

The description of a sample program, and additional figures for the paper

1st supplementary file for article

Can varying activation energy be determined reliably from
thermogravimetric experiments?

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1. Introduction

The presented supplementary files aimed at demonstrating the reliability of the results of the paper. The reader can produce and compare the α or da/dt curves of the paper by a small, simple program and can check whether the curves belonging to first order kinetics with $E=200 \text{ kJ mol}^{-1}$ can really be approximated well by $E(\alpha)$ kinetics at a given set of heating rates. The obtained data can also be used for other purposes, e.g., for testing the various isoconversional evaluation methods of the literature.

2. The sample program

The source code of a sample program is given in the 2nd and 3rd supplementary files. Its description is given here. The code was written in standard C/C++ language and efforts were made to keep it readable for readers not familiar with C/C++. Ample comments aid its understanding. A syntax highlighting was also employed to facilitate the reading. (This syntax highlighting came from Microsoft Visual Studio.) The numerical solution of the kinetic differential equation is carried out by a Runge–Kutta algorithm which requested 15 lines in the presented source code. The program can be compiled by a modern C/C++ compiler and can be run in a console / terminal / command-prompt under Windows or Linux.

After compilation, the program can produce the data of 36 curves from the paper. The obtained data can be used for testing the results presented as well as for testing evaluation methods not covered in the paper.

Besides, the author used the data produced by this code for testing his own evaluation software. The evaluation software is a complex system of programs which have been developed in decades and written mainly in Fortran 90. Contrary to the code presented here, the evaluation software package uses parameter transformations and expresses the polynomials by Chebyshev polynomials of the first kind when it is used for evaluations with the empirical model

$$da/dt = \exp[p(\alpha) - \frac{E(\alpha)}{RT}] (1-\alpha)$$

The results of these tests (i.e., comparison of the curves) are shown in the figures of the next section.

COMPILATION AND RUNNING. The source code of the program is given in a Microsoft Word document which is in the 2nd supplementary file. It can be copied from Word into any modern text editor by a *Select All – Copy – Past* sequence. (If the text editor did not recognize the UTF-8 character encoding automatically, this encoding should be set manually before or during the saving of the file.) Alternatively, the *Save as Plain Text* menu item of Microsoft Word can also be employed, selecting UTF-8 when Word asks about the character encoding. Afterward the file extension of the obtained text file should obviously be changed to **.cpp** or **.cxx**.

The same source code can be run with different kinetic parameter sets. Seven parameter sets are in the third supplementary file, which is also a Word document. The parameter set employed in a given calculation is supposed to be in an include file named **parameters.h**. Perhaps it may be simpler to copy a parameter set from the Word file directly into the program code, replacing the line

```
#include "parameters.h"
```

The heating rates and the name of the output files is also defined in the included program lines; they can be changed easily if needed.

The program itself is a console application (terminal application). It can be compiled and run either from a consol or from a terminal window or by command prompts. If Microsoft Visual Studio is used for the compilation, the command line option **/utf-8** is beneficial. For other compilers the UTF-8 character encoding of the source files is supposed to be the default.

USAGE. The program writes only ASCII characters on the screen of a consol or terminal window (as a short message). However, its output files have UTF-8 character encoding. It is not supposed to cause problems during their usage. They could be opened smoothly by Notepad, Sublime Text, Microsoft Excel, and LibreOffice Calc. Two series of files are produced. One series list

```
t/min      T/°C      1-α      (da/dt)/s-1
```

while the other series list

```
t/min      T/°C      100(1-α)  100(da/dt)/s-1
```

The latter was needed for the tests carried out by the author. The content and the format of the output can easily be changed by searching for the **fprintf** functions in the source code and modifying them.

2. Figures

The first figure supplements the article by showing the curve fitting at parabolic $E(\alpha)$. Its notation is identical to the figures of the paper.

The further figures presented here compare the curves shown in the paper to their counterparts generated by the present sample code. The thick dashed lines were produced by the regular evaluation software of the author while the thin gray lines were generated by the sample program presented here.

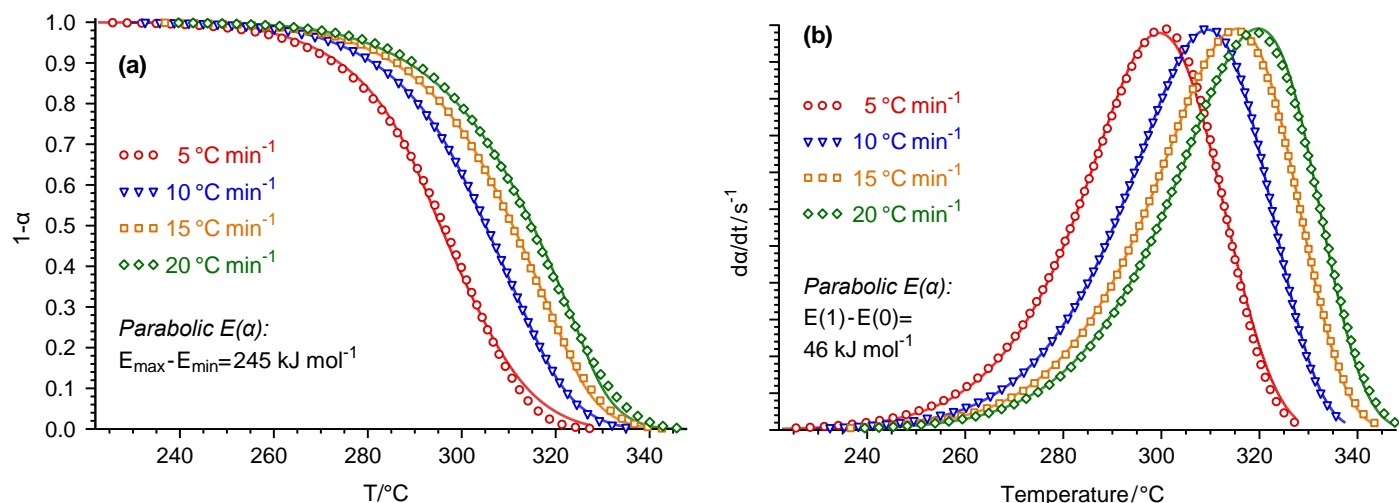


Fig. S1. A figure supplementing the paper. Curves at $E=200 \text{ kJ mol}^{-1}$ (\circ , ∇ , \square , \diamond) and their counterparts simulated with parabolic $E(\alpha)$ functions (solid lines) are shown in heating rate domain $\beta_{\max}/\beta_{\min}=4$.

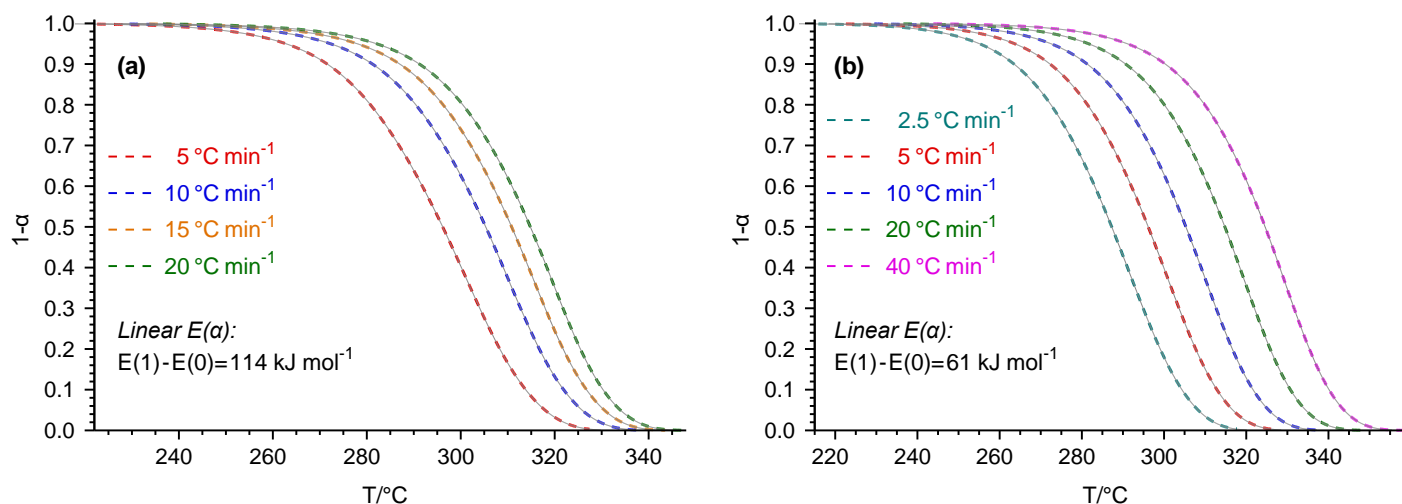


Fig. S2. Testing the curves with linear $E(\alpha)$ in Figure 2 of the paper. Dashed lines: curves from the paper, thin solid line: curves generated by the sample program presented here.

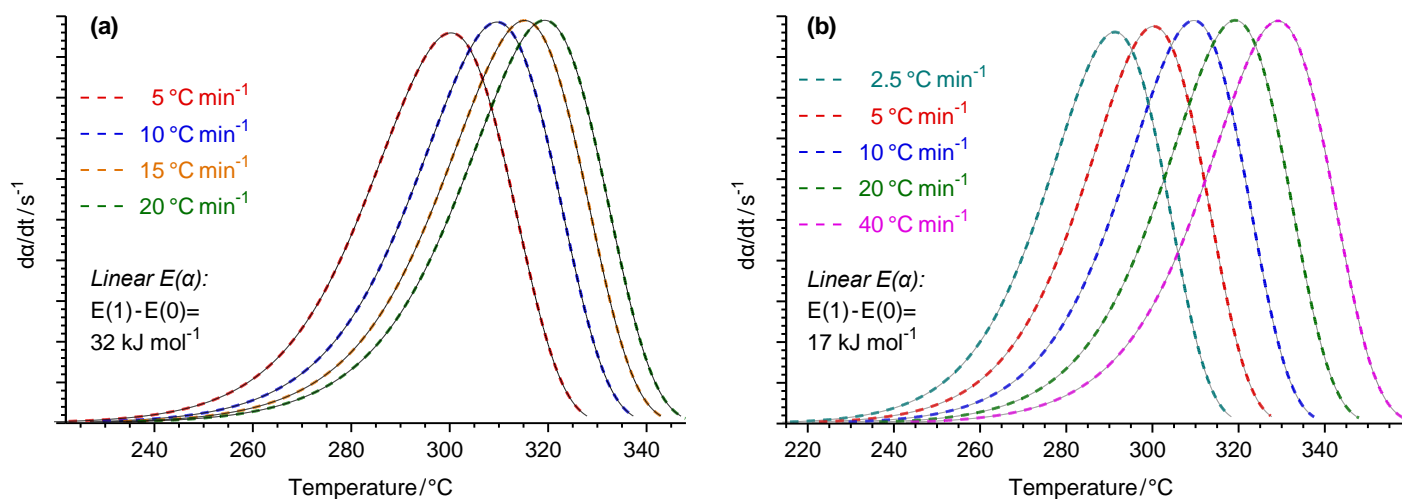


Fig. S3. Testing the curves with linear $E(\alpha)$ in Figure 4 of the paper. Dashed lines: curves from the paper, thin solid line: curves generated by the sample program presented here.

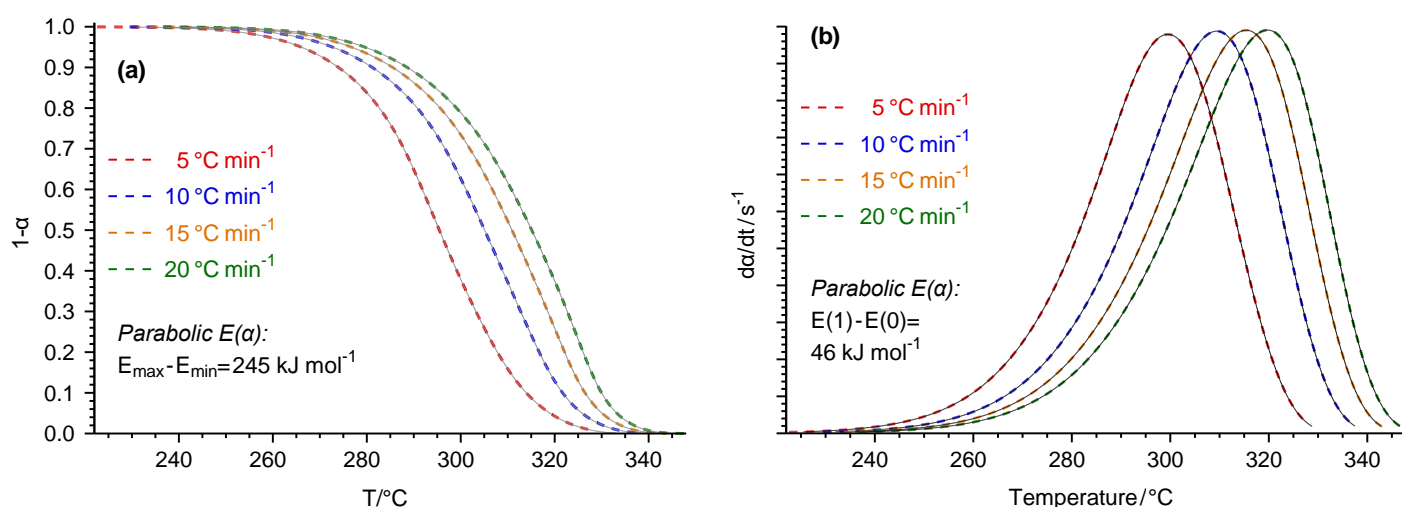


Fig. S4. Testing the curves with parabolic $E(\alpha)$ in Figure S1 of the present supplementary information. Dashed lines: curves obtained by the evaluation software, thin solid line: curves generated by the sample program presented here.

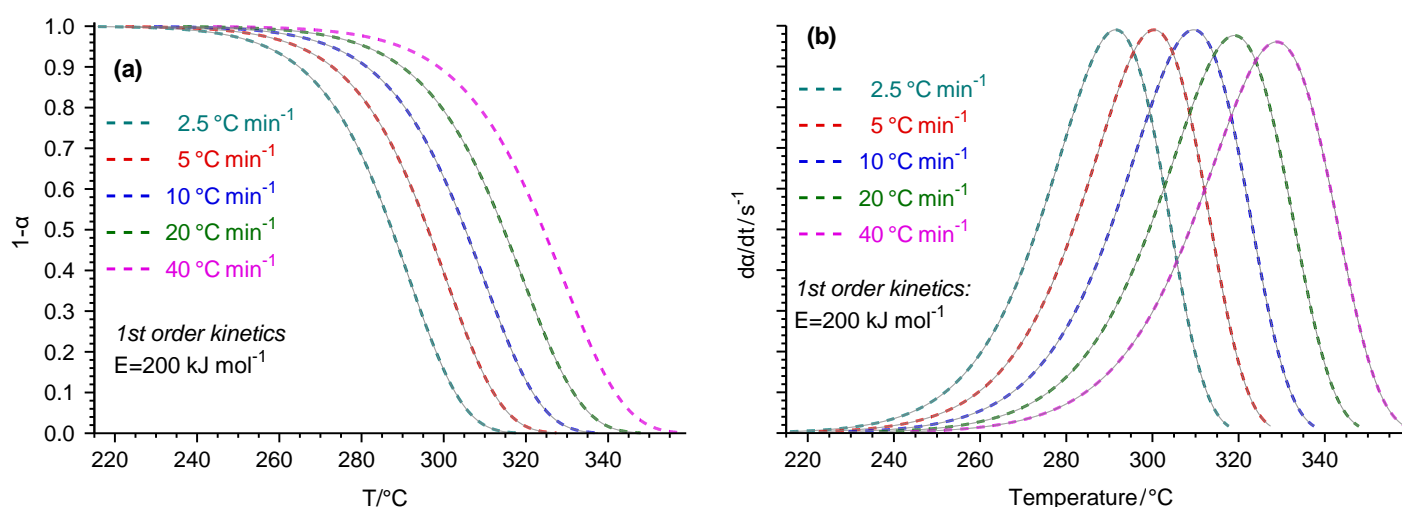


Fig. S5. Testing the curves belonging to first order kinetics with $E=200 \text{ kJ mol}^{-1}$ at five heating rates. (Dashed lines: curves from the paper, thin solid line: curves generated by the sample program presented here.)