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Research paper

# MOD-AGE: An age-depth model construction algorithm

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ABSTRACT

We present MOD-AGE, a new system for chronology construction. MOD-AGE can be used for profiles that have been dated using other techniques. The system uses three basic measurements for input data: activities, the atomic ratio or age, and the depth measurement. Based on the measurement results (probability distributions), MOD-AGE estimates the confidence bands of the age-depth model and uses nonparametric methods to avoid the consequences of failure to meet assumptions. Using the normal distribution of the measured data (activities, atomic ratios, depths, etc.), we applied a Monte Carlo simulation to the model age and depth values. Several fitting models could be applied to estimate the relationships. Following multiple tests, we chose the locally weighted scatterplot smoothing (LOESS) method.

The stratigraphic correction procedure applied in the MOD-AGE program uses a probability calculus, which assumes that all of the sample ages are correctly estimated. The probability age distribution from the samples was used to estimate the most probable sequence in accordance with the superposition rule.

This study presents MOD-AGE as a tool for the chronology construction of speleothems that have been analyzed with the U-series method and compares MOD-AGE to the StalAge algorithm presented by Scholz and Hoffmann (2011).

The MOD-AGE software was written in, made by Borland, RAD STUDIO 2007 and is available from the authors as freeware.



## 1. Introduction

All change, including change in paleoenvironmental indicators, is a function of time. Time information is gained from isotope dating, but the samples for environmental indicator studies commonly have much higher resolutions (number of samples per depth unit) than the samples for age estimation. Hence, age-depth model construction with reliable estimation of confidence bands is an important challenge for paleoenvironmental studies.

Interest in the investigation of speleothems has increased over the last ten years. There are many reasons why speleothem research is attractive: (i) speleothem profiles provide good records of the land environment; (ii) preserved profile records are usually continuous and long-lasting; (iii) U-series methods offer the possibility of precise dating; and (iv) the chemical composition of calcite reflects the chemical composition of water, and the composition of water reflects climatic conditions such as the average rainfall and the mean annual temperature near the cave. In recent years, an abundance of palaeoclimatic information has been obtained from high-resolution geochemical studies based on high density sampling profiles from speleothems. The samples are analyzed in two ways: (i) the stable isotopic composition of O and C and (ii) the proportions of rare elements such as Mg, Sr, Ba, and Ca, which yield information on water circulation times and precipitation intensity. Such studies are possible with a resolution of one calendar year (Baker et al., 1993; Frisia et al., 2003; Roberts et al., 1998; Hu et al., 2008; Yuan et al., 2004; Wang et al., 2001, 2005). Aside from “classical palaeoclimatic reconstruction” (temperature, humidity), the data from high resolution speleothems records are used for setting precise boundaries for climatic episodes (Dansgaard-Oeschger and Heinrich episode) or for determining the internal structure and duration of climate events such as the 8.2 ka event and the reconstruction of the North Atlantic Oscillation (NAO) index. The creation of a reliable chronology is the most crucial challenge in paleoenvironment reconstructions, particularly for high-resolution analyses.

Age-depth model (chronology) construction is a subset of a more general problem, the estimation of spatial uncertainty. The final solution should consider the uncertainties of both variables and provide the result (relation estimation) with its confidence bands.

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Several age-depth model systems were proposed for the radiocarbon profiles (Blaauw and Christen, 2011; Blaauw, 2010; Blockey et al., 2007; Heegard et al., 2005; Ramsey, 2008). The referred models commonly use calibrated radiocarbon dates with a well-defined 2σ band and with the assumption that depth (sample position in a profile) is known with certainty. However, Heegard et al. (2005) use the assumption that organic samples taken from the examined layer could not reflect the age of its layer origin, introducing a new error source to the model. The MOD-AGE system was constructed for speleothems analyzed with the U-series method. Samples analyzed by the U-series method are usually part of the layer and reflect its origin age. However, MOD-AGE assumes that the profile position for the aged samples is not known with absolute certainty. All measurement results have specific uncertainties.

Recently, StalAge was proposed as an age-depth model construction tool for "speleothem researchers". It was published with an R script by Scholz and Hoffmann (2011). The appearance of this tool aroused great interest. The published description of the StalAge algorithm (with the source code) allowed the direct application of data to chronology. Several months after the StalAge algorithm was published, several researchers attempted to apply it to time-scale construction. They used StalAge, as its authors suggested, as a type of "black-box" for age-depth modeling. This demonstrates the great demand within the "speleothems-community" for chronology construction tools.

We propose an alternative tool for chronology construction, the MOD-AGE system, which was built using Borland RAD Studio software. The MOD-AGE software is compatible with the Microsoft Windows operating systems. MOD-AGE can be used with profiles that have been dated previously with different methods. The system uses three basic measurements for input data: activities, the atomic ratio (age), and the depth measurement. Based on the measurement results (probability distributions), MOD-AGE estimates the age–depth relationship and its confidence bands. To avoid the consequences of failure to meet assumptions, MOD-AGE uses nonparametric methods. We applied a Monte Carlo simulation to the model age and the depth values based on the real distribution of the tracked data (activities, atomic ratios, depths, etc.). Several fitting methods could be applied for estimating the relationships, but after several tests, we decided to use the LOESS method (locally weighted scatterplot smoothing).

## 2. Basic ideas and assumptions

The construction of the age–depth model is a case of general problem – the estimation of the relation between two values known from measurements. Both variables are subject to measurement uncertainties. In order to build an adequate model, three major problems must be solved:

(i) the method used must be capable of taking into account the uncertainties of both variables;
(ii) the method used should allow the use of the stratigraphic information describing the sample position in the profile;
(iii) the method used must allow the determination of not only the best age–depth relation, but also its confidence interval.

Additionally, the best-fitting method for modeling must be chosen. The method chosen should reflect the real relationship between the modeled parameters (age and depth) and be as simple as possible. The criteria for evaluating the model must be clearly defined. The model should meet the following criterion: simplest possible solution, compatibility with experimental data (sample age and positions in the profile), in terms of their uncertainty.

## 3. MOD-AGE algorithm

The MOD-AGE algorithm is used for estimating the relation between two variables determined by measurements. In the case of age–depth modeling, there are two variables: depth and age. A normal distribution has been assumed for the depth measurements (distances from the base). The measurement uncertainty of the depth can be estimated by repeating the depth measurement for a given point many times. The age distribution is determined by examining either the atomic ratios (MC-ICPMS, TIMS) or activities (alpha spectrometry). It is possible to estimate the age distribution using Monte Carlo methods by assuming a normal distribution for the basic measurements and using a standard procedure for age estimation.

In the U-series method, age is calculated on the basis of the activity ratios ($^{230}Th/^{234}U$ and $^{234}U/^{238}U$). The measurements of activities or atomic ratios vary in terms of their counting methods (alpha spectrometry or mass spectrometry, respectively) and are used as the basic data for the MOD-AGE algorithm (Fig. 1A). A normal distribution is assumed to describe these measurements (Fig. 2A). Applying the Monte Carlo method enables the MOD-AGE algorithm to estimate the real age distribution (Fig. 1A–C). An age–depth model is built using this real age distribution. The age distribution of young samples is similar to the normal distribution. However, the age distribution of older samples tends to be skewed. For any randomly selected dataset (depths and atomic ratios/

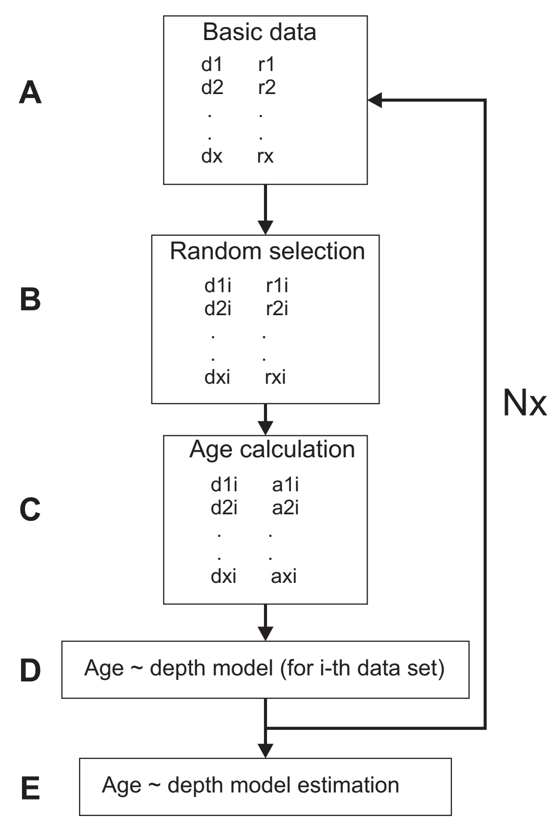


**Fig. 1.** Schematic diagram of the MOD-AGE algorithm. A – basic data; B – random selection from the probability distributions describing the measurement results; C - age calculations using randomly selected data; D – age–depth model calculations for ages and depths from random selections; E – final age–depth model with confidence band estimation. Dp, IZO – basic measurement results of the depth and isotope data respectively, which are assumed to be normally distributed. Dp1i, Izo1i, Dp2i, Izo2i… – random i-th realization of the depth and isotope measurements. Ag1i, Ag2i… – ages calculated for i-th dataset. N – number of random selections.