DOCTORAL SCHOOL OF GEOSCIENCES

MICROSTRUCTURE, GEOMETRY AND HYDROGEOLOGY OF THE FRACTURE NETWORK OF THE BODA CLAYSTONE FORMATION

A BODAI AGYAGKŐ FORMÁCIÓ TÖRÉSHÁLÓZATÁNAK MIKROSZERKEZETE, GEOMETRIÁJA ÉS HIDROGEOLÓGIÁJA

THESES OF THE DOCTORAL DISSERTATION

AUTHOR

EMESE TÓTH

SUPERVISORS

TIVADAR M. TÓTH, DSC

FÉLIX SCHUBERT, PHD

DEPARTMENT OF MINERALOGY, GEOCHEMISTRY AND PETROLOGY

FACULTY OF SCIENCE AND INFORMATICS

UNIVERSITY OF SZEGED

SZEGED

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I. INTRODUCTION AND AIMS

This dissertation extensively examines the brittle structural elements of the Boda Claystone Formation (BCF), which could serve as a host formation for high-level radioactive waste in Hungary (Konrád & Hámos, 2006). Despite the formation's low porosity and permeability, which give its retentive features, it is crucial to assess the tectonic setting of the rock body to comprehend the timing and magnitude of faults and folds. This analysis enables an evaluation of the tectonic development of the host rock and the hydrogeological significance of the tectonic features (Delay, 2010).

The idea behind the research is that each successive phase of the study examines the problem at an increasing scale, from microstructural observations to models of the fracture network based on more than one borehole. Even the microscale investigations of individual fracture network segments contribute to the understanding of the behaviour of the whole fracture network. The main goals of this study were to identify the geometry and hydrogeological properties of the fracture network of the Boda Claystone Formation as well as the investigation of the spatial extensibility of the properties of the fracture network.

The BAF–2 well was regarded as a base well in this study because it explores the maximum thickness of the formation (917 m) with almost 100% core recovery and offers unique opportunity to evaluate its brittle structural elements. In addition, the analysis of the BAF–4 well was also done to investigate the extensibility of the properties of the fracture system.

II. APPLIED METHODS

This study used a wide range of techniques to thoroughly examine the brittle structures of the formation at various scales. Petrographic analysis was carried out in thin sections with a standard Olympus BX41 polarising microscope equipped with Olympus DP73 digital microscope camera.

Three distinct techniques were used in the analysis of the shear zones to estimate the volume change and the shear strain of the shear zones. The first method is based on the shape of the sigmoidal veins. According to Lisle (2013), sigmoidal veins can form in two ways, namely the passive rotation and the folded bridge models. These offer different methods for calculating the shear strain and volume change within the shear zone based on measurable geometric parameters, such as the angle

between the sigmoidal tip and the shear zone boundary, shear zone thickness, etc.

In the second method applied, mass-balance calculations on the bulk chemical components of the wall rock and shear zone were used. The bulk rock chemical analyses were performed in the Bureau Veritas Mineral Laboratories, Canada, using the LF100 and XF702 analytical packages.

Gresens (1967) investigated the composition and volume relationship of the metasomatic modification process and developed equations for computing gains and losses from chemical analyses. The following equation were used to determine the interrelationships between volume change, composition, and density between unaltered and altered types of the same rock:

$$\Delta m_i = f_v(\rho_a/\rho_0)C_a^i - C_0^i \quad (1)$$

where Δm_i is the mass change in component i, f_v is the volume factor, the ratio of the final volume to the initial volume, ρ_0 and ρ_a represent the original and the altered rock densities, C^i_a and C^i_0 are the initial and the final concentrations of component i. If $f_v = 1$, the alteration process occurred on the constant volume. When $f_v < 1$ volume loss, fv > 1 volume gain occurs in the alteration (Gresens, 1967).

The isocon approach, which is a visual solution to the problem of Gresens (1967), was later proposed by Grant (1986). Concentration of a component in the original and altered rocks shows a linear relationship in the isocon diagram. In the diagram points indicate the proportions of elements of the altered and unaltered rock. The immobile elements must lie along an isochemical line or isocon that goes through the origin. In the altered rock, if the points are above the isocon line the concentration of the element increased while those fall below the isocon line are lowered.

In order to verify the density-change of the shear zone, a Bruker Skyscan 2211 cone-beam scanner was used to perform the micro-CT (micro-computed tomography) scan measurements. The following X-ray source settings were used: 168 kV source voltage, 50 a source current, and a 50 ms exposure duration for each measurement. To perform this measurement, the representative elementary rock volume (REV) of the specimens was determined with image analysis using ImageJ software (version 1.51).

Independent of the lithology and structural history, fracture networks typically follow a fractal-like structure (Barton and Larsen, 1985). This characteristic enables to use the observed geometric data to

simulate fracture networks at any scale. Discrete fracture network (DFN) models are built on an understanding of two components: the geometry of the fracture system and the aperture of each individual fracture (Barcelona et al., 2020). This modelling approach enables the estimation of interconnectivity, porosity and permeability of the fracture system.

To generate a discrete fracture network model, Infress fracture network modelling program was used in this study. Fracture length, fracture density, fracture orientation, and fracture aperture are the necessary variables to create DFN models. The P10 parameter and the fractal dimension were used to determine the fracture density. The P10 parameter gives the number of fractures per meter.

According to M. Tóth (2010), calculating the fracture length requires the knowledge of the number of fractures determined by two distinct techniques of different resolution limits. The parameters of the fracture length distribution can be computed based on this difference and the detection limits of the methods used. The number of fractures detected by the less sensitive approach is unavoidably less than that seen by the more sensitive way.

In our study, we calculated the exponents of the fracture length distribution using acoustic borehole televiewer (BHTV) data and core images. Orientation of the fractures are determined by their dip and dip direction, which is recorded by the BHTV. Fracture aperture coefficient was calculated with aperture calibration, which is based the well aquifer test and the DFN model. The effective porosity of the fracture system can be obtained from the aperture of the fractures.

The flow zone indicator (FZI) was used to define the hydrodynamic characteristics of the rock body. This indicator, based on the relationship between permeability and porosity, is frequently used to assess the quality of reservoirs. Additionally, this index can establish hydraulic flow units (HFU) where the geological and petrophysical characteristics that govern fluid flow are internally consistent (Amaefule et al., 1993). FZI can be calculated as:

$$FZI = \frac{RQI}{NPI} = \frac{0.0314\sqrt{\frac{K}{\Phi}}}{\frac{\Phi}{(1-\Phi)}} \quad (2)$$

where FZI is the flow zone indicator in μm, NPI is the normalized porosity index, RQI is the reservoir quality index, k is the permeability in mD, and Φ is the porosity in a volume fraction.

Multiple linear regression analysis was used to determine the relationship between the fracture density and the geophysical log data. Multiple linear regression analysis is a statistical technique used to determine how closely one dependent variable (Y) relates to a cluster of independent variables X_k ($k = 1, 2, \dots, p-1$):

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_{p-1} x_{i,p-1} + \varepsilon_i \qquad (3)$$

where β_0 represents the intercept, also called the constant (the mean of Y when all $X_k = 0$), and each βk represents a slope with respect to X_k, ε_i is the *ith* error. The β_k are called partial regression coefficients (Eberly, 2007).

In this case, fracture density is the estimated dependent variable. The independent variables are those that have an impact on fracture density. In the current study, the independent variables are the geophysical well data. The correlation coefficient is a numerical assessment of the degree of the linear relationship between the properties. In our work, we used the statistical program IBM SPSS to evaluate the relationship between the geophysical logs and the fracture density of the formation.

III. NEW SCIENTIFIC RESULTS

1. *En échelon* veins of the BCF can be interpreted as pennant veins whose kinematics are controlled by Riedel conjugate fractures. Sigmoidal shaped *en échelon* veins are peculiar structures of the BCF. The veins developed without the sign of pressure solution in shear zones in contrast to the general model. Their formation begins from initial flaws of the shear zone; triangular terminations arise at the tip of these localised shear planes. This triangular shape at the end of the veins is formed with rotation and slip of the shear fractures. Between these initial shear planes, rhombus-shaped vein segments could develop during the evolution of the shear zone with the rotation of these a sigmoidal-shaped vein could form. Mineral precipitation can also occur in the middle part of these shear planes if the orientation becomes favourable for vein opening induced by rotation by the shear zone. At the end of the process, a sigmoidal-shaped vein could form by connecting vein segments and continuous mineral precipitation.

2. The shear zones of the BCF underwent volume loss despite vein formation and the precipitation of minerals. Based on the isocon-method and the micro-CT measurements, 5–8% volume loss occurred in the shear zones. Despite the volume loss, the mass of the shear zone increased based on the isocon method. Assuming immobile

Ti, the shear zone enriched in Ca, Mn, Ba, Sr and S relative to the host rock. The mineral composition of the veins explains the enrichment of these elements. Precipitation of minerals may have been responsible for the mass gain and could also cause volume gain. However, the shear zone carries volume loss. Consequently, the rate of volume loss must have been higher than the overall volume gain generated by mineral precipitation. The volume loss occurred in the rock bridges between the veins, where the 2D porosity is significantly less than in the wall rock outside the shear zone. Micro-CT measurements showed that the density of the rock bridges was also higher than the wall rock. I propose that the volume loss is the result of the partial porosity reduction of the shear zones that is caused by tectonic compaction.

3. A large-scale fault can be interpreted in the BAF–2 well at 400 m based on fracture density, geophysical well log data and sedimentological observations. The rock body of the BCF in the BAF–2 well can be divided into two major sections based on the properties of the fracture network. The characteristics of the fracture density differ significantly in the upper half (0–400 m) and the lower half (400–915 m) of the well. The upper section is intensively and uniformly fractured, while the lower half contains significantly fewer fractures. In the lower half three distinct fractured zones could be traced where the fracture density increases. The lithology of the well is relatively homogeneous, although coarser-grained layers appear more frequently with depth. While changing grain size may impact the fracture density, tectonic processes predominantly determine where the highly fractured zones are located. At 400 m, the geophysical parameters of the formation change significantly, and there are stratigraphic irregularities, such as overturned beds and changes in graded sequences, indicating a large-scale structural element.

4. Seven hydraulic flow unit and two poro-perm trends can describe the hydraulic behaviour of the rock body in the BAF–2 well. The most part of the rock body conforms to one trend; the homogenous lithology of the well comes with uniform hydrodynamic characteristics. Only three narrow sections (at 100, 400, and 700 m) differ from this primary poro-perm trend. These sections define individual hydraulic units based on their flow zone indicator (FZI) value. The first zone occurs between 60 and 110 m. In this section, porosity decreases considerably more than permeability. The hydraulic properties of this section were altered by weathering as a result of the long-term near-surface exposure of the formation. The second zone is

located between 350 and 420 m; the fault zone forms an independent hydraulic unit with elevated FZI. The third zone, where the FZI values are higher than the average, is between 690 and 770 m. In this zone, the lithology changes, and fine-sandstone layers are more common, which could influence the hydraulic behaviour of the rock body. On the other hand, the sonic log disruption in this HFU resembles the behaviour seen at about 400 m; therefore, the effects of a large-scale structure at this depth cannot be ruled out either.

5. **Five possible fracture network geometries could be distinguished based on the modelling in the BAF–2 well.** In some cases, the fracture network forms one communicating group along the well. In many cases, two connected subsystems appear that do not communicate with each another. In other modelling runs, the subgroup boundaries can be found at 300, 400 or 700 meters. Most models suggest that the fracture system of the well is separated at 100, 400, and 700 m into four fracture subgroups. The same horizons are designated by the interconnecting fracture clusters and the hydraulic flow units in the well.

6. **Fracture density can be predicted in the BCF based on the density and resistivity logs.** Based on multiple linear regression density and resistivity are the primary determinants of the fracture density in BAF–4 and BAF–2 wells. In the upper part of the BAF–4 well, which was the training section of the regression analysis, a strong relationship was identified with a good fit, $R^2 = 0.767$. The correlation equation was validated in the lower part of the BAF–4 well ($R^2 = 0.630$). I predicted the fracture density of the BAF–2 well using the same method ($R^2 = 0.701$). The fracture density could be predicted with high accuracy in sections with the typical lithology of the BCF. The prediction is less precise in other situations where the lithological characteristics of the claystone are untypical. Fine sandstone layers are present in the lower part of the formation and this grain size variation affects the geophysical characteristics of the rock body. The regression function underestimates the fracture density of the rock body in these sandy areas. Fracture density of the BCF can be predicted with relatively high accuracy with the established regression equation in wells without BHTV from conventional geophysical well log data.

ÖSSZEFOGLALÁS

Jelen értekezés a Bodai Agyagkő Formáció (BAF) töréses szerkezeti elemeit vizsgálja igen széles vizsgálati tartományban. A tanulmány fő

célja töréshálózat geometriájának és hidrodinamikai tulajdonságainak, valamint a repedésrendszer tulajdonságainak térbeli kiterjeszthetőségének meghatározása két fúrás alapján.

Dolgozatomban a nyírási zónákban található szigmoidális erek petrográfiai vizsgálata vékonycsiszolatokon történt. A nyírási zónák térfogat- és sűrűségváltozását az erek geometriája alapján (Lisle, 2013), izokon-módszerrel (Grant, 1986) és mikro-komputertomográfiával elemeztem. A töréshálózat geometriáját diszkrét törésekből felépülő töréshálózat modellezési módszerrel vizsgáltam (Barton és Larsen, 1985), míg hidrológiai tulajdonságait az áramlási zóna indikátorral jellemeztem (Amaefule et al., 1993). Ez a mutató a porozitás és permeabilitás alapján hidraulikus áramlási egységeket jelöl ki. A töréshálózat és a lyukgeofizikai szelvények kapcsolatát többszörös lineáris regressziós analízissel vizsgáltam.

Petrográfiai megfigyelések alapján a BAF-ban található szigmoidális hasadékok „pennant" erekként értelmezhetők, amelyek kialakulását Riedel konjugált törések okozták. A nyírási zónákban az érképződés ellenére 5-8%-os térfogatcsökkenés ment végbe. A töréshálózati modellezés alapján a BAF–2 fúrásban öt töréshálózati geometria különböztethető meg. Némely modellben a töréshálózat kommunikáló rendszert alkot a fúrás teljes hosszában, míg más esetekben egymással nem kommunikáló alrendszerekre bomlik 100, 400 vagy 700 m mélységben. A törésrendszer hét hidraulikai egységre bontható, amelyek határai egybeesnek a töréshálózat konnektivitása alapján kijelölt határokkal. A fúrás felső 100 méterében a kőzet hidrológiai tulajdonságait a mállás befolyásolta. A fúrás által harántolt kőzetoszlop a töréshálózat tulajdonságai alapján két, egymástól igen eltérő szakaszra osztható fel, amelyek között 400 m-es mélységben egy vető található. A képződmény hidrológiai tulajdonságai 700 méteren a finomszemű homokkő rétegek befolyásolták.

Többszörös lineáris regressziós analízis alapján a BAF töréssűrűsége megbecsülhető a sűrűség és ellenállás szelvények alapján. A regressziós egyenlet alkalmazásával az akusztikus lyukfaltelevíziós adatokkal nem rendelkező fúrásokban is becsülhető a töréssűrűség.

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CO-AUTHOR STATEMENTS

I, Ervin Hrabovszki, hereby declare that the role of the doctoral candidate in the publication of

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was decisive that I have not used it to obtain a scientific degree and will not do so in the future.

Szeged, 20.02.2023.

Ervin Hrabovszki

I, Félix Schubert, hereby declare that the role of the doctoral candidate in the publication of

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Félix Schubert

I, Tivadar M. Tóth, hereby declare that the role of the doctoral candidate in the publication of

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Szeged, 20.02.2023.

Tivadar M. Tóth

DECLARATION OF THE SUPERVISOR

I, Tivadar M. Tóth, hereby confirm that the content of the dissertation is based on the independent work of the doctoral candidate and that she has contributed decisively to the results through her independent creative activity. I consider the entire dissertation to be eligible for support from a professional and academic point of view and recommend its acceptance.

Szeged, 20.02.2023.

Tivadar M. Tóth

I, Félix Schubert, hereby confirm that the content of the dissertation is based on the independent work of the doctoral candidate and that she has contributed decisively to the results through her independent creative activity. I consider the entire dissertation to be eligible for support from a professional and academic point of view and recommend its acceptance.

Szeged, 20.02.2023.

Félix Schubert

UNIL | Université de Lausanne
Institut des sciences de la Terre
bâtiment Géopolis bureau 4893
CH-1015 Lausanne

To Whom It May Concern

Lausanne, 17.02.2023

Subject: Letter of acceptance

Dear Miss Tóth,

I am pleased to inform you that following peer-review, the Editorial Board of *Acta Geodaetica et Geophysica* has accepted for publication your manuscript entitled "Using geophysical log data to predict the fracture density in a claystone host rock for storing high-level nuclear waste", with you being first author and Ervin Hrabovszki and Tivadar M. Tóth being co-authors. The study will be published in 2023, either in the March or in the June issue of the journal. The verified proof will become available at https://www.springer.com/journal/40328 as soon as it is ready. The manuscript ID was AGGE-D-22-00148, a DOI is not yet available as of today.

Wishing you good success for your future,

Prof. György Hetényi

Editor-in-Chief
Acta Geodaetica et Geophysica

University of Lausanne
Institute of Earth Sciences
UNIL-Mouline, Géopolis-4893
1015 Lausanne
Switzerland