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Evaluation of the US DOE's conceptual model of hydrothermal activity at Yucca Mountain, Nevada

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Abstract

A unique conceptual model envisaging conductive heating of rocks in the thick unsaturated zone of Yucca Mountain, Nevada by a silicic pluton emplaced several kilometers away is accepted by the US Department of Energy (DOE) as an explanation of the elevated depositional temperatures measured in fluid inclusions in secondary fluorite and calcite. Acceptance of this model allowed the DOE not to consider hydrothermal activity in the performance assessment of the proposed high-level nuclear waste disposal facility. Evaluation shows that validation of the model by computational modeling and by observations at a natural analog site was unsuccessful. Due to the lack of validation, the reliance on this model must be discontinued and the scientific defensibility of decisions which rely on this model must be re-evaluated.

1 Introduction

Yucca Mountain in southern Nevada was studied by the US Department of Energy (DOE) between 1983 and 2005 as a prospective host for the first United States' facility for geological disposal of spent nuclear fuel and high-level nuclear waste. The prolonged period of studies at the site culminated in June 2008 when DOE filed its License Application with the US Nuclear Regulatory Commission (DOE, 2008). In 2009, however, the administration of President Obama decided to terminate the Yucca Mountain project, for reasons purportedly unrelated to the safety or technical suitability of the site (GAO, 2011). Accordingly, in 2010 the DOE filed a motion with Nuclear Regulatory Commission to withdraw the license application. Despite the continued uncertainty regarding the legal standing of this decision, in 2009–2011 the repository program was dismantled and effectively shut down.

At Yucca Mountain nuclear waste was to be emplaced in the thick unsaturated (vadose) hydrogeologic zone. The safety case for the disposal facility rests heavily on the concept that water is and always has been scarce in this zone (i.e., during the last

11.6 myr; DOE, 2008). In the course of the Yucca Mountain site characterization activities, however, mineralogical and geochemical information became available indicating that waters with elevated temperatures (up to 85–90 °C) moved through the unsaturated zone in the past. A conceptual model proposed by the US Geological Survey (USGS) explained these temperatures by the conductive heating of the unsaturated-zone rocks by a large magma body emplaced in the late Miocene (ca. 11 Ma) under the Timber Mountain caldera, some 7–9 km north of the repository site (Marshall and Whelan, 2000).

The purpose of evaluation of the USGS/DOE conceptual model presented in this paper is to establish whether or not validation of the model can be considered successful; in other words, whether or not the model is viable. The need for this evaluation stems from two facts: (1) no formal evaluations of this model have been published; and (2) despite that, the model has become entrenched in the literature, and was relied upon in the decision-making related to high-level nuclear waste disposal in the USA (e.g., Dublyansky, 2007). Evaluation presented in this paper was performed according to a generic protocol for evaluation of geoscientific models (Grewe et al., 2012).

2 Thermal waters in the unsaturated zone of Yucca Mountain

2.1 Paleotemperatures determined from secondary minerals

Volcanic tuffs in the thick unsaturated zone of Yucca Mountain host secondary minerals that are ubiquitous (primarily, calcite and silica). The minerals were initially interpreted as having been deposited from rain waters that had percolated from the surface (Szabo and Kyser, 1990; Paces et al., 2001; Whelan et al., 2001; 2002). Subsequently, however, it was established on the basis of fluid inclusion studies of minerals collected in the ESF tunnel complex (Exploratory Studies Facility, a 7.8 km-long C-shaped tunnel excavated into the host formation of the planned repository) that the minerals were deposited from waters whose temperature reached 85–90 °C (Dublyansky et al., 2001;

Wilson et al., 2003; Whelan et al., 2008). The age of the oldest fluid inclusion temperature (ca. 77 °C) was constrained to 9.4 ± 0.7 Ma by U-Pb dating (Whelan et al., 2008; Table 4). Deposition of the secondary minerals took place at depths of 30 to 300 m from contemporaneous surface of the Mountain. Temperature increases related to a "normal" geothermal gradient would not be expected to exceed ca. 25–28 °C. An important question arose: how to explain the movement of the conspicuously thermal waters through the rock which, according to the accepted geological understanding (e.g., DOE, 2001), had always been a few hundred meters above the water table during the last 11.6 myr?

2.2 Thermal history of Yucca Mountain: what is known?

Cooling of tuffs – The rhyolitic tuffs of the Paintbrush Group that comprise most of the unsaturated zone of Yucca Mountain were emplaced during large-scale silicic eruptions 12.7 myr ago. The cooling of the 350 m-thick sheet of ash-fall tuff from its estimated temperature of emplacement (680–720 °C) to ambient temperatures took about 7000 yr (Buesch and Riehle, 2007). The younger Timber Mountain Group tuffs (ca. 11.45 Ma) may have been deposited on top of the already cooled Paintbrush Tuff. Subsequently this later layer has been largely eroded away; the maximum estimate of its thickness is 100 m (DOE, 1995). Therefore, any thermal water that circulated through the unsaturated zone of Yucca Mountain after ca. 11.4 myr cannot be related to the residual heat of the tuffs.

The Timber Mountain caldera hydrothermal event – A large silicic magma body was emplaced beneath the Timber Mountain caldera, 7–9 km to the north of Yucca Mountain shortly after the final climactic eruption at 11.45 Ma. This resulted in the development of a large-scale southward flowing hydrothermal plume. According to Bish and Aronson (1993), the system included an upflow zone in the area of the Claim Canyon caldera, where thermal waters likely discharged at the surface (Fig. 1). Further to the south they affected only deep parts of the rock sequence (under Yucca Mountain – ca. 1000 m and deeper). A pronounced north-south thermal gradient has been noted:

"it is apparent that a significant thermal event has occurred in the northern end of Yucca Mountain but has not significantly affected the southern end" (Bish and Aronson, 1993, p. 153). The authors also argued that the upper ca. 1000 m of the Yucca Mountain rocks were significantly cooled by infiltration of meteoric water (the "rain curtain" effect). It is thus apparent from Fig. 1 that temperatures of 75–90° C at the ESF level cannot be attributed to the Timber Mountain caldera hydrothermal event.

Another constraint is provided by the ages. The Timber Mountain caldera hydrothermal system was active between ca. 10.5–11.0 Ma (Bish and Aronson, 1993, p. 159); i.e. the event ended well before the time when the oldest elevated-temperature secondary minerals sampled in the ESF were deposited.

3 The MICH thermal model

According to the model proposed by Marshall and Whelan (2000), the unsaturated zone of Yucca Mountain was heated conductively by a magma body emplaced beneath the Timber Mountain caldera, approximately 7–9 km to the north of the ESF. In this conceptual model, the cooling of the magma body and the associated heating of the surrounding rocks lasted for 5 to 8 myr. Purportedly, waters from which secondary minerals in the Yucca Mountain tuffs were deposited were meteoric precipitation in origin, which infiltrated from the topographic surface along fractures and became heated upon contact with the bedrock. In text below this will be designated the *meteoric infiltration-conductive heating* or MICH model.

Significance of the MICH model for the Yucca Mountain Project – The MICH model possesses two features that are critically important from the standpoint of the suitability of Yucca Mountain for hosting the high-level nuclear waste disposal facility. First, the model is consistent with the postulated long-term (i.e. over the last 11.6 myr) stability of the unsaturated zone at Yucca Mountain, the postulate that is one of the keystones of the Yucca Mountain safety case. Second, the MICH model relates the past elevated temperatures in the unsaturated zone to the large-scale silicic volcanism of the Southwestern Nevada Volcanic Field which ceased between 9 and 11 Ma. The regional tectonic conditions that led to the development of this volcanism in the late Miocene have not been present in the area over the last several million years (Sawyer et al., 1994), and the likelihood of the recurrence of any caldera-scale volcanism is considered to be negligible (DOE, 2008). If the mineral-forming thermal waters were demonstrated to be related to the Miocene silicic volcanism, then recurrence of such hydrothermal activity would also be unlikely. As a consequence, there would be no need to include it in the performance assessment for the Yucca Mountain repository. Alternatively, if the fluid inclusion temperatures were shown not to be related to the silicic volcanism, this would be of regulatory concern, and such hydrothermal activity would have to be formally considered in the performance assessment.

Because the MICH model is the only model proposed so far that explains away the presence of thermal waters in the unsaturated zone in a “benign” manner in which the safety case of the Yucca Mountain facility is not affected, thorough validation of this model is important. Validation becomes even more important considering the apparently extraordinary nature of the MICH model, which contemplates heating of near-surface rocks by conductance over distances of several kilometers and to very high temperatures, and maintaining these elevated temperatures for millions of years. Initially, the model does not seem to be plausible.

4 Validating the MICH model through computational modeling

Validation means “determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model” (AIAA, 1998) or “building confidence that a model adequately represents a real system for a specific purpose” (IAEA, 2003). The DOE administrative procedure, Analyses and Models (AP-3.10Q), stipulates that: *“... model validation shall consist of comparing analysis results against data acquired from the laboratory, field experiments, natural and man-made analog studies, or other relevant observations”.* (p. 13). Validation through *computational modeling* involves the construction of a numerical model and comparison of the computational outcomes with the experimental outcomes. Failure to pass the quantitative comparison test would result in a need to revise the conceptual model; failure to achieve the acceptable agreement through revisions must lead to the abandonment of the conceptual model (Thacker et al., 2004).

For validation purposes, the outcomes of computational modeling must be compared to a *benchmark*. For the MICH model the benchmark consists of the coupled temperature-age data characteristic of a certain distance from the heat source (magma chamber). The empirical data constraining the “thermal history” of the unsaturated zone of Yucca Mountain were obtained by studying secondary minerals in the ESF tunnel complex, as noted. The results are summarized in graphical form in Fig. 2. The graph was first presented in Whelan at al. (2003, Fig. 4) and then reproduced in Whelan et al. (2008, Fig. 8b), where it was used as a benchmark for the computational modeling. A simplified version of this graph was used as a benchmark in Dublyansky and Polyansky (2007).

4.1 Evaluation of the benchmark

The age- and temperature data used in the benchmark come from three different sources.

Fluid inclusions – Homogenization temperatures obtained from calcite and fluorite coupled with the ^{235}U/^{207}Pb age dates measured in closely associated chalcedony and opal are shown in Fig. 2 by filled symbols. The data points for which only minimum ages are available (triangles and dotted lines) have too large uncertainties in the time scale and therefore are not useful. In addition, errors of the temperature determinations (typically, 3–7 °C) are not shown on the graph.

Stable isotope calculations – Circled dots in Fig. 2 show the temperatures calculated from δ^{18}O values of calcite. The symbols carry no error bars, which creates a false impression of the robustness of the data. The ages of the calcite were constrained by U-Pb or U-series ages of silica phases, and were interpolated or extrapolated by assuming a constant rate of mineral deposition (Whelan et al., 2008, Sect. 5.2.2). Considering that known variations of the growth rate in the Yucca Mountain samples exceed one order of magnitude (0.5 to 5 mm Ma^{-1} – Neymark et al. (2002), Paces et al. (2004); up to 10 mm Ma^{-1} – Wilson et al., 2003, Fig. 8b), the 1 mm-error in determining the position of the sample corresponds to up to 0.5 myr. Given the complexity of growth textures observed in the Yucca Mountain samples, age uncertainties up to 1–2 myr can be expected for the stable isotope data points.

The uncertainty in the isotopic temperatures shown in Fig. 2 is, primarily, the uncertainty of the method. Calculation of the temperature from δ^{18}O of calcite involves a number of assumptions, namely: (1) that deposition occurred in isotopic equilibrium with the mineral-forming solution; (2) that the equation selected, O'Neil et al. (1969), faithfully describes the temperature-dependent fractionation of oxygen isotopes between calcite and water; and (3) that the mineral-forming water has retained a constant δ^{18}O = −11 ‰ throughout the last 10 myr. None of these assumptions appears defensible. *Assumption 1* – Deposition under isotopic equilibrium may be theoretically compatible with the MICH conceptual model envisaging exceedingly slow mineral deposition but it has not been independently confirmed. *Assumption 2* – Several equations describing "equilibrium" fractionation in the system calcite-water are available (Craig 1965; O'Neil et al., 1969; Friedman and O'Neil, 1977; Kim and O'Neil, 1997; Coplen, 2007; Tremaine et al., 2011). The choice of equation affects the calculated temperatures; for example, application of Coplen (2007) yields temperatures 8–10 °C warmer than those of O'Neil et al. (1969). *Assumption 3* – Between ca. 1.0 and 2.7 Ma the isotopic composition of meteoric precipitation in the southern Great Basin was significantly enriched (by 2.5–3.0 ‰) in ^{18}O relative to modern-day values (Winograd et al., 1985; Dublyansky et al., 2011). Meteoric water in the unsaturated zone of Yucca Mountain was similarly enriched in ^{18}O around 11 Ma (Feng et al., 1999, Sect. 4.1). Indications that δ^{18}O of mineral-forming water could have varied in space and/or time are also found in the Yucca Mountain data. Pairing the fluid inclusion temperatures with δ^{18}O of host calcite, Wilson et al. (2003, Sect. 7.1) calculated δ^{18}O of the parent water to range between −15 and −5 ‰. With similar calculations Whelan et al. (2008, Sect. 5.2) obtained δ^{18}O ranging −13 to −7 ‰. Finally, Dublyansky and Spötl (2010) reported that the oxygen in fluid inclusion waters in the Yucca Mountain calcite is significantly enriched (2 to 8 ‰) in ^{18}O compared to the "normal" meteoric water compositions, apparently due to the water-rock exchange. Because the assumption of constant isotopic properties in waters at Yucca Mountain is demonstrably not true, the merit of using a fixed δ^{18}O value for paleotemperature reconstructions for the calcite precipitates there appears to be questionable.

The effect of any or all of the assumptions discussed above being incorrect will be discrepancy between the calculated and the true temperatures. To check whether this is the case for the Yucca Mountain samples, "isotopic" temperatures calculated using the approach of Whelan et al. (2002) were compared with fluid inclusion temperatures measured from the same calcite (data from Wilson et al., 2003; Whelan et al., 2008). The differences between the measured and the calculated temperatures ranged from −13 °C to +32 °C. In summary, the temporal trends observed in δ^{18}O values of calcite do reflect the overall decrease of temperature with time. The large uncertainties associated with the method of calculation, however, render the δ^{18}O temperatures unsuitable for quantitative benchmarking purposes.

Best-fit curves – The dark blue curve in Fig. 2 is the third-order polynomial fit to the data points obtained by isotopic calculations; two other curves are calculated using the δ^{18}O values that are greater and smaller by 2 ‰. The curves, thus, inherit all of the uncertainties of isotopic calculation discussed in previous section. In addition, the curves were constructed in a methodologically erroneous way: the polynomial fit calculation included several data points for which only minimum ages were known (dotted arrows in Fig. 2). The best-fit curves thus have substantial uncertainty for temperatures below 40 °C and become entirely unreliable for the temperatures exceeding 40 °C (ages greater than 6 Ma).

4.2 Improvement of the benchmark

The currently available data (from Wilson et al., 2003, Fig. 8; Whelan et al., 2008, Table 4) along with associated uncertainties are summarized in Fig. 3. In some cases inclusions from the same samples and of the same age show fluid temperatures that differ by 15–30 °C (dashed oval in Fig. 3). The MICH model envisages conductive heating and subsequent cooling of a large rock mass. Abrupt temperature changes are not possible in this model. Because of this conceptual constraint, the observed difference of the temperatures can only be explained by the secondary or pseudo-secondary character of the lower-temperature inclusions (i.e., these inclusions were trapped after the formation of the given part of the mineral). Since the time of entrapment for these inclusions is not known, they cannot be used to constrain the thermal history. The end-point of thermal history (zero time) is constrained by the temperatures expected in the unsaturated zone of Yucca Mountain during different Pleistocene climate states.

The two benchmarks (Figs. 2 and 3) are mutually consistent for times older than ca. 7 Ma. Between 7 and 2 Ma, the benchmark of Whelan and co-authors produces faster cooling (the same temperatures are attained up to 1.5 myr earlier).

4.3 Comparison of modeling results with the benchmark

Two versions of the computational modeling on the MICH conceptual model have been reported (Marshall and Whelan, 2001; Whelan et al., 2008). In Fig. 4 the results of this modeling are compared with the improved benchmark. Both versions were run using the HEAT code (K. Wohletz, Copyright®1998–2001, The Regents of the University of California). Marshall and Whelan (2001) modeled a 30 km-wide, 7 km-thick magma body, emplaced at 2.5 km below surface (2-D simulations). The temperature of the chamber was held constant for 4 myr (crustal pre-heating), after which cooling was allowed. Thermal convection was allowed for a depth interval 0–2 km above the magma chamber. Partial evaluation of this modeling exercise can be found in BSC (2004a). The conclusion of this study was that modeling failed to match the empirical temperature-time data, which is also obvious from Fig. 4a.

The latest results of thermal simulations were reported in Whelan et al. (2008, Sect. 6.3, Fig. 8). The updated model retains most attributes of the earlier model setup, including the geometry and depth of emplacement of the magma chamber. Modifications included (a) hydrothermal convection in the rocks adjacent to the magma chamber, (b) a 100 m-thicker unsaturated zone following deposition of the younger Timber Mountain Group tuffs, and (c) subsequent, constant rate, thinning of the overburden due to erosion. The description of the model in Whelan et al. (2008) is not sufficiently detailed to allow serious evaluation (i.e., model setup, crustal stratigraphy, thermophysical and filtration properties of rocks, initial and boundary conditions, model scenarios, etc. are not described). Therefore, the evaluation is restricted to the analysis of the two thermal history curves presented in Whelan et al. (2008, Fig. 8).

It is apparent from the comparison of Fig. 4a and b that convection in the rocks adjacent to magma chamber brings more heat to the reference points and slows down the cooling; the overall result being the temperature-time curves that plot closer to the benchmark. The model scenario included several changes in the regime of convection: it was "limited to shallower zones" at 10 Ma and terminated at 8 Ma. Limiting and terminating the convection produced abrupt drops on the cooling trajectories in Fig. 4b. Although it is obvious that the initiation of different convection states was explicitly prescribed by the model scenario, no information is available regarding the geological processes causing these drastic changes. Other two abrupt changes in cooling regime (from fast to slow cooling, at ca. 9.7 Ma and 7.9 Ma) are also not explained. It is not possible, therefore, to assess whether the model setup, assumptions, initial and boundary conditions, and scenarios employed by Whelan et al. (2008) were plausible, reasonable, and consistent with the site-specific geological information. The thermal histories of Whelan et al. (2008) and, particularly, the maximum simulated temperatures are significantly different from those obtained by Dublyansky and Polyansky (2007, Fig. 10), for a similar model setup and configuration. The latter authors used the code HYDROTHERM (Hayba and Ingebritsen, 1994), which is better suited for modeling convective two-phase flow through a porous medium than the HEAT code (Wohletz et al., 1999) used by Whelan et al. (2008). Attempts to reproduce the thermal histories of Whelan et al. (2008) using the HEAT 3-D code and model parameters indicated in the paper were unsuccessful; at a distance of 8 km from magma body, the thermal curves were much more similar to that shown in Fig. 4a than to 4b.

The most important message contained in Fig. 4b, however, is that the inclusion of convection and additional overburden does not result in agreement between the simulation outcomes and the benchmark. The discrepancies range up to 30–40 °C and 3–5 myr. The updated version of the model, therefore, fails to produce an acceptable match with the benchmark data.

4.4 Conservativeness of modeling

A question remains whether the mismatch between the computational outcomes of Whelan et al., 2008) and the benchmark can be removed by using less conservative model parameters. Analysis shows that this is very unlikely, primarily because the parameters used for computing the thermal histories shown in Fig. 4 were non-conservative already. The major source of uncertainty in the MICH model pertains to poorly known parameters of the plutons (dimensions, locations, depths of emplacement, residence time, etc.). Estimates of these parameters for the Timber Mountain caldera system depend on the petrogenetic model selected, which varies from that of a single magma chamber (Lipman et al., 1966), to successive emplacement of magma chambers (Broxton et al., 1989), to multiple magma batches (Schuraytz et al., 1989; Huysken et al., 1994; Cambray et al., 1995; Mills et al., 1997), to vertically separated magma bodies and re-intrusion (Bindeman and Valley, 2003). Temperatures, emplacement dynamics, depth, and residence times of magma, will all vary dramatically between these models. For example, a very shallow depth of emplacement of 2.5 km was used in the simulations shown in Fig. 4; greater emplacement depths decrease the simulated temperatures at the reference points. However, although the depth of 2–3 km was proposed for the Timber Mountain plutons on the basis of geometrical consideration of the calderas (Byers et al., 1976), these estimates were subsequently revised by Warren et al. (1989) and Mills et al. (1997) who, using mineral geo-barometers, estimated the depth of emplacement as 10 km to 12.5 km. Comparison of selected parameters in Table 1 shows that the modeling of Marshal and Whelan (2001) and Whelan et al. (2008) was non-conservative and likely overestimated both the temperatures and the cooling times.

4.5 Reproducibility of modeling

Reproducibility is one of the principal tenets of the scientific method. The temperature-time trajectories simulated by Whelan and Marshall (2001) were independently reproduced. Dobson (2003) using TOUGH2, and Dublyansky and Polyansky (2007) using HEAT 3-D and HYDROTHERM codes, obtained "thermal histories" similar to those of Whelan and Marshall (2001). Dobson (2003) and Dublyansky and Polyansky (2007) however, offered different interpretations of modeling outcomes. Having acknowledged uncertainties in the scaling approach that was used, Dobson (2003) nevertheless concluded that results of his simulations *"do not concur with the conclusions of Marshall and Whelan (2001) that the presence of the Timber Mountain volcanic center could account for the sustained elevated temperatures recorded for Yucca Mountain between 10 and 5 Ma."* (p. 57). In addition to the base-case model setup involving only conductive heating, Dublyansky and Polyansky (2007) evaluated the role of advective heat transfer by moving water. The modeled "thermal histories" were generally similar to the early results of Marshall and Whelan (2001), and they did not match the benchmark, which led Dublyansky and Polyansky to conclude that the MICH model *"does not appear to constitute a plausible explanation for the circulation in the past of thermal waters (up to 70–90° C, according to fluid inclusion data) in the vadose zone of Yucca Mountain."* (p. 1).

In contrast, attempts to reproduce the latest "thermal histories" of Whelan et al. (2008) were unsuccessful (cf. Sect. 4.3). Further reproducibility tests will require disclosure by the authors of the original model parameters; this information is not presently available (author's requests for this information were declined by the authors of the model).

5 Auxiliary sub-models

Several auxiliary sub-models proposed in the literature in order to bring the computational result of the MICH model in agreement with the benchmark (BSC, 2004a; Houseworth, and Hardin, 2010; Whelan et al., 2008) are discussed below. The final sub-model discussed in this section, the cooling action of meteoric infiltration, has not been considered in conjunction with the MICH model before.

5.1 Continued injection of magma, including injections close to Yucca Mountain

Continued injection of magma into the shallow crust in the vicinity of the Timber Mountain volcanic center after 11 Ma, and/or intrusion of magma closer to Yucca Mountain were proposed in (BSC, 2004a) to resolve the discrepancy between the computational results of Marshall and Whelan (2001) and the benchmark data. However, geological or geophysical information supporting this conjecture is lacking (NRC, 2005, p. 16). Before it can be accepted, the purported magma body or bodies would need to be identified, their locations, sizes and time of intrusion would have to be determined, and the thermal effect would have to be numerically modeled. Results compatible with the benchmark so far have been obtained only in simulations where reference point was located immediately above the margin of the pluton; this means that a hypothetical magma body would have to extend southward as far as Yucca Mountain (the ESF tunnel complex).

5.2 Lateral subsurface flow

Lateral subsurface flow of thermal water from the Timber Mountain caldera toward Yucca Mountain was proposed in BSC (2004a) to explain the elevated fluid inclusion temperatures. The unsaturated zone at Yucca Mountain is thought to have formed shortly after ca. 11.6 Ma, and to have persisted since that time (DOE, 2001, 2008). The vitric tuffs of the unsaturated zone do not exhibit devitrification or pervasive alteration, as would be expected if heated waters had moved through them en masse for any extended period of time. This means that the "lateral subsurface flow" of thermal waters could only have occurred within the saturated zone; heating of the unsaturated zone rocks above would still have had to be by conductance. The lateral outflow of thermal water from Timber Mountain is known to have occurred at 10.5 to 11.0 Ma (cf. Sect. 2.2, Fig. 1). Near Yucca Mountain it affected only the deep-seated rocks, below ca. 1000 m. Mineralogical and isotopic evidence (Bish and Aronson, 1993, Sect. Paleogeothermal conditions; Feng et al., 1999, Sect. 4.1) as well as thermal modeling (Dublyansky and Polyansky, 2007, Sect. 4.3.3) indicate that this hydrothermal system did not cause heating of the unsaturated zone at the ESF level that is commensurate with the fluid inclusion temperatures.

5.3 The presence of additional overburden

The presence of additional overburden, later removed by erosion, would increase the depth and, respectively, the temperatures at the reference points in early stages of the process (BSC, 2004a; Houseworth and Hardin, 2010). It is thought that no more than ca. 100 m of the overburden can have been removed from Yucca Mountain over the last 10 myr (YMP, 1993; DOE, 1998). A 100 m-overburden was implicitly included in the simulations of Marshall and Whelan (2001), which calculated the temperatures at a depth of 250 m (BSC, 2004a), whereas the ESF minerals with highest homogenization temperatures (>70 °C) were collected from depths of 30 to 80 m. It was then explicitly modeled by Whelan et al. (2008). Sensitivity simulations of Dublyansky and

Polyansky (2007) have shown that in order to bring the modeling results into approximate agreement with the empirical data, up to 1000 m of overburden would have to be added. Recently Houseworth and Hardin (2010) pointed out that the thermal conductivity of the overburden tuffs could have been smaller than that used in sensitivity simulations of Dublyansky and Polyansky (2007) ($0.5\,\mathrm{W\,m^{-1}\,K}$ instead of $1.3\,\mathrm{W\,m^{-1}\,K}$). New simulations, employing this lower thermal conductivity showed that the thickness of overburden still would have to be at least 700 m. The hypothetical addition of such deep overburden would significantly increase the long-term erosion rate; because the latter is a regulatory concern, acceptance of the "additional overburden" conjecture would require a revision of the Yucca Mountain safety case.

5.4 Heating by vapor-phase convection

Whelan et al. (2008) suggested that vapor-phase convection cells could have developed within the volcanic tuffs above the water table when the latter had a high temperature, and speculated that circulation of this vapor heated the unsaturated-zone rocks:

> *"Preliminary simulations of vapor-phase flux in the unsaturated zone above a water table at near-boiling temperatures indicate that vapor-phase convection cells could develop within the TSw . . . (M. A. Walvoord, US Geological Survey, written communication, 2003). . . . preliminary simulations indicate that heat transport by vapor-phase convection may account for the high temperatures near the TSw–PTn contact."* (p. 1071)

Because neither the technical details nor the numerical results of these preliminary simulations are provided in the paper, the claim that the proposed mechanism may indeed account for the high temperatures in the unsaturated zone of Yucca Mountain cannot be verified. It is unusual that a paper published in 2008 relies on anecdotal preliminary simulations performed five years earlier, particularly considering that the latter represent the only test which purports to validate the author's conceptual model. Conceptually, the proposed mechanism faces at least two serious objections.

Objection 1 – The mechanism postulates near-boiling temperatures at the water table. There is no geological, geochemical, or mineralogical evidence suggesting that the water table under the repository block has ever been at such high temperatures. During the last large-scale hydrothermal event in the area, the Timber Mountain Caldera episode (10.5–11.0 Ma) when the convective outflow occurred under Yucca Mountain, the temperatures at the water table were substantially lower than 100 °C (Bish and Aronson, 1993) (cf. Fig. 1). To make the proposed mechanism acceptable, it must first be reconciled with the hydrogeological history of the area, and independent evidence for near-boiling temperatures at the water table must be presented.

Objection 2 – The elevated temperatures at Yucca Mountain have been determined from fluid inclusions in secondary calcite. This means that the elevated temperatures and the physical-chemical conditions suitable for deposition of calcite must have been present simultaneously. The model envisages a convective rise of the hot/warm vapor phase (a mixture of underground air and water vapor) from a hot water table upward into the fractured rock. Because the overlying rock becomes cooler with decreasing distance to the surface, condensation of the water vapor is expected on the fracture walls. The resulting condensate would dissolve the CO_2 present in the subterranean atmosphere and thus become acidic, aggressive with respect to calcite. This mechanism, known as *condensation corrosion*, produces sizable chambers in some hypogene carbonate caves (Ford and Williams, 2007, Sect. 7.11; Dublyansky, 2012). According to the general conceptual model of Whelan et al. (2004, 2008), calcite in the unsaturated zone of Yucca Mountain was deposited from small amounts of water infiltrating from the soil zone. Due to the nonlinear relation between the calcium equilibrium concentration and carbon dioxide pressure, mixing of slightly supersaturated infiltration water with aggressive condensate would necessarily produce water, which is aggressive with respect to calcite (*mixing corrosion*; e.g., Ford and Williams, 2007, Sect. 3.7.6). Deposition of calcite does not seem to be possible within the proposed vapor-phase convection mechanism.

5.5 Elevated heat flows related to extensional tectonics

Houseworth and Hardin (2010) postulated that the thermal history at Yucca Mountain has been affected not only by nearby magmatic activity, but also by the regional heat flux caused by tectonic extension. They contended that the heat flow could have been as large as 300 $\mathrm{mW\,m^{-2}}$ at 13 Ma and gradually decreased to less than 100 $\mathrm{mW\,m^{-2}}$ at present, and opined that these high heat flows explain the elevated temperatures in the unsaturated zone at Yucca Mountain. This contention is based on the relationship between the heat flow and the extension rates in the Basin and Range (Lachenbruch and Sass, 1978, Figs. 9–14) and the history of extension at Yucca Mountain over the last 16 myr (Snow and Wernicke, 2000, Fig. 12). The postulated, extremely high Late Miocene heat flows in the area, however, are in conflict with the site-specific geological data.

For example, conodonts with a colour alteration index (CAI) of 3 were reported from Late Silurian dolostone at a depth of ca. 1800 m in Borehole UE25p#1, located ca. 2 km to the east of Yucca Mountain (Carr et al., 1986, App. III). This low CAI indicates that the highest temperature the rock was exposed to since Late Silurian time was 140–180 °C. Assuming that these temperatures were caused by the elevated Late Miocene heat flows, as postulated by Houseworth and Hardin (2010) – although these temperatures could just as well be related to much older, post-Silurian burial of the rock – the corresponding (maximum) heat flows for the area are 110–150 $\mathrm{mW\,m^{-2}}$. The paleotemperature gradients that existed during the large-scale hydrothermal event at 10.5–11.0 Ma were reconstructed by Bish and Aronson (1993, Fig. 6) for three Yucca Mountain boreholes from illite-smectite mineralogy and fluid inclusion data (cf. Fig. 1). For the upper ca. 1000 m of the rock mass, the paleogradients are in the 30–36 °C/km-range, corresponding to heat flows of ca. 50–65 $\mathrm{mW\,m^{-2}}$. The hypothesis of Houseworth and Hardin (2010) is thus untenable.

5.6 Cooling action of meteoric infiltration

Infiltration (and, in the fractured near-surface zone, air movement) leads to an additional cooling of the rocks in the unsaturated zone. The intensity of cooling depends on the infiltration rates; the link between the two parameters is so strong that the temperature measured in boreholes was used to assess the infiltration fluxes at Yucca Mountain (Bodvarsson et al., 2003). The cooling may be slight when the climate is semi-arid and infiltration rates are low, as is the case at Yucca Mountain today (Sass et al., 1988). It should have been substantially greater in the past, when climate in the area was cooler and wetter (Hay et al., 1986; Sharpe, 2007). The cooling action of infiltration can create a "rain curtain" state of near-isothermal conditions from the surface to depths of 800–1000 m. Such an effect has been observed at one modern geothermal system in Oregon (Swanberg and Combs, 1986). A rain curtain occurred in the Yucca Mountain unsaturated zone during the Timber Mountain Caldera hydrothermal episode 10.5–11.0 myr ago (Bish and Aronson, 1993, Sect. Paleohydrologic conditions). The inclusion of the effect of cooling by infiltration would lower the temperatures computed for the MICH model in the depth interval of interest (100–300 m). In fact, the temperatures in this zone could have been entirely controlled by this effect, as illustrated in Fig. 1.

6 Additional approaches to validation of the MICH model

6.1 The analog-system observations

Observations from natural analogs are an integral part of the process of development of models in programs related to geological disposal of nuclear waste (DOE, 2004). The term "natural analog" refers to natural systems in which processes similar to those expected to occur in a nuclear waste repository are thought to have occurred. Analog investigations may determine the conditions under which the processes occur, the effects of the processes, as well as the magnitude and duration of the processes

(Simmons, 2003). Natural analog studies represent a somewhat weaker form of validation: while they may confirm that an hypothesized process is generally possible, and has occurred elsewhere, this does not necessarily imply that the process has occurred at the site which is being evaluated.

The Long Valley caldera in California has been proposed as a useful analog for examining the processes postulated in the MICH model (BSC, 2004a). The parameters of the parent magma chamber at Long Valley appear to be similar to those of Timber Mountain (an elliptical form measuring 20 km × 30 km and 2 km thick, with a depth of emplacement of 5–7 km (Bailey et al., 1976); the estimated magma temperature is ca. 800 °C (Hildreth and Spera, 1974). Silicic volcanism at the Long Valley igneous system began at ca. 2 Ma and continued intermittently until the time of the caldera collapse at 0.7 Ma (Bailey et al., 1976). Shortly after the collapse a resurgent dome formed, and silicic and intermediate volcanic material has been discharging around it virtually up to the present time. Heat flow was measured in 11 shallow boreholes (150–300 m) in the vicinity of the caldera by Lachenbruch et al. (1976), who concluded that although the magma chamber has likely been replenished during its 2 myr-long eruptive history, no conspicuous indications of thermal anomalies related to this chamber could be detected outside the caldera margins. This conclusion was upheld in BSC (2004a): *"...a thermal anomaly outside of the Long Valley caldera would not be detectable 700 000 yr after the last major phase of magmatic activity".* (p. H-21). Observations at this natural analog system, therefore, do not support the validity of the MICH model, which envisages a strong thermal anomaly at a distance of several km from caldera margin existing for several million years.

6.2 Observations on spatial structure of the thermal field

In previous sections we evaluated primarily the temperature-time relationships, while the spatial information was reduced to a single parameter, distance from a hypothetical magma body. Another potentially relevant feature is the spatial structure of the thermal field. The field expected in the MICH model is characterized by a strong lateral gradient with highest temperatures immediately adjoining the magma body and decreasing rapidly with increasing distance away from its margin. A critical validation test would consist of a comparison of the actual spatial distributions of paleotemperatures around the proposed heat source, the Timber Mountain magma body, and those expected from the model.

The temperature data obtained from the ESF tunnel cover an area of a few square kilometers which, in the evaluations of the MICH model given above, has been considered a single point for the sake of simplicity. The distribution of maximum fluid inclusion temperatures within this area exhibits a pronounced east-west gradient, orthogonal to the gradient expected within the MICH model (Fig. 5). This distribution requires that the source of heat be located to the east of the repository block.

Fluid inclusion homogenization temperatures from calcite from Borehole USW G-2 located ca. 3 km to the north of the ESF complex (i.e. closer to the presumed heat source, where higher temperatures would be expected) are reported in USGS (2002) and Whelan et al. (2008, Table 1). The temperatures (42–47 °C at −437 m and 45–60 °C at −477 m) are lower than those measured at the ESF. This led the authors of USGS (2002) to speculate that *“the heat source may have been farther to the east than previously thought”*; Whelan et al. (2008) did not discuss the significance of these data for the MICH model. The idea of “relocating” the magmatic heat source to the east of Yucca Mountain is in conflict with the site-specific geological evidence because no significant buried magma bodies are known in this direction. The low conodont color alteration index of the Late Silurian rocks penetrated by the UE25 p#1 borehole ca. 2 km to the east of Yucca Mountain (Carr et al., 1986) speaks strongly against such a possibility.

The spatial structure of the paleotemperature field, as recorded by fluid inclusions, effectively falsifies the MICH model: the temperatures do not increase toward the presumed heat source, Timber Mountain, as they should do. (For discussion of alternative interpretations put forth to explain the paleothermal gradients in the unsaturated zone of Yucca Mountain see Appendix A).

7 Discussion and conclusions

The development and validation of scientific models associated with geological disposal of nuclear waste in the United States are regulated by the US Department of Energy's Quality Assurance Requirements and Description (DOE, 2004) and by a set of administrative procedures (e.g., AP-3.10Q – Analyses and Models and AP-3.11Q – Technical Reports). The development of the MICH model does not seem to have been in compliance with this guidance and regulations. Detailed evaluation of the non-compliance is beyond the scope of this publication; suffice it to say that 12 yr after the introduction of the MICH model by Marshall and Whelan (2000), there is no technical report which demonstrates validity of the model and provides sufficient information for technical evaluation of the computational modeling. The analysis presented above demonstrates that none of the three approaches to validate the model, computational modeling, analog-system observations, and observations on the structure of the paleotemperature distribution, result in validation of the MICH model.

Nevertheless, the model has become entrenched in the scientific record. This was aided by the (erroneous) notion that the conceptual model of the conductive heating at Yucca Mountain has been validated by means of computational modeling. Statements to this effect have appeared in publications by the authors of the model (Marshall and Whelan, 2000, p. A-259; 2001, p. A-375; Whelan et al., 2002, Sect. 5.3; 2003, Sect. IV; 2004, Sect. 3.2; 2008, Sect. 6.3, Sect. 7; Marshall et al., 2005, Sect. 2; see also Appendix B). Other researchers relied on the MICH model to interpret their data (Wilson et al., 2003, Sect. 7.6; Bryan et al., 2009, Sect. 3). The model was incorporated, implicitly or explicitly, into the DOE program documents, such as the Yucca Mountain Science and Engineering Report (DOE, 2001, p. 4–402) and the Yucca Mountain Site Description (BSC, 2004b, p. 7–81). It served as one of the key arguments for the exclusion of the FEP (feature, event, process) "Hydrothermal Activity" from consideration in the Yucca Mountain Total System Performance Assessment (BSC, 2004c; SNL, 2008; cf. Dublyansky, 2007).

Fluid inclusions in secondary minerals in the unsaturated-zone of Yucca Mountain provide direct and unequivocal evidence that thermal waters accessed this zone in the past. Flow of thermal water is a process that could seriously compromise the performance and the safety of the nuclear waste disposal facility. The MICH model is the only model accepted in the DOE Yucca Mountain technical documentation to explain the presence of thermal waters in the unsaturated zone of Yucca Mountain. The lack of validation of the model and information strongly suggesting that the model is not viable, presented in this paper, implies that the DOE Yucca Mountain safety case does not have plausible explanation for this natural phenomenon, potentially detrimental to the safety of nuclear waste disposal.

A defensible phenomenological model must be proposed to explain the origin of the past hydrothermal activity at Yucca Mountain. The model must be thoroughly validated and included in the Total System Performance Assessment calculations. Any safety case which does not consider this potentially disruptive process would be critically deficient.

Appendix A

Evaluation of the paleothermal field at Yucca Mountain

When evaluating information regarding the paleothermal field in the Yucca Mountain unsaturated zone, one needs to address two questions: (1) are there indications of spatial gradients in the paleothermometric data? And, (2) if yes, how may these gradients be interpreted?

A1 Observation of spatial paleotemperature gradients

The non-uniform character of fluid inclusion paleotemperatures in samples from the ESF tunnel was first noted by Dublyansky (1998):

> *"In terms of the spatial distribution of measured homogenization temperatures, the following observation may be important. Two samples that yielded temperatures higher than other samples . . . are both from Tiva Canyon tuff. Also, both these samples are from the eastern part of the exploratory block . . . , closest to the Paintbrush (~ 2 km to the east of the repository block) fault zone which might have served as major avenue for upwelling fluids."* (Sect. 6.8)

The observation was based on the limited number data available at that time and was, therefore, considered tentative:

> *"Although it is premature to make strong conclusions on the basis of only two samples, this hypothesis needs to be addressed in the future, when the spatial structure of the ancient upwelling system is studied."* (Dublyansky, 1998, Sect. 6.8)

More data became available in the course of the UNLV Yucca Mountain Thermochronology project in 1999–2000. In the final report from this Project, Wilson and co-authors asserted that

> *". . . temperatures recorded across the Yucca Mountain repository horizon do not exhibit a central hot plume and large lateral thermal gradients that are present in geothermal and epithermal systems . . . The lack of a significant temperature gradient and presence, instead, of relatively uniform temperatures argues against an upwelling hot fluid model".* (Wilson et al., 2002, Sect. 6.1)

In the follow-up publication, a similar statement appears (Wilson et al., 2003, Sect. 7.3). These statements purport that the early tentative information on the non-uniform character of the paleothermal field at Yucca Mountain was not confirmed. Further, Wilson et al. (2003) proposed the presence of "spatially localized high-temperature fluids" near the north portal of the ESF; no interpretation was offered as to the nature of these localized fluids. In contrast, gradients in paleothermometric data were reported by Whelan et al. (2003):

> “*Fluid inclusion T_h* [temperatures of homogenization] *in calcite decrease from east to west along the ESF north ramp in the north bend (from about 90°C to about 60°C), from northeast to southwest along the ECRB Cross Drift from about 60 to 50°C, and from north to south along the ESF main drift from about 60°C to about 45°C (Fig. 2)”.* (Sect. A3)

One reconstruction of the paleotemperature field based on fluid inclusion data is shown in Fig. 5. It must be emphasized that homogenization temperatures shown on this graph were obtained from the basal, oldest parts of mineral crusts and, therefore, characterize the early stages of mineral deposition. The temperatures decreased with time and eventually attained the ambient values.

Additionally, an important observation is that the distribution of δ^{18}O values in early calcite in the repository block virtually mimics that of the paleotemperatures (Fig. A1c, d). This can be explained by the temperature-dependent isotopic fractionation in the $CaCO_3$-H_2O system:

> “*The fractionation of oxygen isotopes between calcite and water is a function of temperature, with the calcite δ^{18}O value increasing as temperature decreases. The trends in the δ^{18}O values of early-stage calcite . . . are, therefore, consistent with the temperature trends displayed by the FIA* [Fluid Inclusion Assemblage] *T_h measurements.”* (Whelan et al., 2003, Sect. B3)

The data from temperature-sensitive δ^{18}O in calcite, thus further corroborate the fluid inclusion spatial temperature trends.

In summary, although one may put forth different interpretations, and attach different significance to the non-uniform thermal field revealed by fluid inclusions and stable isotopes, characterization of the data as exhibiting “lack of a significant temperature gradient and presence, instead, of relatively uniform temperatures” is clearly unwarranted.

A2 Interpretation of spatial paleotemperature gradients

Dublyansky and Smirnov (2003, Sect. 2.4) and Dublyansky et al. (2005, Sect. 2) considered the temperature gradients apparent in Fig. 5 as a true feature of the paleothermal field, characteristic of the early stages of secondary mineral deposition in the Yucca Mountain unsaturated zone. Alternative interpretations are discussed in subsequent sections.

A2.1 Incomplete sampling

The idea that the gradients are apparent rather than real, and result from the failure to find samples with high-temperature inclusions in the part of ESF where only low homogenization temperatures were measured, was informally put forth in a number of discussions.

Samples for the fluid inclusion studies were collected from the 7.8 km-long ESF tunnel by three research groups in the course of several sampling campaigns. Most of the ESF sites bearing secondary mineralization have been sampled (cf. Wilson et al., 2003, Fig. 2; Whelan et al., 2008, Fig. 2a). The currently available fluid inclusion database consists of ca. 7000 measurements obtained from more than 130 sampling sites (Whelan et al. 2008, Sect. 5.2). The δ^{18}O database exceeds 2000 measurements. Independently obtained fluid inclusion temperatures and stable isotope data are remarkably consistent (Fig. A1). The possibility that some occurrences containing either the high-temperature fluid inclusions or characteristically low δ^{18}O values were not sampled in the north-south drift of the ESF (where the paleothermal field shows the lowermost values) appears therefore remote.

A2.2 Temporal rather than spatial gradients

With respect to the non-uniform temperatures of early fluids, Wilson et al. (2002) opined that:

> *"These temperatures . . . are not related to lateral temperature gradient across the site because the temperature variations occurred at different times ".* (Sect. 4.3)

and

> *"The distribution of fluid temperatures is related to the timing of mineral precipitation at various sites. Where present, elevated temperatures are recorded in early to early-intermediate calcite, and the presence or absence of this record is related to whether or not early fluids with elevated temperatures reached precipitation sites."* (Sect. 6.1)

This hypothesis (presented in an assertive form) is supported by only tenuous argumentation. At Yucca Mountain, secondary minerals are found in two types of openings in the rock: lithophysal cavities and fractures/breccias. Lithophysal cavities formed shortly after the emplacement of host tuffs and were subject to vapor-phase alteration; surfaces of some early fractures are also altered. Fractures which bear no traces of vapor-phase alteration should have formed later than lithophysal cavities. Wilson and Cline (2002, Sect. 7.2) stretch this simple logical premise to argue that "secondary minerals in fractures and breccias began to precipitate later than secondary minerals in lithophysal cavities".

The latter statement is a non-sequitur. The vapor-phase alteration ended shortly after the emplacement of the ash material, its compaction and conversion into welded tuffs. The complete cooling of the 350 m-thick sequence of Topopah Spring ash-fall tuff from its estimated temperature of emplacement to ambient temperatures took about 7000 yr (Buesch and Riehle, 2007). The vapor-phase alteration took only a fraction of this time. A fracture which was not affected by vapor-phase alteration could be just a few thousand years younger than a cavity affected by it; a tiny fraction of their more than 12 myr-long history.

The contention of Wilson and Cline (2002) is also not supported by the data. The U-Pb dating results (Neymark et al., 2002; Wilson et al., 2002, 2003; Whelan et al., 2008) indicate that (a) *all* secondary minerals at Yucca Mountain post-date the vapor-phase alteration by 1 to 1.5 myr and (b) many fractures contain minerals, which are as old as their counterparts from the lithophysal cavities (Fig. A1b). Figure A1b shows also, that areas in the ESF characterized by different early paleofluid temperatures were accessed by these fluids at essentially the same time (within the error of the U-Pb dating method).

The paragenetic age of calcite at Yucca Mountain can be assessed on the basis of its stable isotope properties. Carbon is a conservative component, whose isotopic composition reflects that of the source(s) of dissolved bicarbonate. Fractionation of carbon isotopes is little affected by temperature (e.g. the fractionation coefficient for $HCO_{3(aq)}$-$CaCO_3$ changes by 0.4 ‰ between 20 to 90 °C; Deines et al., 1974). In the Yucca Mountain samples δ^{13}C decreases from 8 to 10 ‰ in the earliest calcite to −8 to −10 ‰ in the latest one (Wilson and Cline, 2002, Sect. 6.4; Whelan et al., 2002). The earliest calcite with characteristic, strongly positive δ^{13}C values is present throughout the repository zone (Fig. A1e), from areas near the North and South portals where the highest paleotemperatures were measured to the N-S drift. This is consistent with the conclusion of Whelan et al. (2002, Sect. 4.4): *"The large range of δ^{13}C values, as plotted against location in the ESF ... , shows that the entire paragenetic sequence is present in mineral coatings throughout the ESF"*.

A2.3 Early fumarolic activity

Whelan et al. (2003, Sect. IV) and Whelan et al. (2008, Sect. 6.2) suggested that the two highest-temperature samples from the first 500 m of the ESF tunnel, one of calcite and one of fluorite, were formed as a result of the transient fumarolic activity. The authors noted the presence of the thin bleached rims on the fractures hosting the minerals at these two locations and interpret these rims as an indication that the fractures transported hot, fumarolic, fluids produced during the initial cooling of the Tiva Canyon Tuff. Although the evidence presented in support of the fumarolic origin of these samples is by no means definitive, we note that even if the highest-temperature calcite sample is excluded (fluorite thermometric data were not used for paleothermometric reconstructions because of their lower reliability at Yucca Mountain), the east-west gradient remains (Fig. A1c). The possible fumarolic activity is thus not relevant for the gradients of the paleothermal field in the Yucca Mountain unsaturated zone.

A2.4 Link with zeolite alteration

Describing the paleotemperature gradients observed in their fluid inclusion and δ^{18}O data Whelan et al. (2008) noted:

> *"Similar temperature trends are suggested by the intensity of zeolitization in the upper Calico Hills Formation (Bish et al., 2003, Fig. 8). . . . this temperature trend more likely reflects a lateral, east–west, temperature gradient, perhaps correlative with zeolitization intensity in the Calico Hills Formation . . . ."* (Sect. 5.2.1)

Genetic implications of the apparent correlation between the temperatures measured in secondary minerals in the ESF and the abundance of zeolites in the layer of vitric tuffs located several hundred meters deeper are not discussed by Whelan and co-authors. Without such a discussion, the above statement represents a causal fallacy (correlation does not imply causation).

It is to be noted that zeolitization of the Calico Hill formation likely occurred between 12.9 Ma (the age of the tuff; Sawier et al., 1994) and 11.3 Ma (Broxton et al., 1987, p. 101). As was stated above, none of the secondary minerals from ESF yielded a U-Pb age exceeding 10 Ma, implying a more than 1 myr-long gap between the two processes. Further, it was demonstrated that the latest large-scale hydrothermal system (10.5–11.0 Ma; Bish and Aronson, 1993), which likely produced zeolitization, only affected the deep parts of the Yucca Mountain rock sequence (> 1000 m). During this hydrothermal event the temperatures in the unsaturated zone remained below those indicated by fluid inclusions (Bish and Aronson, 1993; Feng et al., 1999, Sect. 4.1; Dublyansky and Polyansky, 2007, Sect. 4.3.3).

A3 Conclusions

1. Paleothermal gradients revealed by fluid inclusion homogenization temperatures and the δ^{18}O compositions of early calcite must be considered real unless and until convincing evidence otherwise is presented.
2. No coherent explanation of the origin of gradients can be found in the literature (cf. “localized high-temperature fluids” of Wilson et al. (2003), “fumarolic activity” of Whelan et al. (2003), and trends “correlative with zeolitization intensity in the Calico Hills Formation” of Whelan et al., 2008).
3. The observed, east-west gradients in the ESF area require the heat source to be located to the east of the ESF. This is in direct conflict with the MICH model, in which the source of heat is located to the north of the ESF, under the Timber Mountain caldera. The observed structure of the paleothermal field is a strong argument against the MICH model.
4. An argument can be made that the exact configuration of the paleothermal field depicted in Fig. 5 is uncertain because for some areas in the ESF it is constrained by a limited number of measurements; therefore, different configurations of isotherms can be drawn (Wilson and Cline, 2005, Sect. 2.1). This argument is legitimate. The paleothermal field shown in Fig. 5 must be viewed as a first-order feature only. This, however, does not diminish its significance.
5. Any further development of this line of enquiry would have to include fluid inclusion and stable isotope studies of secondary minerals from numerous boreholes drilled within and outside the ESF footprint. In addition to providing better lateral coverage, such studies would provide sorely needed information on distribution of temperatures with depth.

Appendix B

Introduction, promotion, acceptance, and entrenchment of the MICH thermal model

B1 Introduction and promotion of the MICH model

The meteoric infiltration – conductive heating (MICH) thermal model was introduced by the USGS researchers in 2000 and 2001 at the annual meeting of the Geological Society of America. Two short abstracts (Marshall and Whelan, 2000; 2001) mention thermal modeling and assert that the results of simulations are in agreement with the age, and empirical thermometric data obtained from secondary minerals at Yucca Mountain (emphasis is added in all quotations below):

> *"…this trend indicates a gradual cooling of the rocks over millions of years,* ***in agreement with thermal modeling*** *of magma beneath the 12-Ma Timber Mountain caldera just north of Yucca Mountain. This model predicts that temperatures significantly exceeding current geotherm values occurred prior to 6 Ma."* (Marshall and Whelan, 2000, p. A-259)

> *"…the* ***simulations indicate*** *that modern geothermal gradients were reached at 6 Ma to 3 Ma. These results are in general agreement with paleotemperature data from fluid inclusions and isotopic compositions of secondary calcite at Yucca Mountain."* (Marshall and Whelan, 2001, p. A-375)

On 9 May 2001, J. Whelan presented the USGS results at the US Nuclear Waste Technical Review Board Meeting in Arlington, VA. In his presentation, he again asserted that thermal simulations were successful:

> *"So, to conclude, both fluid inclusions and calcite delta O-18 indicate elevated temperatures during the early and intermediate stages of calcite formation. Those temperatures are consistent with a likely thermal history of*

> *the unsaturated zone tuffs as indicated by the age constraint temperature data and by* ***thermal modeling****".* (NWTRB, 2001, p. 151)

The record demonstrates, however, that contrary to these repeated assertions, simulations carried out by USGS researchers in 2001 failed to reproduce the empirical temperatures and times. The document (BSC, 2004a), in which the USGS modeling effort of 2001 was evaluated states:

> *"Marshall and Whelan (2001) concluded that the presence of a long-lived magma chamber at the Timber Mountain volcanic center could account for elevated thermal conditions in the vicinity of the repository up to around 6 Ma. However, closer evaluation of the model results depicted in Fig. H-3 indicate that the magmatic activity at Timber Mountain as represented by these simulations would only produce minor and relatively short-lived thermal perturbations for the Yucca Mountain area."* (p. H-9-H-10)

Despite the failure of the simulations to validate their model, between 2001 and 2008, the authors of the MICH model continued to promote it by repeating assertions regarding the success of thermal modeling:

> *"Warmer depositional temperatures in the past reflect the prolonged thermal input to the UZ from the ongoing regional magmatic activity . . . Yucca Mountain tuffs were erupted between 15 and 11 Ma (Sawyer et al., 1994) from large caldera complexes only ~ 10 km to the north.* ***Simulations indicate*** *that these Miocene magma chambers would have disturbed local heat-flow regimes on the multi-million-year time scales producing elevated UZ temperatures to 6 Ma or younger (Marshall and Whelan, 2000, 2001; Whelan et al., 2001)."* (Whelan et al., 2002, pp. 746–747)

> *"****Modeling of thermal history*** *indicates that the prolonged cooling of the UZ is consistent with heat flow produced by the regional magmatic activity*

responsible for widespread silicic volcanism 15 to 11 Ma, including the tuffs at Yucca Mountain." (Whelan et al., 2003, Sect. IV)

*"**Simulations** of temperatures in the upper crust around a large intrusive heat source to the north indicated that cooling of the UZ at Yucca Mountain could have taken until 4–6 Ma, which is consistent with the fluid inclusion thermochronology . . . ."* (Whelan et al., 2004, p. 1884)

*"These highest temperatures of deposition are explained in Marshall and Whelan (2001) with **a thermal model** . . . that links the slow cooling of the UZ at Yucca Mountain to the cooling magma body beneath the Timber Mountain caldera complex. . . . The driving mechanism is dissipation of a large amount of thermal energy emplaced at shallow crustal levels via magmatic processes."* (Marshall et al., 2005, p. 221)

*"**Simulations using the HEAT code demonstrate** that prolonged cooling of the unsaturated zone is consistent with magmatic heat inputs and deep-seated (sub-water table) hydrothermal activity generated by the large magma body ∼ 8 km to the north that produced the 15–11 Ma ash flows and ash falls that make up Yucca Mountain."* (Whelan et al., 2008, p. 1041)

*"Slow cooling of the unsaturated zone is, however, consistent with thermal models of regional heat flow around the large magma chamber ∼ 8 km north of Yucca Mountain that produced the voluminous 15- to 11-Ma ash flow and ash-fall tuffs that compose Yucca Mountain. **The simulations approximate** the thermochronology of secondary mineral deposition recorded in the unsaturated zone."* (Whelan et al., 2008, p. 1072)

B2 Acceptance by DOE

Despite the lack of documentation and validation of the MICH thermal model, discussed in the previous section, the model was hastily accepted by the US Department of Energy in 2001 and implicitly included in the Yucca Mountain Science and Engineering Report (DOE, 2001). In the latter document, the elevated temperatures measured in fluid inclusions were dismissed by relating them to "...a well-documented thermal period that affected the volcanic rock for a long time after its formation" (p. 4-402). The Report was used in the process of recommending the Yucca Mountain site to President Bush, who accepted the recommendation and sent it to the Congress. The Congressional resolution approving the President's recommendation was signed into law in June 2002. It now appears that both the recommendation of the President and subsequent approval of the Congress were based, at least in part, on untested scientific conclusions that failed to pass the veracity test.

When technical data on the USGS modeling were published by the DOE contractor (BSC, 2004a) the flawed character of the MICH model became apparent. Amazingly, despite the problems discussed in it, the document offered the following overall conclusion regarding the MICH model:

> *"In summary, while the thermal model simulations of Marshall and Whelan (2001, 2004) do not predict a thermal event that is as prolonged and pronounced as that recorded by secondary minerals at Yucca Mountain, their general model provides a mechanism to account for the presence of elevated temperatures between 10 and 6 Ma."* (p. H-12)

The latter statement does not appear to be a sound scientific judgment. It is hard to comprehend how a model which so utterly failed to match the benchmark empirical data (cf. Fig. 4a)"provides a mechanism" to account for these data.

In an Analysis Model report discussing features, events, and processes to be considered in the Yucca Mountain Total System Performance Assessment for License Application, the MICH thermal model was used as a key argument, to base the exclusion of hydrothermal activity from consideration (BSC, 2004b) (see analysis in Dublyansky, 2007). The latest (pre-License Application) version of this report (SNL, 2008) also relies on the purported outcomes of thermal modeling.

In 2004, DOE published a major document, Yucca Mountain Site Description (BSC, 2004c), which supports the Yucca Mountain License Application. This document also contained an inaccurate claim with respect to the validation of the MICH conductive heating model:

> *"Two-dimensional conductive/convective thermal modeling of an idealized upper-crustal section at Yucca Mountain indicates that modern geothermal gradients were established by 6 Ma (Marshall and Whelan, 2000). These results are consistent with the cooling history observed in unsaturated zone secondary minerals."* (BSC 2004c, p. 7–81)
>
> *"Although Yucca Mountain thermal evolution based on these data require that heat dissipation from Miocene magmatic activity extended through longer periods of time than those expected by some (Dublyansky, 2001), results are consistent with heat-flow models involving multiple injections of large magma bodies at shallow crustal levels."* (BSC 2004c, p.7–84)

B3 Acceptance by NRC

The US Nuclear Regulatory Commission staff reviewed the modeling results presented in the (BSC, 2004a) document. The review states:

> *"Additional thermal modeling by Marshall and Whelan (2001) suggests that the long-lived, near-surface thermal perturbation at Yucca Mountain* ***could not be reproduced*** *by their thermal models, which predicted much faster cooling than inferred from oxygen and strontium isotope analyses in secondary minerals. . . ."* (NRC, 2005, p. 15)

The NRC review cites the four auxiliary hypothetical mechanisms proposed in BSC (2004a) to explain greater-than-modeled temperatures and cooling times at Yucca Mountain (i.e., sustained magmatism; magmatic intrusions outside the caldera; additional overburden; and lateral outflow of hydrothermal fluids). The NRC report was explicit in stating that none of these hypothetical mechanisms is supported by site-specific factual evidence:

> *"There is little evidence to support DOE's scenario of sustained magmatism and, thus, sustained heating of crustal rocks within the Timber Mountain caldera."*
> *"... DOE does not cite any information to support the scenario of a hidden magmatic intrusion occurring south of the Timber Mountain or Claim Canyon caldera boundaries."*
> *"... DOE does not provide a technical basis to account for the thickness of potentially missing deposits needed for this scenario. In addition, DOE does not discuss how much additional burial would be needed in this scenario to account for paleotemperatures measured in 6 to 11 million year minerals at Yucca Mountain."*
> *"... DOE does not present a model for advective hydrothermal flow from the cooling Timber Mountain caldera. ..."* (NRC 2005, pp. 16–17)

The NRC review rejects the first three mechanisms, but does accept the fourth:

> *"Subsurface outflow of hydrothermal fluids from the Timber Mountain caldera system, however, appears a credible scenario to account for elevated paleotemperatures preserved in 6 to 11 million year minerals at Yucca Mountain."* (NRC 2005, p. 17)

Astonishingly, the only argument put forth by the NRC staff to justify this acceptance was a vague statement that: *"... such flows are commonly observed in geothermal systems that occur above and adjacent to large-volume magma bodies (e.g., Goff et al., 1988)"* (p. 17). The reason why the NRC reviewers decided to cite general observations on geothermal systems, ignoring the substantial body of site-specific information in this regard, is unclear. Subsurface outflow of thermal fluids is known to have occurred at Yucca Mountain between 10.5–11.0 Ma, but only affected the deep-seated part of the rock sequence (below ca. 1000 m). Mineralogical, fluid inclusion, and isotopic evidence (Bish and Aronson, 1993, Sect. Paleogeothermal conditions; Feng et al., 1999, Sect. 4.1) and thermal modeling (Dublyansky and Polyansky, 2007, Sect. 4.3.3) indicate that this hydrothermal system did not cause heating of the unsaturated zone rocks commensurate with the fluid inclusion temperatures. There is little doubt that if the site-specific information were used, this hypothetical mechanism would also have to be rejected. Tenuous acceptance of the "subsurface outflow" conjecture allowed NRC to accept the MICH model as a whole:

> *"Although studies of secondary minerals at Yucca Mountain by several organizations continue to this date, the NRC staff consider the conceptual model proposed by DOE for secondary mineral deposition at Yucca Mountain is generally consistent with available lines of evidence, notwithstanding remaining uncertainties in the age, timing, and origin* [sic!] *of the thermal perturbations that produced elevated temperatures evidenced by fluid inclusions. . . ."* (NRC, 2005, p. 17)

In view of the discussion above, this NRC decision to accept the MICH model does not seem to be scientifically defensible.

B4 Acceptance by scientific community

The model of Marshall and Whelan (2000) was used to explain the elevated temperatures measured in the Yucca Mountain fluid inclusions by Wilson et al. (2003):

> *"Elevated temperatures within the sequence could be expected for a few million years following intrusion of the Timber Mountain Caldera at around 10 Ma (Marshall, 2000)."* (Sect. 7.6)

Bryan et al. (2009) used the MICH model to constrain thermal history of Yucca Mountain in their study of the dissolution rates of feldspar in the Topopah Spring Tuff:

> *"The available thermochronologic data for the Topopah Spring Tuff were compiled by Whelan et al. (2008). They also generated a **thermal model**, involving magmatic heat input from the nearby Timber Mountain volcanic center, which fit the thermochronologic data . . . ."* (Sect. 3)

B5 Summary

Being cited in many technical publications over the past 9 yr, the notion that the meteoric infiltration – conductive heating (MICH) model has been validated by thermal modeling has become entrenched in the scientific record. Meanwhile, examination of the available modeling results reveals no modeling outcomes which produce a satisfactory match with the empirical benchmark data.

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Table 1. Comparison of parameters used in thermal simulations of the MICH model by Marshal and Whelan (2001) and Whelan et al. (2008) with realistic parameters for the Timber Mountain volcanic center.

Modeled	Realistic
Depth of emplacement	
2.5 km	Up to 10-12.5 km (Warren et al., 1989; Mills et al., 1997).
Thickness of magma body	
7 km	Could be as small as 1–2 km (Bindeman and Valley, 2003)
Shape and dimensions of magma body in plan view	
Circular, diameter 30 km	Rainier Mesa caldera* – ellipse 17 × 12 km; Ammonia Tanks caldera – 9 × 6 km; post-11.45 Ma resurgent dome – between 6.5 × 3.5 km and 9 × 6 km.
Distance to the target block	
4 and 8 km	Rainier Mesa caldera – 9–11 km; Ammonia Tanks caldera – 16–17 km; post-11.45 Ma resurgent dome – 16–19 km.
Initial temperature of magma	
900–1000 °C	700–750 °C (upper part) to 900–950 °C (lower part) (Mills et al., 1997; Bindeman and Valley, 2003)
Residence time of magma	
Permanent emplacement (no evacuation)	Between 10 and 100 thousand years for early plutons, followed by eruptive evacuation (Bindeman and Valley, 2003). Permanent for the post-11.45 million year-old resurgent dome.

[*] Structural boundaries of calderas provide the best estimate of the shapes of the underlying magma chambers (e.g., Smith and Shaw, 1978). Whelan et al. (2008, Sect. 6.3) speculated that the pluton under the Timber Mountain caldera could have had a subsurface footprint that extended beyond the caldera margins (i.e., closer distance to reference point). There is no site-specific information supporting this conjecture.

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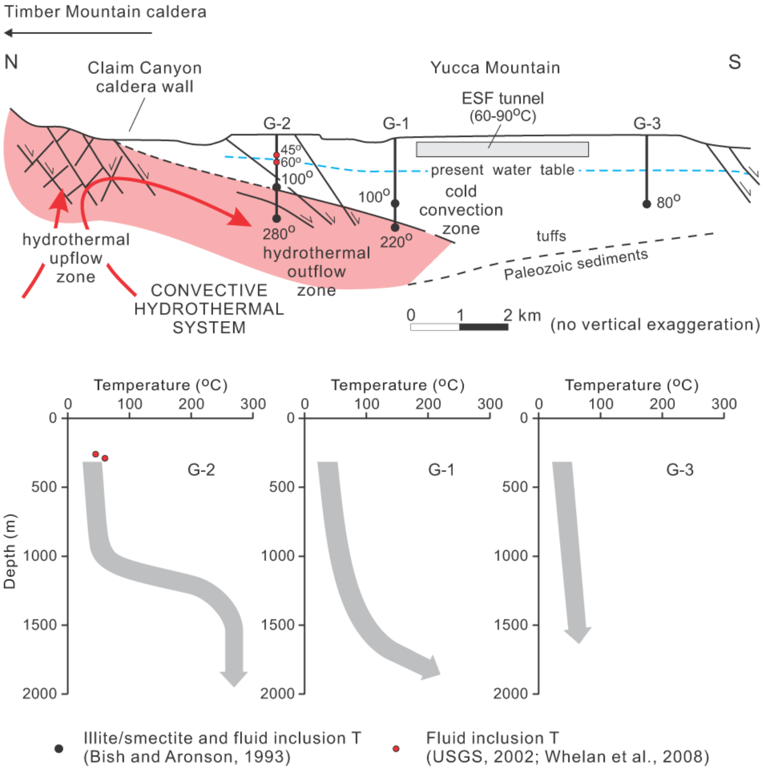

Fig. 1. Reconstruction of the Timber Mountain hydrothermal circulation system near Yucca Mountain 10.0–11.5 myr ago (upper figure) and schematic temperature profiles for boreholes USW G-1, G-2 and G-3 estimated from illite/smectite mineralogy and fluid inclusion data (lower figure). Modified from Bish and Aronson (1993). Box in the upper figure shows the approximate location of the ESF tunnel complex, from which elevated fluid inclusion temperatures were obtained.

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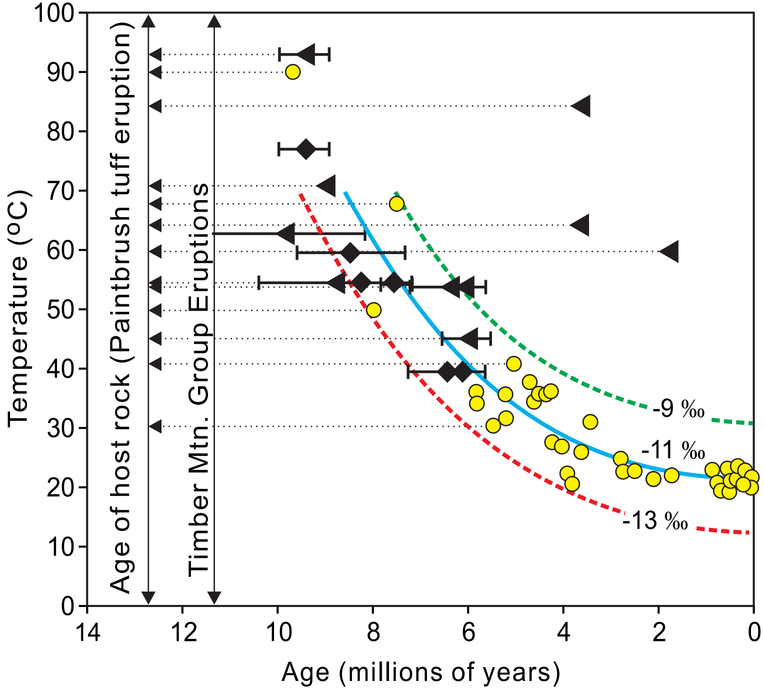

Fig. 2. Fluid inclusion homogenization temperatures and temperatures calculated from calcite δ^{18}O values (from Whelan et al., 2003). Fluid inclusion temperatures tightly constrained by ^{235}U/^{207}Pb ages are plotted as black diamonds. Triangles indicate temperatures for which a ^{235}U/^{207}Pb age provides only a minimum age for calcite. Error bars are shown at 2σ. Temperatures calculated from calcite δ^{18}O values and constrained by U-Pb or U-series ages are shown as circled dots. Curves are best fits to the temperatures calculated from calcite δ^{18}O values for deposition from waters with δ^{18}O = −13 ‰, −11 ‰ or −9 ‰. (Copyright ©2003 by the American Nuclear Society, La Grande Park, IL, USA).

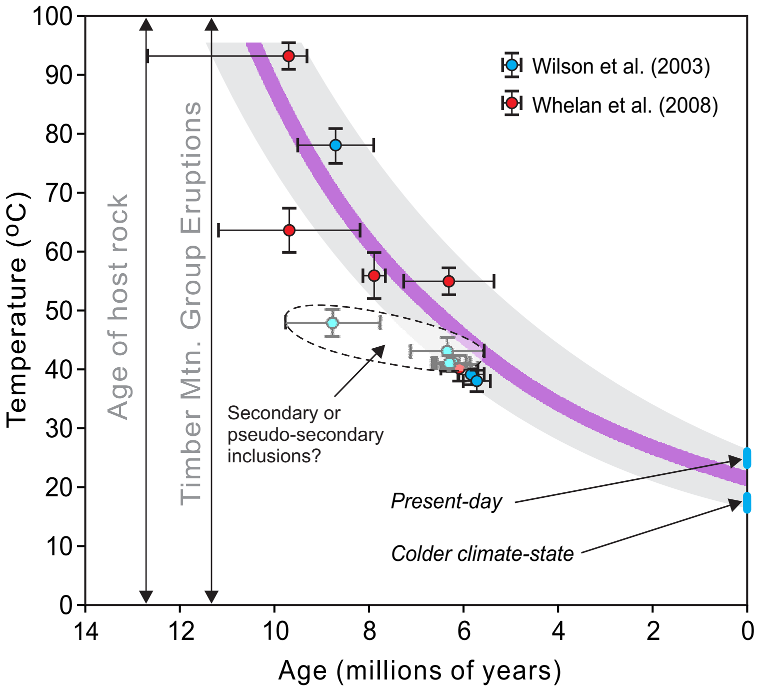

Fig. 3. The proposed benchmark for thermal modeling at Yucca Mountain. The benchmark is constrained by fluid inclusion temperatures paired with ^{235}U/^{207}Pb ages (data from Wilson et al., 2003; Fig. 8 and Whelan et al., 2008; Table 1 and 4) and the range of temperatures expected in the unsaturated zone of Yucca Mountain during different Pleistocene climate states (shown at zero age).

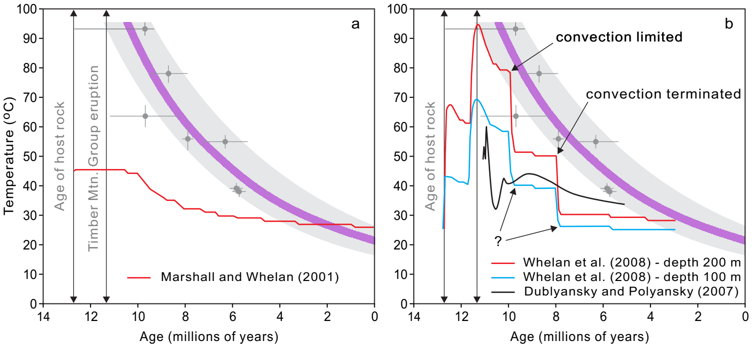

Fig. 4. Comparison of the modeling results with the benchmark. **(a)** The "best" result of Marshal and Whelan (2001; as reposted in BSC, 2004a). Lateral distance from southern limit of the magma chamber is 4 km, depth from surface is 400 m. Modeled scenario included prolonged magmatic pre-heating (15 to 11 Ma) by a very shallow (2.5-km-deep) magma chamber, and the presence of a 2-km thick convection system above the magma chamber. **(b)** Results of Whelan et al. (2008; Fig. 8). Lateral distance from southern limit of the magma chamber is 8 km, the present-day depths from surface are 100 m and 200 m. Model scenario included introduction of magma chambers at 12.8 and 11.4 Ma. The simulation considers the effects of convection outside the magma chamber, which was limited to shallow zones at 10 Ma and terminated at 8 Ma (the reasons for abrupt slowing-down of cooling at ca. 9.7 Ma and 7.9 Ma are not clear from description in Whelan et al., 2008). The model also assumes an additional 100 m of volcanic overburden deposited at Timber Mountain time (vertical double-headed arrow) that was subsequently eroded at a constant rate. The result of Dublyansky and Polyansky (2007, Fig. 10b) for lateral distance from pluton of 7 km and depth of 250 m is shown for comparison (non-monotonic character of the line reflects transient convection effects in full-3-D conduction + advection simulations).

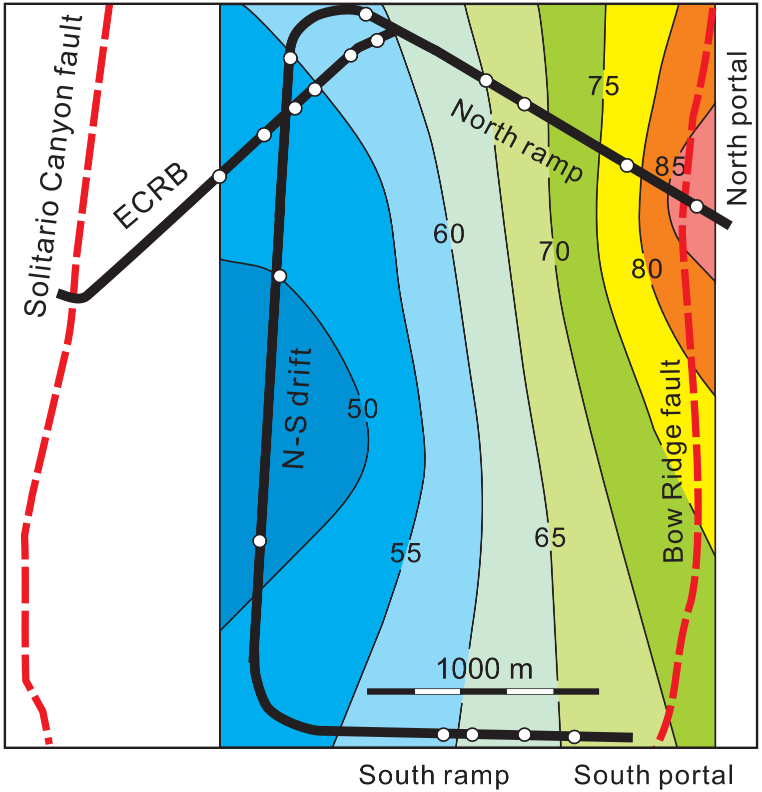

Fig. 5. Reconstructed field of maximum paleotemperatures (°C) in the repository block, at the ESF level (based on the data reported in Dublyansky et al., 2001; Wilson et al., 2003; Whelan et al., 2003, 2008).

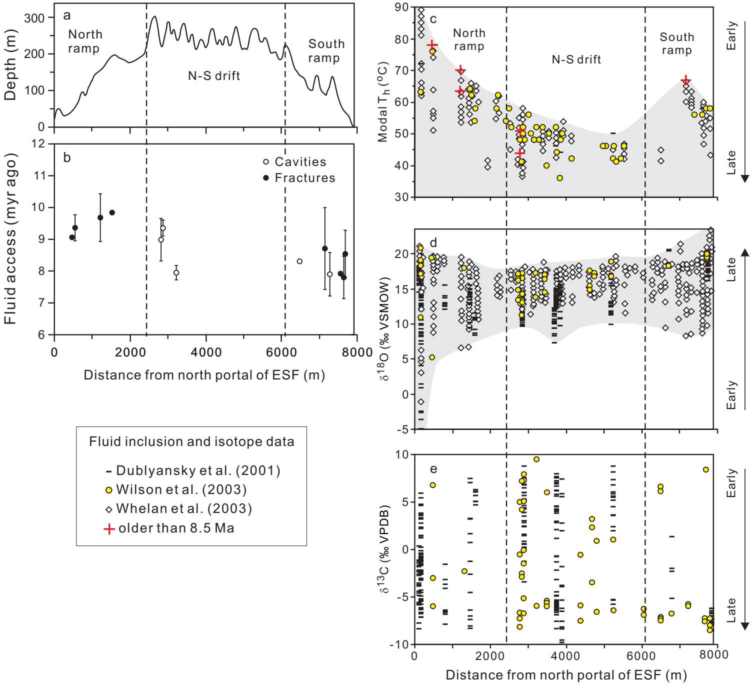

Fig. A1. Characteristics of secondary calcite from ESF tunnel: **(a)** depth from topographic surface along the ESF; **(b)** oldest U-Pb age dates for different locations in the ESF; **(c)** maximum modal values of the homogenization temperatures; **(d)** δ^{18}O properties; and **(e)** δ^{13}C properties. U-Pb ages in b are from Neymark et al. (2002), Wilson et al. (2003), and Whelan et al. (2008). Red crosses in c indicate temperatures older than 8.5 Ma (data from Wilson et al., 2003; Whelan et al., 2008). Each mode shown in c was calculated on the basis of tens to hundreds of individual measurements reported in Dublyansky et al. (2001), Wilson et al. (2003), and Whelan et al. (2003). Vertical dashed lines correspond to the bends in the ESF (cf. Fig. 5).

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