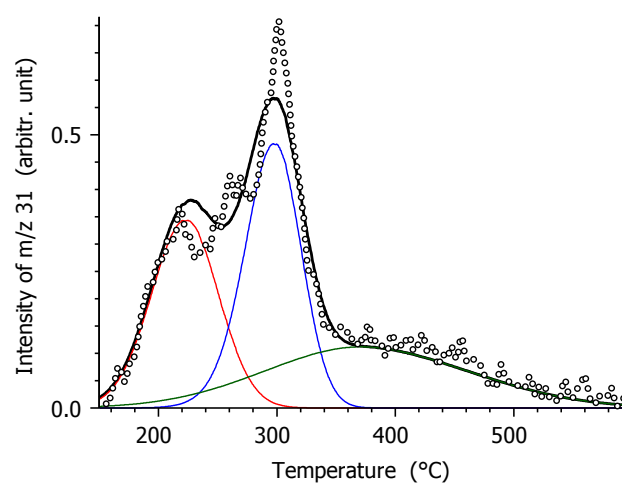
$\text{fit}_1 = 6.05\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.93$ $\sigma(E)=7.8$ scalefactor=1.20

2: $E_0=183.5$ $\log_{10} A=14.07$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.37$ $\sigma(E)=13.1$

scalefactor* c_j : 1188. 661. 446.



Burley blend, $G_0=4.0\text{mg}$, Ar, $4^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

$\text{fit}_1 = 4.94\%$; $\text{fit}_{10} = 4.55\%$

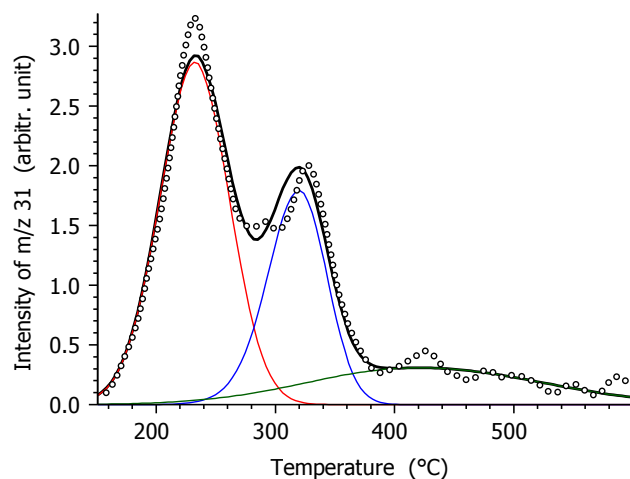
1: $E_0=155.1$ $\log_{10} A=13.87$ $\sigma(E)=7.8$ scalefactor=0.986

2: $E_0=183.5$ $\log_{10} A=14.32$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.60$ $\sigma(E)=13.1$

scalefactor* c_j : 350. 426. 366.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.1\text{mg}$, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

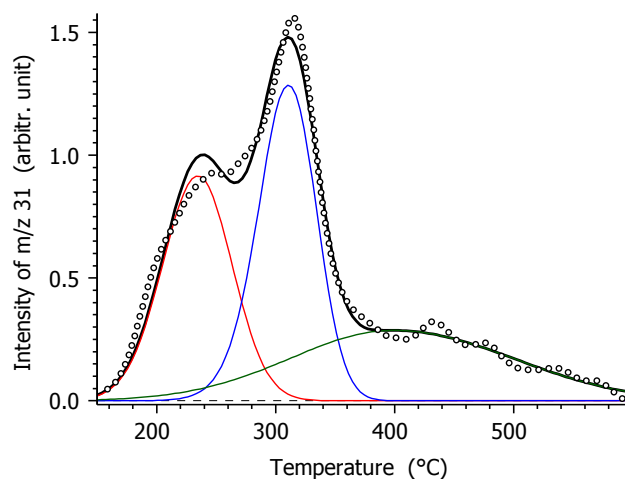
$\text{fit}_1 = 3.38\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.93$ $\sigma(E)=7.8$ scalefactor=1.21

2: $E_0=183.5$ $\log_{10} A=14.07$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.37$ $\sigma(E)=13.1$

scalefactor* c_j : 1200. 668. 450.



Burley blend, $G_0=4.1\text{mg}$, Ar, $10^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

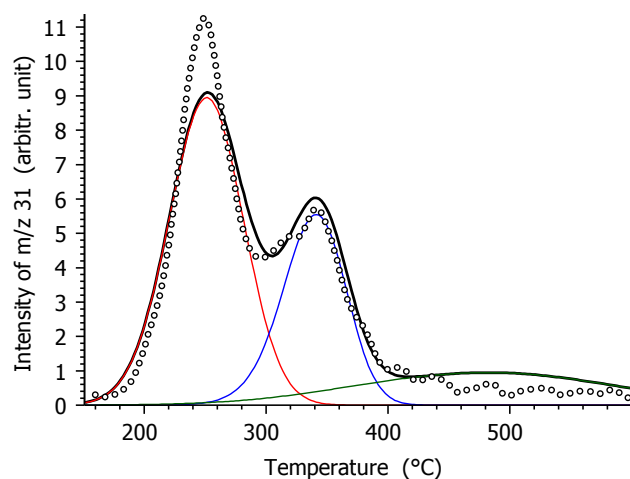
$\text{fit}_1 = 2.99\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.87$ $\sigma(E)=7.8$ scalefactor=1.09

2: $E_0=183.5$ $\log_{10} A=14.32$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.60$ $\sigma(E)=13.1$

scalefactor* c_j : 386. 470. 403.



Virginia blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

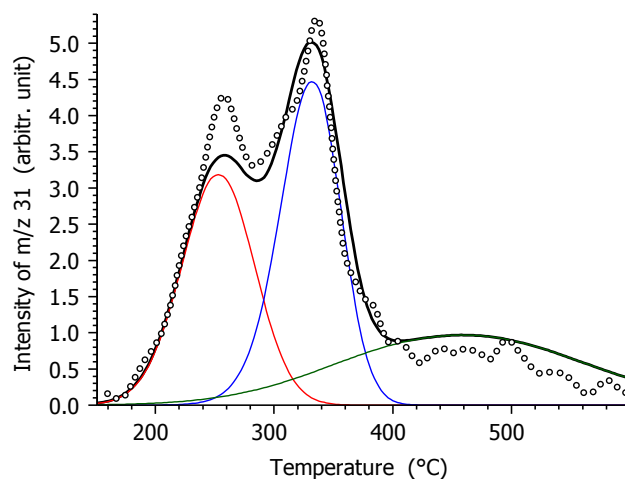
$\text{fit}_1 = 5.46\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.93$ $\sigma(E)=7.8$ scalefactor=1

2: $E_0=183.5$ $\log_{10} A=14.07$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.37$ $\sigma(E)=13.1$

scalefactor* c_j : 988. 550. 371.



Burley blend, $G_0=1.0\text{mg}$, Ar, $40^\circ\text{C}/\text{min}$

DAEM kinetics of intensity m/z 31 (CH_3O^+)

$\text{fit}_1 = 5.62\%$; $\text{fit}_{10} = 4.55\%$

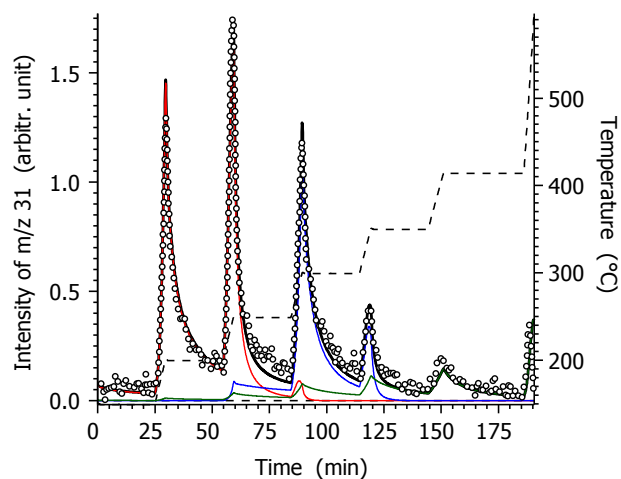
1: $E_0=155.1$ $\log_{10} A=13.87$ $\sigma(E)=7.8$ scalefactor=1

2: $E_0=183.5$ $\log_{10} A=14.32$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.60$ $\sigma(E)=13.1$

scalefactor* c_j : 355. 432. 371.

Fig. 5. (Continued.)



Virginia blend, $G_0=4.0\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity $m/z\ 31\ (\text{CH}_3\text{O}^+)$

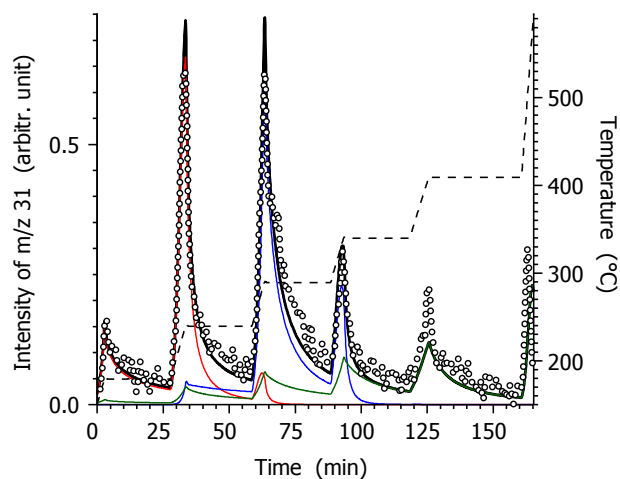
$\text{fit}_1 = 3.01\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.93$ $\sigma(E)=7.8$ scalefactor=1.28

2: $E_0=183.5$ $\log_{10} A=14.07$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.37$ $\sigma(E)=13.1$

scalefactor* c_j : 1269. 706. 476.



Burley blend, $G_0=4.1\text{mg}$, Ar, stepwise $T(t)$

DAEM kinetics of intensity $m/z\ 31\ (\text{CH}_3\text{O}^+)$

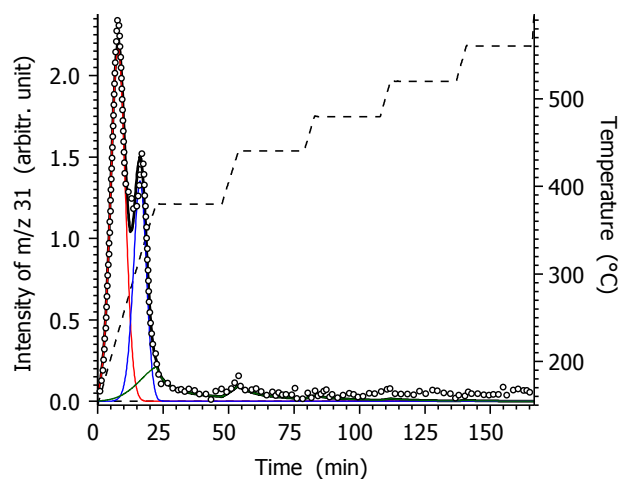
$\text{fit}_1 = 5.69\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.87$ $\sigma(E)=7.8$ scalefactor=0.933

2: $E_0=183.5$ $\log_{10} A=14.32$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.60$ $\sigma(E)=13.1$

scalefactor* c_j : 331. 403. 346.



Virginia blend, $G_0=4.2\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity $m/z\ 31\ (\text{CH}_3\text{O}^+)$

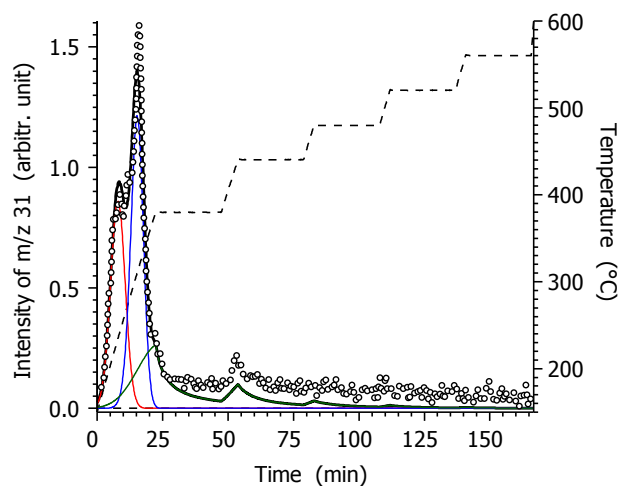
$\text{fit}_1 = 2.21\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.93$ $\sigma(E)=7.8$ scalefactor=0.917

2: $E_0=183.5$ $\log_{10} A=14.07$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.37$ $\sigma(E)=13.1$

scalefactor* c_j : 906. 504. 340.



Burley blend, $G_0=4.1\text{mg}$, Ar, steps at higher T

DAEM kinetics of intensity $m/z\ 31\ (\text{CH}_3\text{O}^+)$

$\text{fit}_1 = 4.21\%$; $\text{fit}_{10} = 4.55\%$

1: $E_0=155.1$ $\log_{10} A=13.87$ $\sigma(E)=7.8$ scalefactor=1.02

2: $E_0=183.5$ $\log_{10} A=14.32$ $\sigma(E)=5.7$

3: $E_0=106.0$ $\log_{10} A=5.60$ $\sigma(E)=13.1$

scalefactor* c_j : 363. 441. 379.

Fig. 5. (Continued.)