

1. About DECOMP (version 1.1; for WindowsXP®)

This program (DECOMP) is designed to calculate age evolution curves for U-Th-He thermochronology (Forward modeling). It is an amendment to the papers of Meesters & Dunai (2002, part I and II) and is described in chapter 10 of this RiMG volume (Dunai 2005). DECOMP allows to compute age evolution curves for spherical symmetry. As demonstrated in above papers the spherical geometry can be used as an accurate approximation for other geometries if spheres of identical surface to volume ratio and properly transposed zonation of parent nuclides are used.

The target group for DECOMP are beginners as well as experienced practitioners in thermochronology. The functionality of the software lends itself to following applications:

1. Qualitative assessment of how changes of sample parameters (diffusion parameters, surface/volume ratios, emission distance) and model temperature histories affect ages. This aspect is particularly useful for teaching/learning what the most sensitive parameters for a certain system are.
2. Quantitative forward modeling of any time temperature history
3. Qualitative assessment of the effect of parent nuclide zonation (The calculation is quantitative, however, input with in most cases be qualitative, consequently also the results).
4. While DECOMP was originally designed for forward modeling of (U-Th)/He ages, forward modeling of any thermochronological system that is governed by volume diffusion, and of which the diffusion parameters (D_0 , E_a) of the radionuclide are known, is possible

2. Conditions of use

DECOMP was created for **scientific purposes** and if used for these purposes its use is **free of charge**. It may be dispersed freely within the scientific community. Any results obtained with this program must be properly referenced if they are used in publications and presentations. Proper referencing is referring to *both* Meesters & Dunai (2002, part II) *and* the program (DECOMP; by Bikker, A.; Meesters A.G.C.A. and Dunai T.J.). The program can be freely used in university teaching and teaching in non-profit organizations. If DECOMP is used as a part of another program the same conditions of use as for DECOMP must apply to that other program.

Although DECOMP has been created and tested with great care to avoid errors the authors can not be made responsible for any consequences of eventual errors or malfunctioning of DECOMP. We are grateful for any feedback on errors or other suggestion that might improve later versions of DECOMP (please contact: dunt@geo.vu.nl).

3. How to use DECOMP

We aimed at a user-friendly interface that allows repeating calculations of Meesters & Dunai (2002, part I and II) and of course to perform own forward modeling calculations. The results can be exported to standard spreadsheet programs. On first starting the program the user is asked to fill in, step by step, the parameters necessary for a computation. In most cases default values or exemplary temperature histories are supplied, which of course can be changed. Both the left and right buttons of the mouse can be used to have access to options (such as adding and/or editing points to the temperature histories). On finishing this introduction the actual window of DECOMP will appear. Once DECOMP was quit for the first time the introduction will not reappear on restarting DECOMP. Starting DECOMP is straightforward: double click on the icon of the executable file (DECOMP.EXE).

In the following features of the DECOMP window (screenshot: Fig. 3; Dunai 2005) are described:

Button panel

Save and open geometric parameters, temperature histories, constants and annotations

Quit the program

Recalculate the age evolution diagram

Edit constants: number of eigenvalues used for computation; activation energy (the non-SI unit [cal/mol] is used here as currently most values are still published in [cal/mol], for conversion 1 joule = 0.239 cal); pre-exponential factor D_0 [cm²/s].

Input parameters describing the geometry of a sample:

Sphere radius: Radius (in microns) of a sphere of identical surface to volume ratio as the sample

Outer and inner zone radius: Gives the outer and inner radius (in microns) of the zone containing the parent nuclides. The shape of the zone containing the parent nuclides is visualized by the red zone in the circle to the right of the input field that is changing simultaneously while changing values. Samples with a homogenous parent nuclide distribution have outer zone radius equal to the sphere radius and an inner radius of 0 microns.

Emission distance: Emission distance (in microns) of alpha particles.

Temperature history diagram

(real time [Ma] vs. temperature [°C]; real time = time elapsed since beginning of the model)

right mouse button:

copy the numeric values of temperature history (table comma delimited) to be pasted e.g. in a spreadsheet program.

add and delete points to/from the temperature history

table edit: edit the numeric values of existing points of the temperature history

left mouse button:

drag axis to scale

drag existing points

The temperature and real time at the position of the tip of the cursor are indicated in the frame at the top right of the diagram

Age evolution diagram

(real time [Ma] vs. calculated age [Ma]; calculated age = age as would be calculated from U, Th and He concentrations in a sample)

Initially this diagram is blank, on pressing the recalculation button the age evolution is calculated for the current temperature history.

The numeric values curve can be copied (right mouse button) and pasted into a spreadsheet program (table comma delimited). The calculated age and real time at the position of the tip of the cursor are given in the frame at the top right of the diagram.

Annotation field

For annotations to be saved with the model parameters (save with the save button)

4. References:

Meesters, A.G.C.A. and Dunai T.J. (2002) Solving the production-diffusion equation for finite diffusion domains of various shapes (part I): implications for low-temperature (U-Th)/He thermochronometry, *Chemical Geology* **186/3-4**, 337-348

Meesters, A.G.C.A. and Dunai T.J. (2002) Solving the production-diffusion equation for finite diffusion domains of various shapes (part II): Application to cases with alpha-ejection and non-homogenous distribution of the source" *Chemical Geology* **186/3-4**, 351-369

Dunai T.J. (2005) Forward modeling and interpretation of (U-Th)/He ages, *Reviews in Mineralogy and Geochemistry*, Vol. 58