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Foreword

The Geo-mapping for Energy and Minerals (GEM) program is laying the foundation for sustainable economic development in the North. The Program provides modern public geoscience that will set the stage for long-term decision making related to investment in responsible resource development. Geoscience knowledge produced by GEM supports evidence-based exploration for new energy and mineral resources and enables northern communities to make informed decisions about their land, economy and society. Building upon the success of its first five-years, GEM has been renewed until 2020 to continue producing new, publically available, regional-scale geoscience knowledge in Canada's North.

During the summer 2016, GEM program has successfully carried out 17 research activities that include geological, geochemical and geophysical surveying. These activities have been undertaken in collaboration with provincial and territorial governments, northerners and their institutions, academia and the private sector. GEM will continue to work with these key collaborators as the program advances.

Project Summary

Sedimentary basins can host numerous types of mineral and petroleum deposits and temperature history is a key parameter for assessing and exploring for these resources. Multi-kinetic apatite fission track (MK-AFT) thermochronology is a powerful and rapidly-evolving state-of-the-art technique for reconstructing the low temperature (<200°C) thermal history of sedimentary basins within the upper 4-6 km of the Earth's surface. It exploits the experimentally-observed, composition-dependent temperature sensitivity of AFT parameters to resolve more details of the thermal history than the conventional methods currently used by the thermochronology community. New methods of data interpretation and modelling have been developed at GSC Calgary and are being applied to the study of northern Canadian basins where multi-compositional detrital apatite grains are common in sedimentary rocks such as sandstone. This report discusses some of the procedures that are used and presents MK-AFT thermal modelling results for an example in the northern Yukon, a geologically complicated region where much of the stratigraphic record has been removed by erosion. The MK-AFT method is able to resolve multiple thermal events in the study area because it treats different apatite compositional groups as separate thermochronometers that are sensitive to different parts of the thermal history.

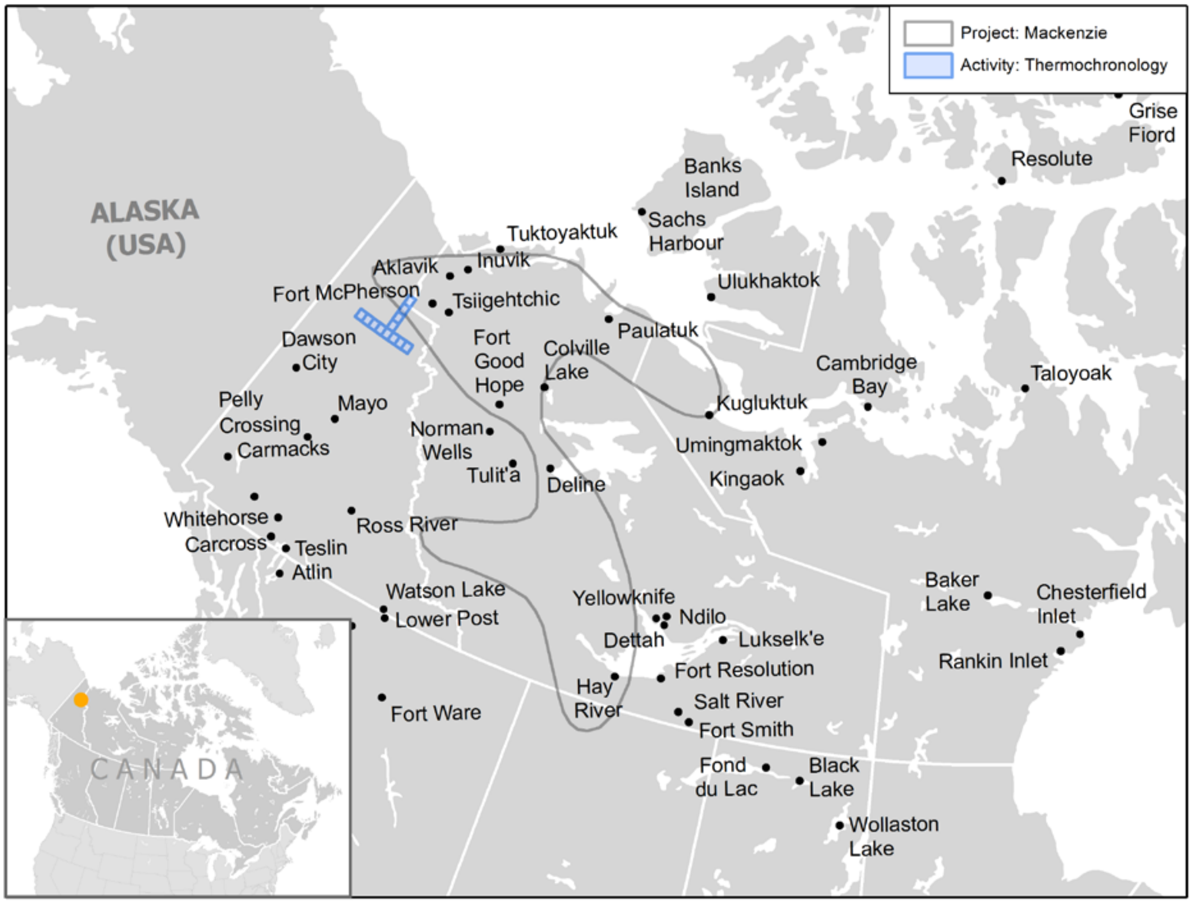

Figure 1: Current thermochronology modelling transects under this activity.

Introduction

Although MK-AFT studies are in progress in the Northwest Territories in the Mackenzie Delta region and in areas to the south, the main focus of activity for the current fiscal year (FY) has been in northern Yukon along transects (shown in blue in Figure 1) through the Peel Plateau, Eagle Plain and Richardson Mountains. Two AFT sample sets from the study region were processed in FY 2015-16 and the resultant data are the subject of study for the current FY. Multi-parameter data were acquired in close consultation with the laboratories in order to try and optimize the amount of information that can be extracted from these complicated samples. Data for 12 cuttings samples from three wells in Eagle Plain were received initially in May 2015 but careful examination of the data indicated that further work was required. The data were reprocessed and supplemented with additional data from extra sample aliquots and these new data were received in December 2015. Data for a second sample set consisting of 9 mainly outcrop samples from northern Yukon were received in March 2016. Final interpretations and modelling results for these two data sets will be published in scientific journals and corresponding data will be published in GSC Open File reports. In addition, during the previous FY, 12 legacy northern Yukon samples (data collected during 2011-2013) were interpreted and modelled. Preliminary results document a significant Carboniferous thermal event related to Ellesmerian foredeep deposition for a sample from the southern Richardson Mountains (Lane *et al.*, 2015).

The goal of this study is to acquire regional high-resolution thermochronology data to constrain the burial/exhumation and thermal history of this geologically complicated area. MK-AFT samples from this region are able to resolve multiple thermal events that occur between 50°C to 200°C, a temperature range that encompasses petroleum generation reactions and certain mineralization processes. Currently no other low-temperature thermochronology methods can operate over such a broad temperature range.

Review of Activities

Much of the activity for the current FY involved compiling and processing of AFT data (generated by GeoSep Services, LLC of Moscow, Idaho) and apatite elemental data (Electron Probe Microanalysis (EPMA) Laboratory of Washington State University), calculating annealing kinetic parameters for individual apatite crystals using the elemental data, and correlating these values with measured AFT age and length parameters to define statistical kinetic populations that are treated as separate thermochronometers for thermal modelling. Preliminary interpretations are complete for most of the FY 2015-16 samples but a few samples still require additional supporting data (which is forthcoming) before interpretations can be finalized. Although AFT age and length measurements are performed on the same apatite grain mount for each sample, the lab data were sent in different files with different grain numbers for each set of measurements. Therefore, x-y coordinate data for age and length measurements were requested from both laboratories so that the apatite grain location data could be used to identify which grains on the sample mounts had duplicate elemental analyses associated with age and length measurements performed on the same grain. These duplicate grain analyses provide important information on typical errors for kinetic parameter values, they help to compensate for some missing or poor elemental data and, by linking age and length measurements to the same grain, they provide more confidence that grains have been sorted into the correct kinetic population. As a result, preliminary kinetic population interpretations were adjusted for each sample based on the new information gained from using the x-y coordinate data. Similarly, x-y coordinate files have been retrieved for the 2011-2013 AFT data and previous interpretations are being refined as necessary prior to publication of the results. Laboratory procedures have been modified so that duplicate grain identifications will be included with future data sets. Model setup files have been prepared for most of the 2015-16 samples and the next step will be to begin modelling the data to extract thermal history information.

Methodology

Conventional AFT methods and applications have been described in numerous publications (e.g. Wagner and Van den Haute, 1992; Gallagher et al., 1998; Gleadow et al., 2002). Apatite grains are common in the heavy mineral fraction of sandstones and they contain trace amounts of ^{238}U that can undergo fission decay through geological time to produce fission tracks. Fission tracks are linear regions of crystal damage that can be observed using an optical microscope after chemical etching of the tracks. Typically AFTs form with an initial etchable length of approximately 16 μm (depending on mineral chemistry) but undergo length reduction (thermal annealing) with increasing temperature. AFTs are only stable below a composition- and heating/cooling rate-dependent total annealing temperature. Any pre-existing AFTs are erased at temperatures higher than the total annealing temperature. At temperatures below the total annealing temperature, AFTs are retained but their length depends on the thermal history they experienced. Track formation is a continuous process and therefore apatite grains from geological samples contain a distribution of AFT lengths that provide information on maximum temperature and the style and rate of cooling. For a given apatite composition, the oldest tracks are the shortest and have experienced more of the thermal history than the longer, more recently formed tracks. AFT ages are determined using observed track densities but they can be difficult to interpret for sedimentary apatite grains where slow cooling and reheating commonly results in "partially annealed" track lengths and reduced AFT ages. Rather than trying to directly interpret these AFT ages, thermal history information can be extracted from AFT age and length parameters using an appropriate thermal annealing model.

Conventional AFT analysis is based on the interpretation and modelling of a statistically uniform population of apatite crystals within a sample. An inherent assumption is that all crystals in a statistically uniform population behave similarly when exposed to the same thermal history and therefore probably have a similar composition. A χ^2 statistical test is used to assess whether a set of single grain AFT ages could belong to a uniform population. Data interpretation and modelling techniques are well established for single apatite populations and are routinely applied to samples that pass the χ^2 test. However, it should be noted that results of the χ^2 test depend on the precision of single grain ages. Compositionally-variable apatite crystals may still pass the χ^2 test if the single grain ages have low precision (e.g., low U concentration and a low numbers of track counts) and/or there has been minimal annealing. When AFT grain ages are overdispersed (variance of the grain ages is greater than expected for the analytical error), samples fail the χ^2 test and conventional methods can break down. Although analytical error may sometimes be a contributing factor, the most common and likely reason for AFT age dispersion is the geological variability of mixed apatite populations related to composition-dependent thermal annealing (e.g. Carlson *et al*., 1999; Ketcham *et al*., 1999; Barbarand *et al*., 2003) and/or the variable provenance of detrital apatite grains. Mixed AFT populations are the normal situation for Phanerozoic sedimentary samples from northern Yukon and the Northwest Territories and, unlike conventional AFT analysis, there are no general published procedures for dealing with these types of samples. Therefore, methods for interpreting and modelling these samples were developed in-house.

AFT age data were acquired using the newer LA-ICP-MS method (Hasebe et al. 2004; Donelick et al. 2005; Chew and Donelick 2012) which measures U content directly and avoids exposing the sample to thermal neutrons in a nuclear reactor which is required by the well-established and widely used external detector method (Fleischer et al., 1964; Hurford and Green, 1982). Apatite grains were etched to obtain measurements of the density of spontaneous AFTs intersecting the polished mineral surface. Following age measurement, apatite grain mounts were irradiated with ^{252}Cf and re-etched to increase the number of observed horizontal confined tracks for length measurement by creating more etchant pathways (Donelick and Miller, 1991). D_{par}, a measure of AFT etch figure size (Donelick, 1993), is a commonly used proxy annealing kinetic parameter because of the relationship between apatite solubility and composition. These data are easy to acquire and were collected along with AFT age and length measurements at the microscope. The most commonly used AFT annealing kinetic parameters, Cl content and D_{par} (Donelick *et al*., 2005), are unable to account for the AFT age dispersion observed in samples from northern Yukon. Therefore detailed apatite elemental data were obtained to investigate how apatite composition may be influencing AFT annealing. Apatite elemental data were received from Washington State University as weight % oxide values and these were converted to atoms per formula unit (apfu) values using in-house software (PROBECAL). The apfu values were used to calculate r_{mr0} kinetic parameter values (Carlson et al., 1999) which are expressed as an effective Cl value (apfu) using the r_{mr0}-Cl equation of Ketcham *et al*. (1999). Effective Cl values can be considerably higher than measured Cl values because other cations and anions such as Fe, Mn, Mg and OH are incorporated into the r_{mr0} calculation and contribute to AFT retentivity.

AFT age and length data were received as separate files and were compiled into multi-worksheet Excel spreadsheets along with the elemental data and calculated r_{mr0} and effective Cl values. The r_{mr0} values were matched with corresponding age and length measurements, incorporating any information from duplicate grain analyses obtained from x-y grain coordinate data where possible. Single grain age data were analysed using the latest version of the RadialPlotter program of Vermeesch (2009) which displays single grain ages according to their relative precision and estimates statistical age populations. Single grain ages and track lengths were sorted and plotted with respect to effective Cl values in order to determine statistical AFT kinetic populations for modelling. Final interpretations took into consideration multiple factors that included the results from RadialPlotter, calculated χ^2 values for sorted grain ages, the quality of the elemental data, the characteristics of other samples in the region, and typical errors associated with kinetic parameters that can contribute to population overlap.

We use an extensively modified and upgraded version of the custom modelling software (AFTINV) of Issler (1996) and Issler *et al*. (2005) to extract thermal history information from AFT data. AFTINV is based on the inverse monocompositional AFT model of Willett (1997) and it has been extended to include the multi-kinetic annealing formulation of Ketcham *et al*.

(1999). The model uses a non-directed Monte Carlo method to search for thermal histories that provide statistically acceptable fits to AFT parameters. Geological constraints on temperature and heating/cooling rates can be applied to limit the model search space. Model input parameters and constraints are set up in an Excel spreadsheet and a model pre-processing program, PREAFT, is used to set up a model run. The model constructs random thermal histories as a combination of piecewise thermal history segments representing different thermal history styles over specified time ranges. Examples of thermal history styles include: random heating followed by random cooling (to simulate the effects of burial/exhumation); random cooling (e.g., exhumation of apatite from source area prior to deposition); random heating (e.g., heating only to represent burial of preserved stratigraphic sections); and various other combinations. Thermal maturity data such as percent vitrinite reflectance (%Ro) can be used to help constrain paleotemperatures by using a kinetic model (Nielsen et al., 2015) to calculate %Ro values from the time of deposition to the present for comparison with measured values. AFTINV allows for simultaneous solution of up to four different AFT statistical kinetic populations. Thermal history results are presented as a time-temperature envelope defined by typically 300 statistically-acceptable Monte Carlo solutions (envelope boundaries are not valid solutions) and a smoothed, good-fitting representative thermal history calculated as the exponential mean of the Monte Carlo solutions.

Example Thermal History Result

In this example, a Late Devonian sandstone from Eagle Plain, Yukon at the locality shown in Figure 2 yielded abundant apatite grains with diverse chemistry. Thirty-six single grain AFT ages and 200 track lengths with composition data were used to define two statistical kinetic populations with pooled ages of 144 and 238 Ma, and corresponding mean track lengths of 11.65 and 12.74 μm, respectively (Fig. 3). The nearly 100 Ma difference in population ages and the > 1 μm difference in mean lengths implies that these populations have substantially different annealing kinetics. Elemental data were acquired using the LA-ICP-MS method and, because F cannot be measured using this technique, OH content could not be estimated. Although the populations are reasonably well-defined and pass the χ^2 test ($Q \geq 5\%$), the lack of OH data affects calculated r_{mr0} values and this contributes to some scatter and population overlap which reduces goodness-of-fit probabilities (Q). Similar results were obtained for another sample from the same stratigraphic unit in the area but with elemental data that were acquired using EPMA; these populations are better defined with minimal overlap and high Q values. Both samples have very similar compositions with the higher retentivity population being associated with elevated concentrations of Na, Fe, Cl and Ce, and to a lesser extent, Sr, Mn and Mg. EPMA data indicate that OH contents are quite variable with some very high values of OH (> 0.6 apfu) associated with retentive grains. Effective Cl values are reduced by approximately 0.08 apfu, on average, due to the unavailability of OH data for the r_{mr0} calculations for this example.

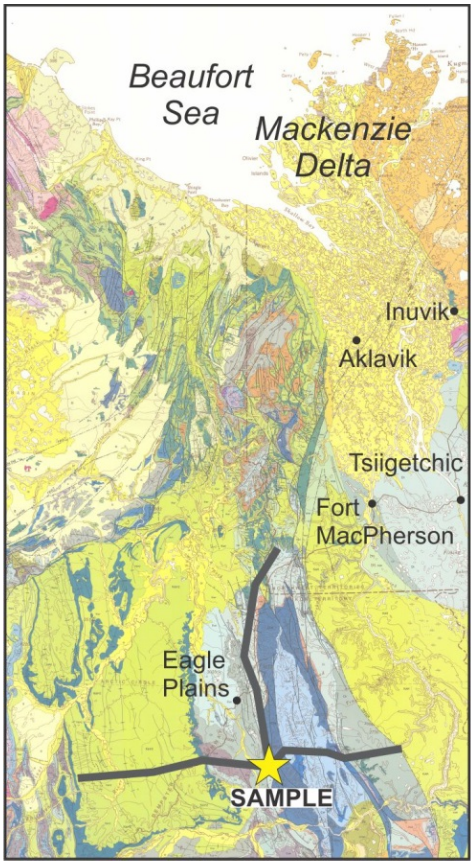

Figure 2. Location of Late Devonian sample (near western margin of Richardson Mountains) used in the example discussed in the text (after Norris, 1984). Heavy lines represent thermochronological transects generalized in Figure 1.

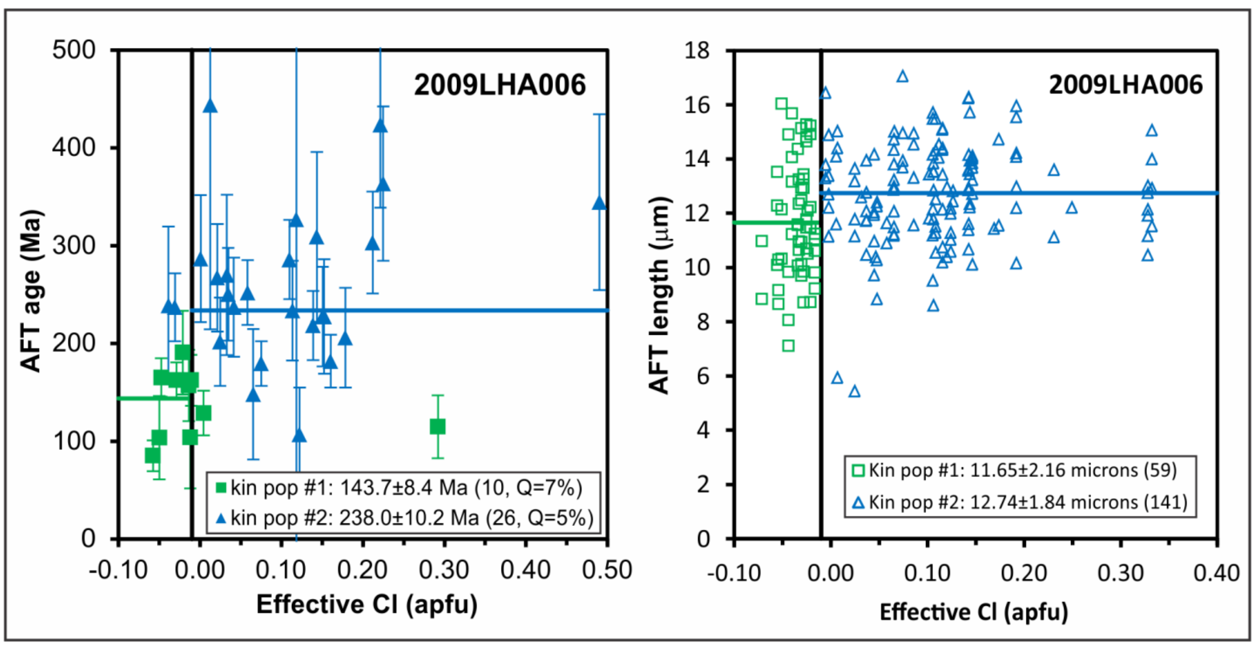

Figure 3. Characterization of two statistical AFT kinetic populations for the Devonian sandstone sample. AFT single grain ages and lengths are grouped according to calculated effective Cl values (derived from r_{mr0}) for kinetic populations 1 (solid and open green squares) and 2 (solid and open blue triangles). Errors on ages are one standard deviation.

An example of a multi-kinetic modelling result is shown in Figure 4. First, careful documentation of the geological setting is required as input to the modelling software. This provides useful information to limit the modelling space interrogated by the software, improve the resolution of the model, and reduce the run time. For example, a sample of the adjacent shale beds yields an indigenous %Ro value of 1.38, equivalent to a maximum temperature near 175-180°C. Also, within the area, ~5 km of overlying Devonian to Permian strata are preserved beneath the sub-Cretaceous unconformity. This indicates that subsidence and heating dominated the post-depositional history into Permian time. Thin remnants of Triassic strata are preserved in places within the region, suggesting there was a phase Triassic burial of unknown significance. The preserved Cretaceous section (Barremian to Cenomanian ages are documented in the area) indicates a second period dominated by deposition, subsidence and heating. Only the post-depositional history, in this case, younger than 375 Ma (black arrow in Fig. 4), has geological relevance for this model because annealing has obscured the provenance history.

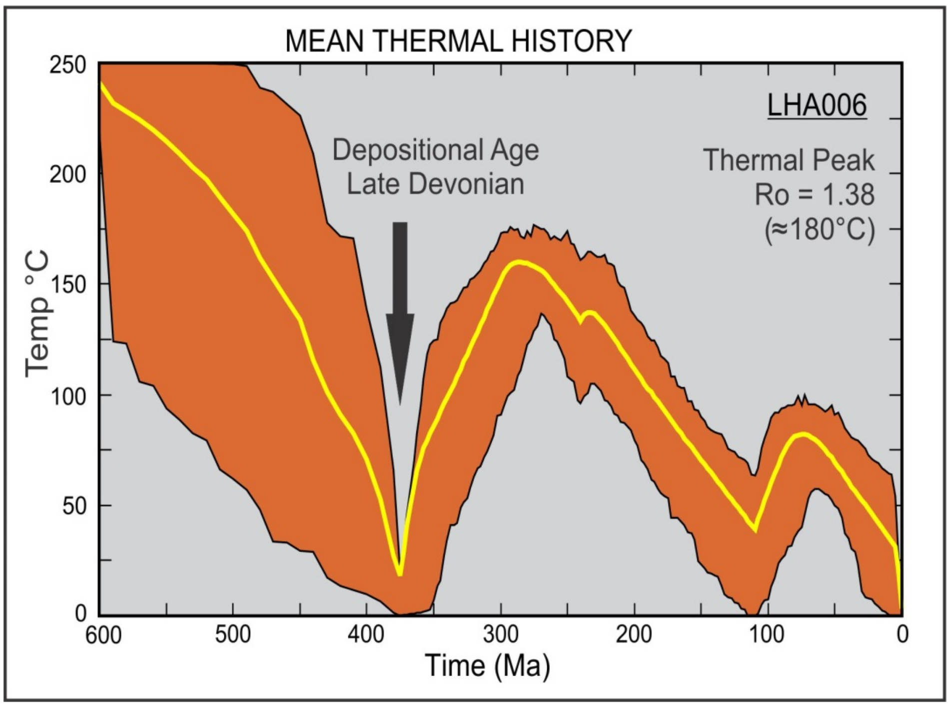

Figure 4. Post-depositional thermal history reveals two main thermal peaks, one in Carboniferous-Permian time and the other in Late Cretaceous-Paleocene time. The early thermal peak is sufficient to generate hydrocarbons, whereas the later peak is potentially within the early stages of the oil window. The secondary peak after 240 Ma is not required to fit the AFT data but is included because thin remnants of Triassic strata in the general area (not at this location) suggest there was a minor phase of Triassic burial superimposed on overall Permian-Early Cretaceous regional exhumation.

Multi-kinetic thermal modelling uses the differential annealing kinetics inherent in the apatite compositional variations to access information contained in their AFT ages and lengths. The more track retentive older AFT population constrains the early thermal peak whereas the least retentive younger AFT population is most sensitive to the younger thermal peak. The model result indicates that the sampled unit was heated to between ~160-175°C through Carboniferous time and remained at elevated temperatures through the Permian and Triassic. Cooling ensued from Late Triassic into Early Cretaceous time, followed by the second sedimentation and heating event through the mid-Cretaceous to Paleocene interval. The youngest thermal peak reflects the end of sedimentation and the onset of Cordilleran deformation affecting the sample area.

Thermal modelling reveals that the Carboniferous-Permian thermal event was sufficient to generate hydrocarbons in Paleozoic rocks in Eagle Plain Basin. The younger event, though less severe, was also potentially within the early stages of the oil window.

Discussion

The AFT samples collected in this study contain mixed apatite populations that cannot be properly interpreted and modelled without detailed elemental data. This situation is likely to be common for most sedimentary basins where there are multiple sources for detrital apatite. Very little work has been published on MK-AFT analysis and therefore a very important part of this study has been methods and model development. This has involved a large amount of data manipulation and analysis to determine the best procedures for processing, interpreting and modelling MK-AFT data. We have been working closely with GeoSep Services (and formerly A to Z Inc.) and the EPMA laboratory at Washington State University to improve data acquisition and analysis procedures in order to be able to process these complicated, multi-parameter data sets more efficiently and to maximize the information available to aid interpretation. AFTINV has been continuously upgraded to accommodate various types of geological situations and sample characteristics that have been encountered during the course of the study.

Expected outcomes of these advanced methodologies include:

- greater resolution of thermal histories;
- improved understanding of basin development and inversion;
- more reliable syntheses of regional tectonic history;
- improved regional geological context for petroleum resource assessments.

Conclusions

The MK-AFT samples of this study require detailed elemental data for their proper characterisation and modelling. The compositionally variable apatites in these samples can be grouped into statistical kinetic populations that can be modelled as separate thermochronometers with significantly different annealing temperatures that enable the resolution of multiple thermal events across the northern Yukon study area. The methods being developed as part of this study should lead to more reliable interpretations of MK-AFT data and more widespread application of this powerful thermochronology technique.

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References

Barbarand, J., Carter, A., Wood, I. and Hurford, T. 2003. Compositional and structural control of fission-track annealing in apatite. Chemical Geology, v. 198, p. 107-137.

Carlson, W.D., Donelick, R.A. and Ketcham, R.A. 1999. Variability of apatite fission-track annealing kinetics: I. Experimental results. American Mineralogist, v. 84, p. 1213-1223.

Chew, D.M. and Donelick, R.A. 2012. Combined apatite fission track and U-Pb dating by LA-ICP-MS and its application in apatite provenance analysis. Mineralogical Association of Canada Short Course 42, p. 219-247.

Donelick, R. 1993. A method of fission track analysis utilizing bulk chemical etching of apatite. Patent No, 5,267,274, U.S.A.

Donelick, R.A. and Miller, D.S. 1991. Enhanced TINT fission track densities in low spontaneous track density apatites using ^{252}Cf-derived fission fragment tracks: A model and experimental observations. Nuclear Tracks and Radiation Measurements, v. 18, p. 301-307.

Donelick, R.A., O'Sullivan, P.B. and Ketcham, R.A. 2005. Apatite fission-track analysis. Reviews in Mineralogy and Geochemistry, v. 58, p. 49-94.

Fleischer, R.L., Price, P.B. and Walker, R.M. 1964. Fission-track ages of zircons. Journal of Geophysical Research, v. 69, p. 4885-4888.

Gallagher, K., Brown, R. and Johnson, C. 1998. Fission track analysis and its applications to geological problems. Annual Reviews of Earth and Planetary Science, v. 26, p. 519-572.

Gleadow, A.J.W., Belton, D.X., Kohn, B.P. and Brown, R.W. 2002. Fission track dating of phosphate minerals and the thermochronology of apatite. In: Phosphates; Geochemical, Geobiological and Materials Importance. M. J. Kohn, J. Rakovan and J.M. Hughes (eds.). Reviews in Mineralogy and Geochemistry, v. 48, p. 579-630.

Hasebe, N., Barbarand, J., Jarvis, K., Carter, A. and Hurford, A.J. 2004. Apatite fission-track chronometry using laser ablation ICP-MS. Chemical Geology, v. 207, p. 135-145.

Hurford, A.J. and Green, P.F. 1982. A users' guide to fission track dating calibration. Earth and Planetary Science Letters, v. 59, p. 343-354.

Issler, D.R. 1996. An inverse model for extracting thermal histories from apatite fission track data: Instructions and software for the Windows 95 environment. Geological Survey of Canada, Open File 2325, 84p.

Issler, D.R., Grist, A.M. and Stasiuk, L.D. 2005. Post-Early Devonian thermal constraints on hydrocarbon source rock maturation in the Keele Tectonic Zone, Tulita area, NWT, Canada, from multi-kinetic apatite fission track thermochronology, vitrinite reflectance and shale compaction. Bulletin of Canadian Petroleum Geology, v. 53, no. 4, p. 405-431.

Ketcham, R.A., Donelick, R.A. and Carlson, W.D. 1999. Variability of apatite fission-track annealing kinetics: III. Extrapolation to geological time scales. American Mineralogist, v. 84, p. 1235-1255.

Lane, L.S., Issler, D.R. and O'Sullivan, P.B. 2015. Late Paleozoic Thermochronology of Northern Yukon: Implications for Phanerozoic Basin Evolution in Northern Canada. GeoConvention 2015: Geoscience New Horizons, CSPG-CSEG-CWLS Annual Convention, Telus Convention Centre, Calgary, May 4-8.

Nielsen, S.B., Clausen, O.R. and McGregor, E. 2015. basin%Ro: A vitrinite reflectance model derived from basin and laboratory data. Basin Research, doi:10.1111/bre.12160.

Norris, D.K., 1984. Geology of the Northern Yukon and Northwestern District of Mackenzie. Geological Survey of Canada, Map 1581A, scale 1:500,000.

Vermeesch, P. 2009. RadialPlotter: A Java application for fission track, luminescence and other radial plots. Radiation Measurements, v. 44, p. 409-410.

Wagner, G.A. and Van den Haute, P. 1992. Fission track dating. Klewer Academic Publishers, Dordrecht, 285p.

Willett, S.D. 1997. Inverse modeling of annealing of fission tracks in apatite 1: A controlled random search method. American Journal of Science, v. 297, p. 939-969.