EarthChem Workshop on Geochronology for (U-Th)/He

University of Kansas, Lawrence, Kansas 66045
May 10, 2007, 8:30am to 3:30 pm

Report compiled by Doug Walker, Peter Reiners, and Dan Stockli.

Participants:
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Background
EarthChem is a community driven project to facilitate the compilation and dissemination of geochemical data of all types. The project is active at building a home for future data contributions by working with authors, societies, and publishers as well as government organizations. In addition, the EarthChem project responds to community needs to facilitate compiling and serving data.

A recently identified community need is in the area of geochronology. At the GeoEarthScope town hall meeting held in association with the 2006 GSA National Meeting in Philadelphia, attendees discussed the necessity of a home for geochronology and thermochronology data collected by that project. Consensus opinion of attendees and organizers was that EarthChem should be the group to provide management for data collected in association with GeoEarthScope, storing and serving geochronological data submitted by participating facilities. Such a management system would be useful to other workers. EARTHTIME, for example, strongly endorses EarthChem's leadership in this regard and will work to encourage members to contribute data. This emphasis was endorsed by the EarthChem advisory board at its 2006 annual meeting.

To move this effort forward, several small workshops are planned for 2007 to ensure that the proper standards for data and metadata reporting are enforced. To this end, EarthChem is working with experts in the field of U-Pb geochronology (who are also connected with the EarthTime effort) in an April meeting, and experts at (U-Th)/He geochronology/thermochronology at a May meeting. Additional meetings for Ar-Ar and cosmogenic nuclide dating are in the planning stages. This report gives the results of the (U-Th)/He workshop.

Goals
Goals of the meeting were to address important issues for creating a home for geochronology and thermochronology data related to (U-Th)/He.

a. Establish reporting requirements including metadata and classes of measure values.
b. Identify and evaluate methods of data entry and output that will work for the geochronology community.
c. List the important requirements of a geochronology website.
d. Plan approaches and actions for moving forward with the effort.

Workshop Summary

The workshop group focused most of its effort on identifying the important items that must be reported for (U-Th)/He geochronology and thermochronology results. This is presented as a large table at the end of the report. The community involved with (U-Th)/He is still relatively small. However, individual laboratories are extremely productive, so that data providers present a high-density opportunity for getting data into any system. In addition, the nature of (U-Th)/He analyses are such that the technique (like Ar-Ar) is applicable to both geochronology and thermochronology. For simplicity, we refer to geochronological applications below, recognizing the added aspect of thermochronology.

The group addressed the need for an easy path for data entry. Although contributors to a database can enter parameters directly into a spreadsheet or web-based form, the group considered that the most appropriate route would be to take output directly from data reduction programs/spreadsheets. Because of the limited number of groups involved in (U-Th)/He, it is possible that each group's data reductions forms (currently universally done in Excel) could be parsed into the system. Creation of a new, general-purpose reduction program is also a priority for the group. Participants also defined numerous features important to a (U-Th)/He website. These features include data display, data download, and query functions. Visualization using maps and standard diagrams are important to users and to making the data accessible.

Participants created several different *approaches* to making progress on the creation of a geochronology database within EarthChem. These approaches are general goals and aspects of the effort. These approaches were then fit into a plan of *next steps* to be taken over the rest of 2007 and the first half of 2008 to move the effort forward.

Approaches

A basic recommendation of data reporting should be an IGSN for each sample and subsample (mineral separate, aliquot, etc.). To this end, the data entry system will ask for the IGSN identifier. This can be done with a link to the SESAR site during data entry/upload if the IGSN is not present. It is important that users be able to establish their own IGSN for host samples in the field. This may take some work with the SESAR group, but was deemed very desirable so that users/collectors do not create multiple sample identifiers (field vs. IGSN).

One of the most arduous tasks for contributors is to enter data into any system. For (U-Th)/He geochronology many important data parameters are required to make full use of the data. For that reason, the group recommended emphasizing data entry directly from data reduction Excel workbooks. The group recommends that a common output format be established that can be uploaded containing items with controlled vocabulary. This is given in the attached table of important values.

The database itself will be built on XML using a schema that preserves the critical data and metadata (see attached table). This will allow other parties to access the data through the XML if needed; the creation of the XML schema is critical to maintaining interoperability. The group understands that the (U-Th)/He geochronology database will be one of several such geochronology systems. The interoperability of these systems is important for future inquiry. The use of an IGSN identifier will ensure that samples can be tied together in the future. For example, the participants considered the potential value in comparing high- and low-temperature chronometer ages especially appealing, in light of the potential to make powerful new interpretations of locations and regions.

Lastly, the user interface needs to allow complex queries and tailor the output of such queries to the need of the user. For this reason, the interface must allow for simple display and download for casual/non-geochronologist users (probably the vast majority) and complete and rich interactions for experts.

Next Steps

Considering the approaches listed above, the participants recommended the following next steps to move the process of creating a geochronology database. We anticipate that these steps will be done over the next 6 to 18 months.

1) Prepare and circulate the report of this workshop. The report will be posted on the EarthChem, KU and Arizona lab websites as well as being emailed to a list of critical data providers (including most (U-Th)/He geochronologist and the EarthChem advisory board). This will allow for community comments on the critical reporting items included in the attached table. Dan Stockli and Peter Reiners will lead this effort and will consult with Ken Farley about the nature of the data reporting.

2) Start developing the XML schema. This will be done by taking the list of critical items (see table) combined with some sample data to create a structure. The schema should allow for efficient search and retrieval. The schema will be normalized to the extent needed by the amount and complexity of potential data. Exploration of existing schemas (such as OGC, GeoSciML, and GfG) will be done to further foster interoperability. Jason Ash and Eileen Jones (EarthChem programmers) will work on this effort in conjunction with Dan Stockli who will provide reduction program output.

3) Explore developing a data reduction program of wide appeal, which will be distributed freely to the community. This will form the basis for data entry into the geochronology and thermochronology system. Stockli will take the lead on this effort.

4) Prototype a (U-Th)/He geochronology website. This may be stand-alone or, more likely, be part of an integrated geochronology website. Many components may be built off existing components of the EarthChem site. Eileen Jones and Jason Ash will start this.

5) Integrate programs from both individual users and the Mineralogical Society of America website (http://www.minsocam.org/MSA/RIM/software_rim58/) for interpreting thermochronologic data, with the EarthChem website. Make data output generated files in compatible formats for these programs. Explore implementing any programs directly on the website. Basic plotting will include graphs such as age vs. U/Th, age vs. effective U concentration, elevation vs. age, PDF plots of age, contour maps of ages, and time-temperature histories using nominal kinetics.

Supporting Materials

Nature of website output and user interaction.

1. *Because many routine (U-Th)/He methods rely on multiple replicate analyses of individual samples, a helpful user interface would include methods for quickly visualizing ages in the context of histogram, probability density, and cumulative probability plots. Methods for calculating weighted mean ages and uncertainties, easily adapted for user preferences, would also be helpful. Other quick plotting tools that could be considered include the relationships between age and parent or daughter nuclide contents, crystal/grain/aliquot mass or size, or other measured attributes provided in the on-line data. Ideally, the output from these plotting tools would at least have the aesthetic standards of typical IsoPlot output, and also be easily exported to other graphics programs for custom modification.*
2. *Qualitative judgements of crystal/grain suitability for (U-Th)/He dating methods is often important. For this reason it would be nice if users could easily download a reasonably-sized (e.g., <200 kbyte) image/photomicrograph of each aliquot associated with a datafile.*
3. *Commonly used interpretational software for (U-Th)/He (and other thermochronologic) data include HeFTy, TERRA, BINOMFIT, and other programs (e.g., http://www.minsocam.org/MSA/RIM/software_rim58/). Being able to export (U-Th)/He data directly from the EarthChem website into formats ready to upload into these programs would benefit rapid and versatile interpretation.*

EarthChem Workshop on Geochronology – (U-Th)/He

Nichols Hall, University of Kansas – May 10, 2007

Agenda

8:30	Overview of Geoinformatics and examples. Demonstration of NAVDAT and EarthChem systems.
9:30	Discussion of reporting requirements for (U-Th)/He data. What are the critical items that must be reported? Can we link to IGSN/SESAR for sample information?
11:00	Demonstration of NAVDAT data entry.
11:15	Discussion of how data entry and submission should work for geochronology. Do we need digital lab books? How do legacy data and new data differ? Do data reduction programs contain enough metadata? What level/depth of data documentation is needed or desirable?

Lunch (1:00 – 2:15)

2:15	Nature of (U-Th)/He geochronology/thermochronology website and geochronology websites in general. What ways do providers and users want to interact with the data? Is it critical to allow reprocessing of data at some level? What sorts of age calculation utilities are needed?
3:00	Wrap up and listing of goals. Identify next steps and key providers/users to move the effort forward.

General Comments on Table:
AEC = Alpha Ejection Corrected or Alpha Ejection Correction
C = common parameter applicable to all analyses in an experiment (or batch); I = individual parameter applicable only to one analysis

Item	Type	Units	Use	Comment
General Information about host sample				
Sample Name (IGSN)	text string		C	The sample name refers to the primary sample for which positional, elevation, lithologic and other metadata were established
Sample Metadata (IGSN)	text string		C	The metadata for a sample name include positional, lithologic data, etc. which is captured with the original IGSN designation, or by the host database
Experiment/Batch Name	text string		C	The experiment is a sub-sample of the primary sample name
Experiment/Batch Reference	text string		C	Literature reference for the experiment
Laboratory	text string		C	Laboratory in which the experiment was conducted
Analyst	text string		C	Investigator conducting the experiment
Instrumental Method - He	text string		C	Method used to analyze He
Instrumental Method Reference - He	text string		C	Reference for He analysis method
Instrumental Method - U-Th-Sm	text string		C	Method used to analyze U-Th-Sm (e.g., ICPMS, ID-TIMS)
Instrumental Method Reference - U-Th-Sm	text string		C	Reference for U-Th-Sm analysis method
Alpha Ejection Correction Method	text string		C	Method used for AEC
Alpha Ejection Correction Method Reference	text string		C	Reference for method used for AEC
Comment	text string		C	Text string accommodating a description of any aspect of the sample or experiment
Interpreted Sample Age Information				
Preferred Age Type	text string		C	The preferred Age Type for the experiment sub-sample as intrepreted and stated by the author; Age Types include the list below
Preferred Age	numeric	Ma	C	The preferred Age for the experiment sub-sample as intrepreted and stated by the author
Preferred Age Error	numeric	Ma, absolute 2-sigma	C	The error on the preferred age
Preferred Age Explanation	text string	string	C	A text string describing the details of the preferred age interpretation
Age Type	text string		C	There can be more than one Age Type per Experiment; Age Types include the list below
Age	numeric	Ma	C	"Age" combines one or more analyses into an age interpretation for the Experiment; there can be more than one Age per Experiment
Age Error (Analytical w/o AEC)	numeric	Ma, absolute 2-sigma	C	Analytical error includes counting statistic uncertainties, mass fractionation uncertainties, blank and tracer subtraction uncertainties (without AEC uncertainties)
Age Error (Analytical w/ AEC)	numeric	Ma, absolute 2-sigma	C	Analytical error includes counting statistic uncertainties, mass fractionation uncertainties, blank and tracer subtraction uncertainties (with AEC uncertainties)
Age Error (Systematic)	numeric	Ma, absolute 2-sigma	C	Systematic error includes decay constant uncertainties, tracer calibration uncertainties, and calibration uncertainty.

MSWD	numeric		C	Mean Squared Weighted Deviation
Included Analyses	text string		C	Those analyes included in a given Age
Comment	text string		C	Text string accommodating a description of any aspect of the interpreted sample age information
Age types = weighted mean of mulitple aliquots (AEC), maximum age of population (AEC), minimum age of population (AEC), age mode of population (AEC), weighted mean of mulitple aliquots (raw), maximum age of population (raw), minimum age of population (raw), age mode of population (raw)				
Decay Constant Parameters				
238U Decay Constant	numeric		C	
238U Decay Constant Error	numeric	% 1-sigma	C	
235U Decay Constant	numeric		C	
235U Decay Constant Error	numeric	% 1-sigma	C	
232Th Decay Constant	numeric		C	
232Th Decay Constant Error	numeric	% 1-sigma	C	
230Th Decay Constant	numeric		C	
230Th Decay Constant Error	numeric	% 1-sigma	C	
147Sm Decay Constant	numeric		C	
147Sm Decay Constant Error	numeric		C	
238U/235U	numeric		C	
Decay Constant Reference	text string		C	Literature reference for the utilized decay constants
Comment	text string		C	Text string accommodating a description of any aspect of the utilized decay constants
Data Reduction Parameters				
Spike Type U-Th-Sm	text string		C	Isotope dilution tracer used in ID analysis
Spike Type He	text string		C	Isotope dilution tracer used in ID analysis
Standard Mineral	text string		C	Mineral standard used as an external check on accuracy and reproduceability
Standard Mineral Reference	text string		C	Literature reference for the age standard
Standard True Age	numeric	Ma	C	Accepted (true) age of standard
Standard True Age Error	numeric	abs., 2-sigma s.d.	C	Uncertainty in accepted (true) age of mineral standard
Standard Measured Age	numeric	Ma	C	Measured age of mineral standard
Standard Measured Age Error	numeric	abs., 2-sigma s.d.	C	Uncertainty in accepted (true) age of mineral standard
Comment	text string		C	Comment on the data reduction parameters used in the experiment
Analysis Information				
General				
Analysis (Aliquot) Name	text string		I	An analysis is a sub-sample of the experiment sample name, and is thus a sub-sub-sample of the primary sample name
Grain Image	file	(CL, BSE, Optical, etc.)	I	Link to image file illustrating the aliquot comprising the analysis (multiple for mult-grain aliquots)
Time Stamp	date		I	Time of analysis
Mineral/Phase	text string		I	e.g. zircon, xenotime, monazite, apatite, titanite, rutile, calcite, whole rock, other
Setting	text string		I	(in situ, laser, furnace, flux, foil type)
Number of Grains	numeric		I	Number of grains dissolved for analysis; useful for queries of "single-grain" analyses

Grain Length	numeric	mm, µm	I	Measured Length of mineral grain (multiple for mult-grain aliquots)
Grain Width 1	numeric	mm, µm	I	Measured Length of mineral grain (multiple for mult-grain aliquots)
Grain Width 2	numeric	mm, µm	I	Measured Length of mineral grain (multiple for mult-grain aliquots)
Weight	numeric	mg, µg	I	Weight of the grain(s) analyzed
Physical Abrasion?	boolean		I	Was the grain(s) used for analysis physically abraded prior to dissolution?
Alpha Ejection Correction?	boolean		I	Was an AEC applied
He measurement description	text string		I	ID, peak height, gettered, cryogenic purification
Dissolution technique	text string		I	Acid dissolution (type and mixture), pressure vessle digestion (unwrapped, wrapped), flux melting, etc
U-Th-Sm measurement description	text string		I	ID, peak height, column chemistry
Comment	text string		I	Text string accommodating a description of any aspect of the analysis
Compositional				
U	numeric	atoms, pg, moles, ppm	I	U concentration of analysis
U Error	numeric	atoms, pg, moles, ppm, %, abs., 1-sigma	I	Uncertainty in U concentration of analysis
Th	numeric	atoms, pg, moles, ppm	I	Th concentration of analysis
Th Error	numeric	atoms, pg, moles, ppm, %, abs., 1-sigma	I	Uncertainty in Th concentration of analysis
Sm	numeric	atoms, pg, moles, ppm	I	Sm concentration of analysis
Sm Error	numeric	atoms, pg, moles, ppm, %, abs., 1-sigma	I	Uncertainty in Sm concentration of analysis
He	numeric	atoms, ncc@stp, moles	I	He concentration of analysis
He Error	numeric	atoms, ncc@stp, moles, %, abs., 1-sigma	I	Uncertainty in He concentration of analysis
Blanks				
U Blank	numeric	atoms, pg, moles	I	
U Blank Error	numeric	pg, moles, atoms, %, 1-sigma	I	
Th Blank	numeric	atoms, pg, moles	I	

Th Blank Error	numeric	pg, moles, atoms, %, 1-sigma	I	
Sm Blank	numeric	atoms, pg, moles	I	
Sm Blank Error	numeric	pg, moles, atoms, %, 1-sigma	I	
He Blank	numeric	atoms, ncc@stp, moles	I	
He Blank Error	numeric	pg, moles, ncc@stp, atoms, %, 1-sigma	I	
Comment	text string		I	Text string accommodating a description of any aspect of the analysis
Radiogenic Age				
(U-Th-Sm)/He Age (Raw)	numeric		I	Age Calculated without AEC
(U-Th-Sm)/He Age Error (Raw)	numeric	(abs. 2-sigma)	I	Age Error Calculated without AEC
(U-Th)/He Age (Raw)	numeric		I	Age Calculated without AEC
(U-Th)/He Age Error (Raw)	numeric	(abs. 2-sigma)	I	Age Error Calculated without AEC
(U-Th-Sm)/He Age (AEC)	numeric		I	Age Calculated with AEC
(U-Th-Sm)/He Age Error (AEC)	numeric	(abs. 2-sigma)	I	Age Error Calculated with AEC
(U-Th)/He Age (AEC)	numeric		I	Age Calculated with AEC
(U-Th)/He Age Error (AEC)	numeric	(abs. 2-sigma)	I	Age Error Calculated with AEC
Disequilibrium Corrected?	boolean		I	Was a disequilibrium correction applied to the AEC data
Disequilibrium Method	text string		I	What method was used for disequilibrium correction
Comments	text string		I	
Alpha Ejection Correction Parameters				
Morphology	text string		I	Assumed morphology (e.g., sphere, tetragonal or hexagonal prism with pinacoidal or pyramidal terminations, irregular, etc.)
Surface Area	numeric		I	Computed from morphology and measurements
Volume	numeric		I	Computed from morphology and measurements
AEC/Ft weighted	numeric	% 1-sigma	I	
AEC/Ft weighted homog?	boolean		I	
AEC/Ft numerical	numeric	%/amu	I	
AEC/Ft numerical homog?	boolean	% 1-sigma	I	
147Sm included in AEC/Ft?	boolean		I	
AEC/Ft uncertainty	numeric		I	Qualitative estimates applied to AEC/Ft
AEC/Ft uncertainty comment	text string		I	
Zonation Information	text string		I	
Zonation Data	file		I	
Numerical AEC/Ft Information	text string		I	Information about numerical approach to AEC/Ft if used
AEC/Ft Applied to parents?	boolean		I	Was the AEC/Ft applied to parents rather than age/He
Comments	text string		I	