Preliminary Results of Elaborating a Methodology for Determining the Thermal Conductivity of Clastic Sediments Using Well Logs in Hungary

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ABSTRACT
The thermal conductivity of rocks can be deduced from available data of exploration wells such as core samples, cuttings, lithological descriptions and geophysical well logs. 70% of Hungary’s surface is covered by Neogene and Quaternary clastic sediments. The average sediment thickness is 1–2 km, but in the deepest troughs it reaches 5–8 km. As the thermal conductivity of clastic sediments is lower than the conductivity of the crystalline basement, the sediments have a significant influence on the temperature distribution and heat flow density.

By this time in Hungary most of the temperature measurements were carried out in clastic sediments. Furthermore, the thermal conductivity of more than 300 sediment core samples were measured using the Transient Line Source technique in laboratory conditions. We present a methodology for determining the thermal conductivity of clastic sediments using geophysical well logs and thermal conductivity data measured in laboratory. In general, the method determining thermal conductivity from well logs bears large significance in geothermal studies in Hungary, because orders of more thermal conductivity data can be obtained than presently available. The thermal conductivities determined by high resolution in wells can be interpolated between the boreholes by statistical methods and 3D numerical thermal models can be constructed.

Here we present our preliminary results based on the data of 3 exploration wells. Several well log combinations and thermal conductivity measurements from 96 core samples were used to work out the method. The lithological composition consisting of shale, sand, marl and water were identified and the volumetric fractions of these components were derived from wireline logging data such as natural gamma ray, resistivity, bulk density and neutron porosity logs. The lithological composition is determined with Bayes-inversion applying the weighted least squares method. The effective thermal conductivity was computed with applying an appropriate mixing law using the thermal conductivity values of the lithological components. The thermal conductivity derived from well logs were tested using the temperature and pressure corrected archive thermal conductivity measurements of core samples.

1. INTRODUCTION
The utilization of geothermal energy in Hungary has a long tradition, because several geothermal reservoirs exist in the Tertiary sediments and buried karstified and fractured carbonates. Almost 70% of Hungary’s surface is covered by Neogene and Quaternary clastic sediments. The average sediment thickness is 1–2 km, but in the deepest troughs it reaches 5–8 km (Fig. 1.). As the thermal conductivity of clastic sediments is lower than the conductivity of the crystalline basement, the sediments have a significant influence on the temperature distribution and heat flow density. The heat flow density is one of the most important quantities in geothermal exploration, because it allows the prediction of subsurface temperature, and its local variations may originate from groundwater flow, which indicates the presence of a reservoir. Its large scale distribution is also influenced by mantle and lithospheric processes, therefore it is an important control parameter in geodynamic models. The heat flow density is determined using Fourier’s Law as the product of the thermal conductivity of rocks and the temperature gradient measured in boreholes and wells.
Figure 1: The locations of the drilling projects in Hungary. The color scale represents the thickness of Neogene sediments.

The knowledge of detailed thermal conductivity data is required to separate the conductive and convective heat flow density for instance in numerical models. It is impossible to acquire thermal conductivity data with such resolution from laboratory measurements alone. Coring processes to obtain core samples are such expensive techniques to reach a good spatial and depth resolution. This important source of data can get damaged during its transportation and analysis. However, well log data offer good resolution thus one of the main goals of the project is to develop a method to determine thermal conductivity of the Neogene clastic sediments using well logs.

In this project we have more than 300 thermal conductivity measurements on core samples which come from 12 available exploration wells (Fig. 1). By this time the whole dataset of three drillings labeled Ifrámosberény-I (Ib-I), Szirák-2/a (Szi-2/a) and Mikepércs-1 (Mp-1) were successfully collected, quality controlled and digitized. In the listed wells the following log types were accessible: spontaneous potential, natural gamma ray, resistivity, neutron porosity and bulk density logs.

There are two basic ways to establish a relationship between the thermal conductivity and well logs. First is regression analysis where a relationship between thermal conductivity and different well logging parameters (such as natural gamma ray, sonic velocity, bulk density, neutron porosity and resistivity, temperature) is determined by linear, multi-linear or non-linear methods. A review about the method is given in Blackwell and Steele, (1989); Demongodin et al., (1991); Clauser and Huenges, (1995); Hartmann et al., (2005); Fuchs and Förster (2013).

The other method is to compute the lithological composition usually consisting of shale, sand, marl and water using well logs (natural gamma ray, density, neutron porosity, resistivity etc.), and apply an appropriate mixing law amongst the components to obtain the thermal conductivity (Brigaud et al., 1990; Demongodin et al., 1991). The mixture models describing the thermal conductivity of a rock can be grouped in (1) well-defined physical models (Hashin and Shtrikman bounds) and in (2) purely empirical or semi-empirical approaches (geometric, arithmetic or harmonic mean) (Fuchs et al., 2013).

The behavior of different mixing models in case of sedimentary rocks was analyzed by several authors. In the work of Hutt and Berg (1968) bulk thermal conductivities calculated by several mixing models (arithmetic mean, harmonic mean, geometric mean) were compared to values measured with a needle probe on 28 sandstone samples. The harmonic mean showed a good fit, whereas the arithmetic and geometric mean models overestimated the measured data. Brigaud et al., (1990) mentioned the fact that the properties of certain lithotypes containing clay can change during the drilling causing systematic errors. Regarding to their work, the geometric mean model was manifested as a suitable method to calculate the bulk thermal conductivity. Hartmann et al., (2005) also concluded that the geometric mean mixing law can be a reliable choice in case of argillaceous and marly lithology. Fuchs et al., (2013) provided a validity study of simple and generally used mixing models for a two-phase rock system based on the work of Clauser (2009) based on 1147 laboratory measurements conducted on sandstone, mudstone, limestone and dolomite samples with the optical scanning method (Popov et al., 1999). The geometric mean model seemed to be the best choice with a poor coefficient of determination ($R^2=0.62$), thus they developed correction charts to increase the $R^2$ values of mixing models.

The thermal conductivity measurements on core samples were carried out with the Transient Line Source method (Dövényi et al., 1983) based on the work of Cull (1974). The average error of this measurement technique is 10–15%. The preservation of the fluid content was performed by waxing the samples. In the case of Ib-I and Szi-2/a wells more than one measurements were accomplished and documented for one sample, however only the average values of the measurements were available for the core samples of Mp-1.

Our main goal is to elaborate a methodology for determining the thermal conductivity of clastic sediments using geophysical well logs and thermal conductivity data measured in laboratory. Thus, improving the method of the determination of the thermal conductivity would significantly increase the precision of the heat flow density calculation and would increase the reliability of the
thermal models. These new heat flow density values carry the opportunity of establishing 3D conductive numerical models with increased precision which allow the detection of unknown anomalies caused by groundwater flow. Here we present our preliminary results of the attempts to elaborate a methodology regarding to the behaviour of common mixing laws in case of a three-component lithological model.

2. METHODOLOGY

2.1 Well log analysis

A geophysical inversion algorithm based on a weighted least squares method was created using the Mathcad software. The main goal of the inversion is to derive the volumetric fractions \( (\lambda_i) \) of the lithological components from wireline logging data such as natural gamma ray, resistivity (potential), compensated bulk density and neutron porosity measurements. The lithological composition — determined with Bayes-inversion — is assumed to be the mixture of clay \((c\ell)\), sandstone \((ss)\), calcite \((ca\ell)\) and water \((w)\).

The conventional inversion is based on maximum likelihood principle and the measurement noise is assumed to be additive centered Gaussian noise. In the case presented the sum of squares of the differences between the measured and the recalculated data is minimized to evaluate the best fitting parameter vector of the volumetric fractions. The correction for the input parameter vector of the inversion \( (\Delta \lambda) \) can be calculated as following (Szatmári, 2010):

\[
\Delta \lambda = R^{-1}F^TW\Delta y
\]

where \( F \) is the Jacobi’s matrix, \( W \) is the weighting matrix, \( \Delta y \) is the difference vector between the observed and the calculated data respectively and \( R \) is the so called iteration matrix described as

\[
R = F^TWF.
\]

The measured data is often characterized by different amount of uncertainties. In order to take into consideration this effect, a given weight proportional to the uncertainties is contributed to the solution. The applied weighting matrix is symmetric and its diagonal elements are the reciprocal of squares of the particular measurement’s standard deviations which were determined by the sample standard deviation formula along a clear lithological zone.

To examine the statistical features of the estimated parameters, theirs covariance matrix has been determined in every depth point which includes the squares of the parameters’ standard deviation values in its main diagonal:

\[
\sigma_i = \sqrt{C_{i,i}}
\]

where \( \sigma_i \) is the standard deviation of the i-th parameter, \( C \) is the covariance matrix of the calculated parameters in a given depth point.

As it was mentioned the lithological composition was assumed to be the mixture of four constituents, however this initial model has resulted in not only high standard deviation values for the estimated volumetric fractions but also has made the inversion process unstable. With the intention of reducing the extent of the standard deviation and making the inversion algorithm more accurate and stable, a new lithological model was created with a decreased number of components excluding calcite. We present the detailed results of the examination of relevance and pertinence of this model in Chapter 3.

2.2 Mixing models

Several mixing models were applied in this work. These are the four mostly used models: arithmetic, geometric, harmonic means and the Hashin-Shtrikman bounds. Calculating the bulk thermal conductivity \((\lambda_b)\) of a two-component rock system involves the thermal conductivity of the matrix \((\lambda_m)\), the effective porosity \((\phi)\), and the thermal conductivity of the pore content \((\lambda_p)\). Using the sensitive relationship between porosity and bulk thermal conductivity is the root of every mixing models: the thermal conductivity of the pore fluid is fairly low regarding to the matrix thermal conductivity. Porosity and the volumetric fraction of matrix can be derived from geophysical well logs.

2.2.1 Arithmetic and harmonic mean

Frequently used approaches are the arithmetic and harmonic mean, which both are based on a layered model where the thermal conductivity depends on the direction of the heat flow density. If the heat flow is parallel to the layering, the bulk thermal conductivity is equal to the arithmetic mean of the lithological components (matrix and pore content) weighted by their volumetric fractions:

\[
\lambda_b = (1-\phi) \cdot \lambda_m + \phi \cdot \lambda_p.
\]

Assuming a heat flow density perpendicular to the layering, the harmonic mean can be used to calculate the bulk thermal conductivity:

\[
\lambda_b = \frac{1}{\frac{1-\phi}{\lambda_m} + \frac{\phi}{\lambda_p}}.
\]
Regarding to Voigt (1928) and Reuss (1929), these mixing models can be defined as the upper (arithmetic) and lower (harmonic) bounds of the thermal conductivity.

2.2.2 Hashin and Shtrikman bound

Narrower bounds can be derived by the theory of Hashin and Shtrikman (1962). The upper bound represents a geometry assuming fluid-filled, spherical pores included in a solid rock matrix:

\[
\lambda_{US}^F = \lambda_m + \frac{\phi}{\frac{1}{\lambda_p} + (1-\phi) \frac{3\lambda_m}{\lambda_m - \lambda_p}}
\]  

The lower bound can be derived by assuming a geometry where the solid fraction is represented as spherical grains suspended in a fluid:

\[
\lambda_{LS}^F = \lambda_p + \frac{(1-\phi)}{\frac{1}{\lambda_m} + \phi \frac{3\lambda_p}{\lambda_m - \lambda_p}}
\]

Theoretically, the thermal conductivities of rock samples should fall in between these bounds.

2.2.3 Geometric mean

The geometric mean model is the most popular approach which is a pure empirical formula providing a simple mathematical expression to calculate the bulk thermal conductivity:

\[
\lambda_b = \sqrt[3]{\lambda_m^p \cdot \lambda_p^m}
\]

2.2.4 Thermal conductivity of lithological components

The most critical part of calculating the bulk thermal conductivity is choosing an appropriate mixing law and using correct thermal conductivity values for the given components. In this work, a three-component lithological model was utilized which means the mixture of clay, sandstone and water as pore fluid. The thermal conductivity of the sandstone and clay parameter was chosen after the work of Dövényi and Horváth (1988). The Neogene sediments of the Pannonian Basin can be divided in two broad lithological categories: pelites (including clay, claystone and marl) and psammites (including sand, sandstone and gravel). This classification was implemented on core samples used in the laboratory measurements. They established thermal conductivity – depth functions and calculated the matrix thermal conductivity of pelites and psammites using the geometric mean (Fig. 2.). Thus, in the present work, the conductivity of the sandstone and clay parameter was 4.2 and 2.8 W/(mK) respectively.

![Figure 2: Thermal conductivity vs. depth functions of pelites (a) and psammites (b) based on laboratory Transient Line Source measurements (Dövényi and Horváth, 1988.).](image)

3. RESULTS

3.1 Lithological model

Our main purpose is determining the thermal conductivity of Neogene clastic sediments for which a lithological model must be built that not only represents realistically the sediments filling in the Pannonian Basin but provides a statistically satisfying result after the inversion process.

According to stratigraphy-sedimentology study Juhasz (1994) synthesized the main lithofacies units common in the Pannonian s.l. sequence of the Neogene subbasins considering the new unified lithostratigraphic nomenclature. On the basin plain basal marls formed beginning with calcareous marl grading into argillaceous marl upwards which consists of the Endröd Formation. The
Szolnok Sandstone Formation represents the deep-water turbidite sequence of fine-grained sandstones transported from the shelf edge to the deep sea (Fig. 3.). Afterwards both the delta and basin slope sediments reach huge thickness built up by argillaceous marls and siltstones with sandstone interbeds. This depositional environment contains the Algyő Formation. In the deltaic environments large amount of littoral sediments deposited forming a thick, sandy, continuous lithofacies association which comprises the Újfalu Formation (Fig. 3.). The Zagyva Formation represents fluvial or alluvial sediments concentrated in particular regions with thin lignite beddings in some areas however in the northern part of the Pannonian Basin thicker lignite and brown coal beds formed — called Bükkalja Member — because of the negligible amount of sediment input.

Figure 3: Generalized cross-section of the characteristic depositional environments in the Late Miocene (Horváth et al., 2015.).

All of the mentioned formations are penetrated by the examined exploration wells, nevertheless the drilling labeled Szirák-2/a reached the Lower Badenian (Middle Miocene) sediments. The Lower Badenian cycle of sedimentation comprises the Hidas Formation forming brown coal beds with argillaceous sand, sandy clay marls and clay interbeddings. The Szilágy Formation represent a pelagic lithofacies with well layered silty or fine-grained sandy clays, clay marls and marls. This sedimentary cycle ended with regression in the end of the Badenian, the Kozárd Formation represents a new period of transgression in the evolutionary of the basin. The sequence deposited in littoral or even paludal, shallow and deep sublittoral environments is diversified mainly built up by arenose sands with aleurit bands. The neritic or shelf facial Tinnye Formation seems to laterally interfinger with the Kozárd Formation consisting of layered clay marls with sandstone and aleurit interbeds.

To emphasize the conclusions of the stratigraphy we summarize the main rocks occurring in this study presented: sandstone, argillaceous sand, sandy clay, silty clay, clay, clay marl, argillaceous marl, marl, aleurit, lignite and brown coal bands. On the basis of the listed elements, a lithological model assumed to be a mixture of clay, sandstone and water is acceptable and appropriate.

It was preliminary expected that the uncertainty of the inversion would increase in case of the lignite and brown coal bands. However these bands are not relevant in the aspect of this study thus the reliability of the inversion is not decreased by these sections (Fig. 4.).
Figure 4: Results of the inversion from the Szi-2/a well consisting of Badenian (Middle Miocene) sediments. This section covers the Hidas Formation where thin brown coal and lignite bands can be detected causing anomalously low bulk density values and higher standard deviations (marked with red-lined intervals). Input curves are light blue and dash lined, recalculated curves: black: natural gamma ray, red: resistivity, orange: bulk density, pink: neutron.
Our results confirm the pertinence of this lithological model which can be verified by the fitting of the recalculated log data and the standard deviations of the estimated parameters. As the example interval presented in Fig. 5, shows that the recalculated gamma ray, bulk density, neutron porosity and resistivity log are fitting satisfyingly well to the original measured data. The model was confirmed not only visually but quantitatively by examining the average standard deviation values of clay, sandstone and water fractions which are 6.7%, 4.9% and 2.7%, respectively. Nevertheless there are depth sections where the inversion is uncertain probably due to poor quality of measurement technique, but fortunately the core sampling intervals are not affected.

Figure 5: Results of the inversion from the Szi-2/a well consisting of Lower Pannonian (Late Miocene) sediments. For description of the logs see the caption of Figure 4.

3.2 Thermal conductivity
The bulk thermal conductivities — calculated by using different mixing models — were compared to laboratory measurements conducted on core samples. The first noticeable phenomenon also concluded by Hartmann et al. (2005) is that in the case of an analogous mineral composition the geometric mean model closely follows the lower Hashin-Shtrikman bound, corresponding to a rock model representing spherical grains suspended in a fluid.
Figure 6: Bulk thermal conductivity values calculated by various mixing models. (a) and (b) represent the results of the Szi-2/a and Mp-1 wells respectively, in case of intervals including clayey, marly, silty sections interbedded with fine grained sandstones contaminated with clay. (c) introduces the result of Szi-2/a representing a section containing multiple sandstone interbeds. The purple circles are the measured thermal conductivities; in case of (b) the red triangles define the error of laboratory measurements. Description of logs: dark red, H-Sh+: upper Hashin-Shtrikman bound, dark yellow, H-Sh-: lower Hashin-Shtrikman bound, green, HM: harmonic mean, dark blue, GM: geometric mean, pink, AM: arithmetic mean.

Seeking after relationships between the bulk and measured conductivities, three main trends can be observed by visual examination. (1) There are samples where the harmonic mean model seems to be an appropriate mixing law for calculating bulk thermal conductivities (Fig. 6a and 6b). (2) A large number of samples fall close to the Hashin-Shtrikman bounds or the geometric mean (Fig. 6a and 6b). (3) In the case of samples described as pure sandstones all of the mixing models used underestimates the thermal conductivity (Fig. 6c).

4. DISCUSSION AND CONCLUSIONS

According to a satisfying fitting between the measured and recalculated log data and low standard deviations of the calculated volumetric fractions, the lithological model was considered to be stable and reliable. Furthermore the agreement between the lithology defined by the inversion and described from core samples with an 80% of accuracy also confirms the pertinence of the model.
During the investigation of various mixing models, two major trends were detected. As can be seen in Fig. 7a the first group contains the mixture of clays, marls and silts, where the harmonic mean produced the best fit on the data with an average relative error of 23.2%. A dual behaviour can be observed for the harmonic mixing model: in case of clays and claymarls, the harmonic mean overestimates the thermal conductivities regarding to the laboratory data; on the other hand the model underestimates the thermal conductivity considering silty samples.

The other group in which pure and fine grained sandstones, sandstones contaminated with clay and silt were represented, the harmonic mean underestimates the conductivities. All the other mixing models are representing a dual behaviour depending on the clay content: considering samples with increased amount of clay, the mixing laws overestimate the thermal conductivity, and underestimate the values relating to pure sandstones (Fig. 7b).

![Figure 7: Crossplots of measured vs. calculated thermal conductivity data for clays, claymarls, silts (a) and for fine grained sandstones contaminated with clay (b).](image)

There can be several reasons for those sections where none of the mixing models fit to the values of laboratory measurements: (1) the dual behaviour of the mixing laws allow to deduce that other values of thermal conductivity need to be applied for clay and sandstone parameter, (2) the vertical resolution of the lithological model (10 cm) is comparable with the length of core samples, thus the model can be insensitive for thin sandstone interbeds. Furthermore, the quality of the well logging data can be a critical point as well.

In our further researches a synthetic model would like to be built on which it is possible to analyse the impact of a given mixing law on the thermal resistance used for the Bullard-plot technique and on the heat flux consequently.

For the validation of our methodology we are planning to log natural gamma ray, temperature and temperature gradient in wells that are in steady-state condition and assuming that groundwater flow does not occur. The application of this log combination is also suitable to recalculate the thermal conductivity of the lithological parameters applying another inversion algorithm and to compare these conductivities to the values used after the work of Dövényi and Horváth (1988), however all of the exploration wells’ data from the project must be processed first.

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