Supporting Information for article

Várhegyi, G.; Czégény, Zs.; Liu, C.; McAdam, K.: Thermogravimetric analysis of tobacco combustion assuming DAEM devolatilization and empirical char-burnoff kinetics.


**Scope of this document:** The simultaneous least squares evaluation of 30 samples is shown in computer-generated figures at three model variants:

**Figure 1.** Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to $m_{\text{char}}$.

**Figure 2.** Model assumptions: DAEM with constant preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.

**Figure 3.** Model assumptions: DAEM with variable preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.

**Arrangement.** Each figure has six pages. Each page shows the five experiments of a tobacco sample at a given oxygen concentration. (Note that two parallels were used from the 40°C/min experiments due to their low sample mass, as described in the paper.)

**Notation.** Experimental DTG curves normalized by the initial sample mass ($o o o$; their calculated counterpart (black $-$ $-$ $-$); and simulated partial curves $-dm_{\text{tar}}/dt$ (red $-$); $-dm_{\text{char}}/dt$ (blue $-$); and $-dm_{\text{ash}}/dt$ (green $-$). The stepwise temperature programs ($+ + +$) are also shown when appropriate.

**Data below the graphics in the figure panels.** The first line beneath the graphics contain the experimental conditions, including the initial sample mass ($G_0$) and the dimensionless V/V concentration of the oxygen ($C_{O_2}$). The next line contains the fit1 and fit30 values, as described in the paper. The following lines list the model parameters. (The first line of parameters in red color belongs to the devolatilization, while the second line in blue contains the char burn-off parameters.)

**Further information.** Please address any question with this document to the corresponding author

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Figure 1/a (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to $m_{\text{char}}$.)
**Figure 1b** (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to $m_{\text{char}}$.)

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Figure 1/c (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to $m_{char}$.)
Figure 1/d  (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to \(m_{\text{char}}\).)
Burley blend, G=2.1mg C_0=0.04, 4°C/min
fit: 7.57%, fit: 7.79%
1: E=185.6 log10 A=15.18 μ(E)=17.2 yield=0.542
2: E= 210.7 log10 A=13.57 μ=0.420 yield=0.487

Burley blend, G=0.4mg (2.027mg) C_0=0.04, 40°C/min
fit: 5.77%, fit: 7.79%
1: E=185.6 log10 A=15.18 μ(E)=17.2 yield=0.542
2: E= 210.7 log10 A=13.57 μ=0.420 yield=0.487

Burley blend, G=1.0mg C_0=0.04 40°C/min, 45° at 409°C
fit: 3.21%, fit: 7.79%
1: E=185.6 log10 A=15.18 μ(E)=17.2 yield=0.542
2: E= 210.7 log10 A=13.57 μ=0.420 yield=0.487

Burley blend, G=2.0mg C_0=0.04 stepwise T(t)
fit: 8.34%, fit: 7.79%
1: E=185.6 log10 A=15.18 μ(E)=17.2 yield=0.542
2: E= 210.7 log10 A=13.57 μ=0.420 yield=0.487

Figure 1/e (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to m_{char}.)
Figure 1/f  (Model assumptions: DAEM with constant preexponential factor and first order char burn-off kinetics with respect to $m_{\text{char}}$.)
**Figure 2a** (Model assumptions: DAEM with constant preexponential factor and an empirical $f(\alpha,m_{\text{char}})$ function in the char burn-off kinetics.)
Figure 2/b (Model assumptions: DAEM with constant preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.)
Figure 2c  (Model assumptions: DAEM with constant preexponential factor and an empirical \( f(\alpha, m_{\text{char}}) \) function in the char burn-off kinetics.)
Figure 2/d (Model assumptions: DAEM with constant preexponential factor and an empirical f(α, mchar) function in the char burn-off kinetics.)
**Figure 2e** (Model assumptions: DAEM with constant preexponential factor and an empirical $f(\alpha, m_{char})$ function in the char burn-off kinetics.)
Figure 2f  (Model assumptions: DAEM with constant preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.)
Virginia blend, G_0=2.0mg  C_{\text{CO}_2}=0.02, 4°C/min
fit: 7.79%  fit_0: 6.99%
1: E_o=181.7  log_{10}A_o=15.37  \delta(E)=52.8  yield=0.402  beta=0.106
2: E=212.4  log_{10}A=14.32  n=1.92  a=3.09  z=0.014
   \nu=0.416  yield=0.197

Figure 3/a (Model assumptions: DAEM with variable preexponential factor and an empirical f(\alpha,m_{\text{char}}) function in the char burn-off kinetics.)
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Figure 3/b  (Model assumptions: DAEM with variable preexponential factor and an empirical f(α,mchar) function in the char burn-off kinetics.)
Figure 3/c (Model assumptions: DAEM with variable preexponential factor and an empirical f(\(\alpha, m_{\text{char}}\)) function in the char burn-off kinetics.)
Figure 3/d  (Model assumptions: DAEM with variable preexponential factor and an empirical f(α, mchar) function in the char burn-off kinetics.)
Figure 3/e (Model assumptions: DAEM with variable preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.)
Figure 3/f  (Model assumptions: DAEM with variable preexponential factor and an empirical $f(\alpha, m_{\text{char}})$ function in the char burn-off kinetics.)