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Prediction of Thermal Properties for Mesozoic Rocks of Southern Germany

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ABSTRACT

In general, the variation for thermal rock properties is too large to constrain thermal characteristics at a specific site. To improve this situation, this project will provide statistically relevant data of thermal and hydraulic properties for the subsurface of Germany. In a first stage, a large number of mesozoic rock samples from the South-West German Molasse basin was studied: About 280 core samples were tested by thermal and petrophysical core scanning yielding high resolution information on thermal conductivity, density, porosity and sonic velocity of the rocks in dry and saturated condition. In addition, 100 core plugs were taken for measurements of specific heat capacity and hydraulic permeability and for XRD and XRF analyses. Thus, thermal properties could be related to the petrophysical characteristics and to the mineralogical and chemical rock composition. The geometric mixing law was confirmed as a fast and robust estimator for thermal conductivity, especially for limestones and dolomites regardless of their stratigraphic age and genetic origin. In a more sophisticated approach, the data were further used to compare and to calibrate theoretical models for thermal conductivity prediction. Rock type specific parameters were determined describing the relations between rock matrix, porosity, rock morphology, and the effective thermal conductivity. This grouping by rock type and rock generation allows an enhanced prediction of thermal properties of the mesozoic strata of German sedimentary basins.

1. INTRODUCTION

In general, the ranges of thermal and hydraulic properties given in compilations of rock properties are too wide to be useful to constrain properties at a specific site. To improve this situation, we performed a systematic study of thermal properties of major rock types in the Molasse Basin in Southern Germany. About 280 core samples were tested by thermal and petrophysical core scanning yielding high resolution information on thermal conductivity, density, porosity and sonic velocity of the rocks in dry and saturated condition. In addition, 100 core plugs were taken for XRD and XRF analysis. Thus, thermal properties could be related to the petrophysical characteristics and to the mineralogical and chemical rock composition.

2. PETROPHYSICAL PROPERTIES

Physical property distribution and statistical values were calculated for the main rock types of sandstones, dolomites and limestones (Fig. 1). Limestone samples only show small variations in the measured properties, even the samples are from different stratigraphic zones and were built under different genetic conditions. Dolomites have significantly higher density values than limestones und exhibit also higher values for the thermal conductivity and porosity. Physical properties of dolomites cover a wider range than as observed for limestones, which can be explained by the secondary building of dolomites from limestones. While rock matrix density increases by substitution of Ca-Ions by Mg-Ions (Fig. 2), rock porosity and sonic velocity decrease due to vesicles and voids formed during dolomitization. The studied dolomites show all transitions to limestones and the differences in matrix density, porosity and thermal conductivity are dependent on the degree of dolomitization.

Physical properties of sandstones show a strong data scattering (Fig. 2). This is especially valid for the thermal conductivity covering a value range from 2.3 W m^{-1} K^{-1} to 5.5 W m^{-1} K^{-1} for saturated samples. In contrast to the limestones and dolomites, thermal conductivity of the sandstones is strongly influenced by stratigraphy and genetic origin. Upper Triassic fluviatile sandstones (e.g. Schilfsandstein) for example are badly sorted heterogeneous sediments with high feldspar contents, while parts of the Lower Triassic Buntsandstein formation (e.g. Kristallsandstein) were deposited as well sorted, quartz dominated sandstones. With respect to the varying quartz/feldspar ratios the Schilfsandstein samples (quartz ≈ 57%, feldspar ≈ 35%) have a much lower thermal conductivity of 2.5 W m^{-1} K^{-1} than the quartz rich Kristallsandstein samples (quartz ≈ 90%, feldspar ≈ 6%) with = 4.5 W m^{-1} K^{-1}.

3. A MODEL FOR THERMAL CONDUCTIVITY

The XRD data collection (Fig. 3) allowed to compare the measured thermal conductivity values with theoretical models. XRD-mineral volumes were combined with matrix properties (Table 1) to calculate rock thermal conductivity on the base of different mixing laws (Fig. 4):

$$l_{arith}(f) = (1-f)\, l_m + f\, l_{fluid} \qquad (1)$$

$$l_{geo}(f) = l_m^{(1-f)} \cdot l_{fluid}^{f} \qquad (2)$$

$$l_{har}(f) = 1/\{(1-f)/\, l_m + f \,/\, l_{fluid}\}, \qquad (3)$$

where $?_m$ is rock matrix thermal conductivity, $?_{fluid}$ rock fluid thermal conductivity, and ϕ porosity.

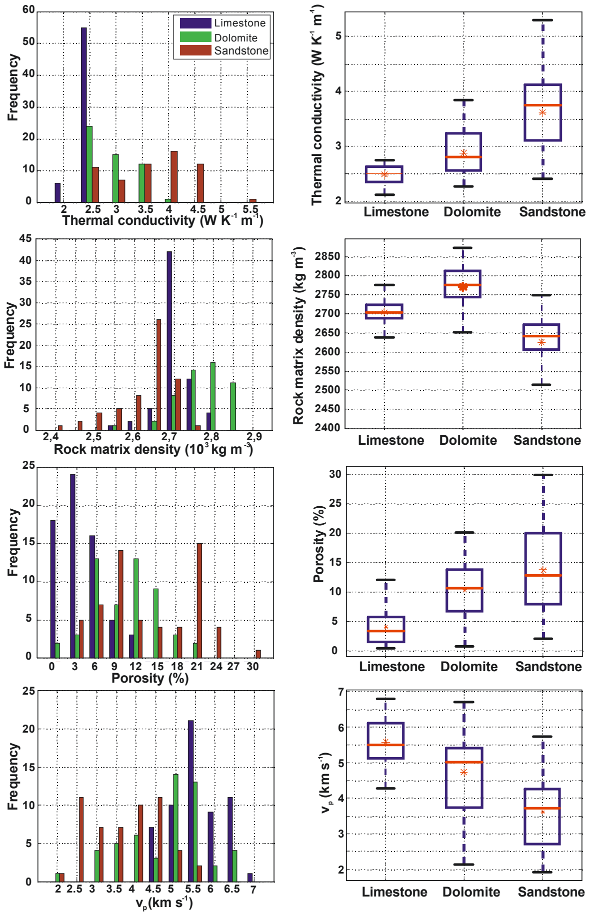


Figure 1: Distribution of petrophysical properties grouped for the main rock types of sandstone, dolomite and limestone. Statistical values displayed as Box-Whisker-Diagrams (red line: median; red star: mean; blue box: 24% and 75% percentile; black lines: 5% and 95% percentile).

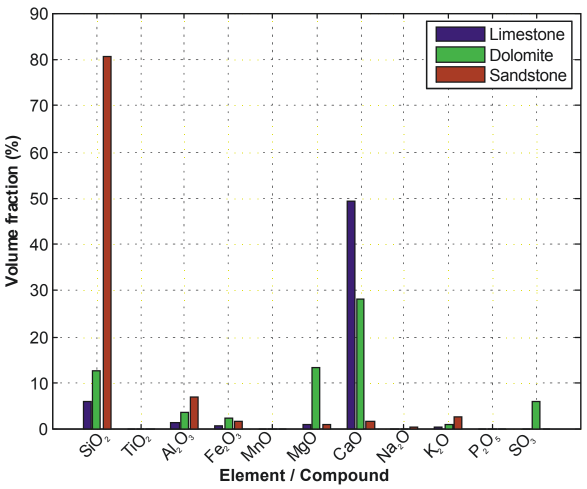


Figure 2: Average chemical composition of the main rock types sandstone, limestone and dolomite from XRF-analysis.

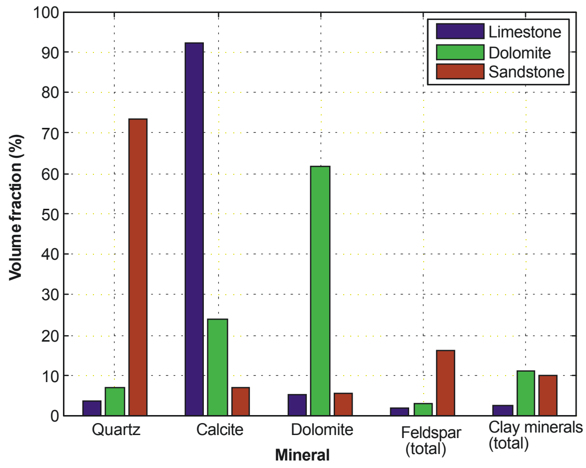


Figure 3: Average mineralogical composition of the main rock types sandstone, limestone and dolomite from XRD-analysis.

The results show that calcite and dolomite literature values generated from measurements on single crystals are much higher than values gained from a dense 100% limestone or dolomite rock sample. As displayed in Fig. 5 the geometric mean, also called Lichtenecker model [3], shows the best fit with the measured data. In general the agreement is better for dry than for saturated samples, which might be attributed to effects of uncomplete saturation. The geometric law also give the best results for sandstones and dolomites.

In order to consider effects of pore geometry and lithification, Asaad [1] modified the Lichtenecker model by incorporating a correlation factor *f* as follows:

$$l(f) = l_m^{(1-ff)} \cdot l_{fluid}^{ff} . \qquad (4)$$

Following this equation we used a Monte Carlo simulation to extract $?_m$ und *f* from the laboratory data. As an example Fig. 6 illustrates the distribution of the randomly generated parameters for the limestone samples. Fig. 7 shows the predicted thermal conductivity after analysing 10^6 random combinations, in comparison with the data. In contrast to the dolomites and limestones, the sandstones have to be divided into at least two stratigraphic groups to come to reasonable results. Table 2 displays the results from Monte Carlo Simulation for matrix thermal conductivity and *f*-factors.

Table 1: Thermal conductivities of the occurring main minerals used for calculation of the rock thermal conductivity.

Mineral	Thermal conductivity (W m^{-1}K^{-1})	Source
Quartz	6.5	[2]
Dolomite	3.9	this study
Limestone	2.8	this study
Feldspar	2.0	[2]
Clay minerals	1.7	[2]
Anhydrite	5.4	[2]

Table 2: Results of the Monte-Carlo simulations, determining matrix thermal conductivity and *f*-factor (mean and standard deviation) according to Asaad's model (Eq. 4).

Rock type	Matrix thermal conductivity (W $m^{-1}K^{-1}$)	*f*-factor
Limestone	2.63 ± 0.13	0.77 ± 0.26
Dolomite	3.71 ± 0.25	0.95 ± 0.13
Sandstone (Buntsandstein)	3.6 ± 0.25	0.25 ± 0.13
Sandstone (Keuper)	3.44 ± 0.42	0.73 ± 0.15

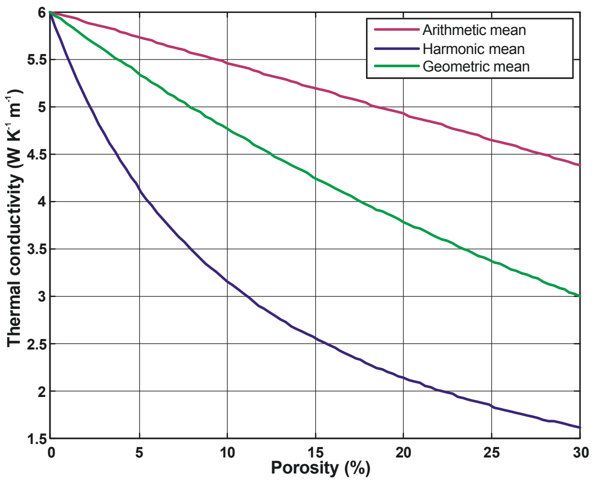
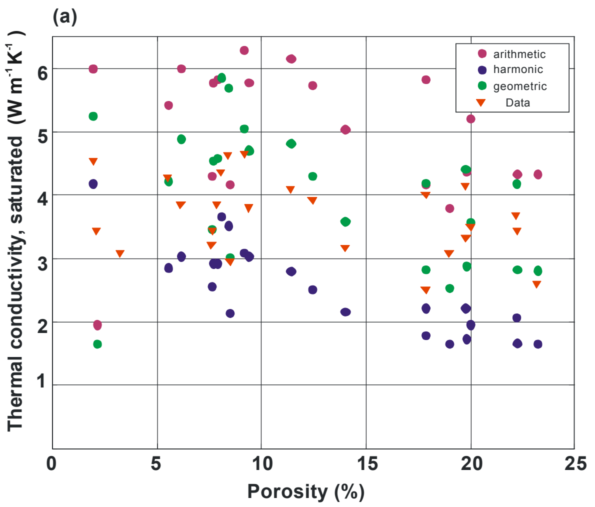


Figure 4: Variation of thermal conductivity with rock porosity calculated with different mixing laws. A value of 6.0 W m^{-1} K^{1} was taken as matrix conductivity.



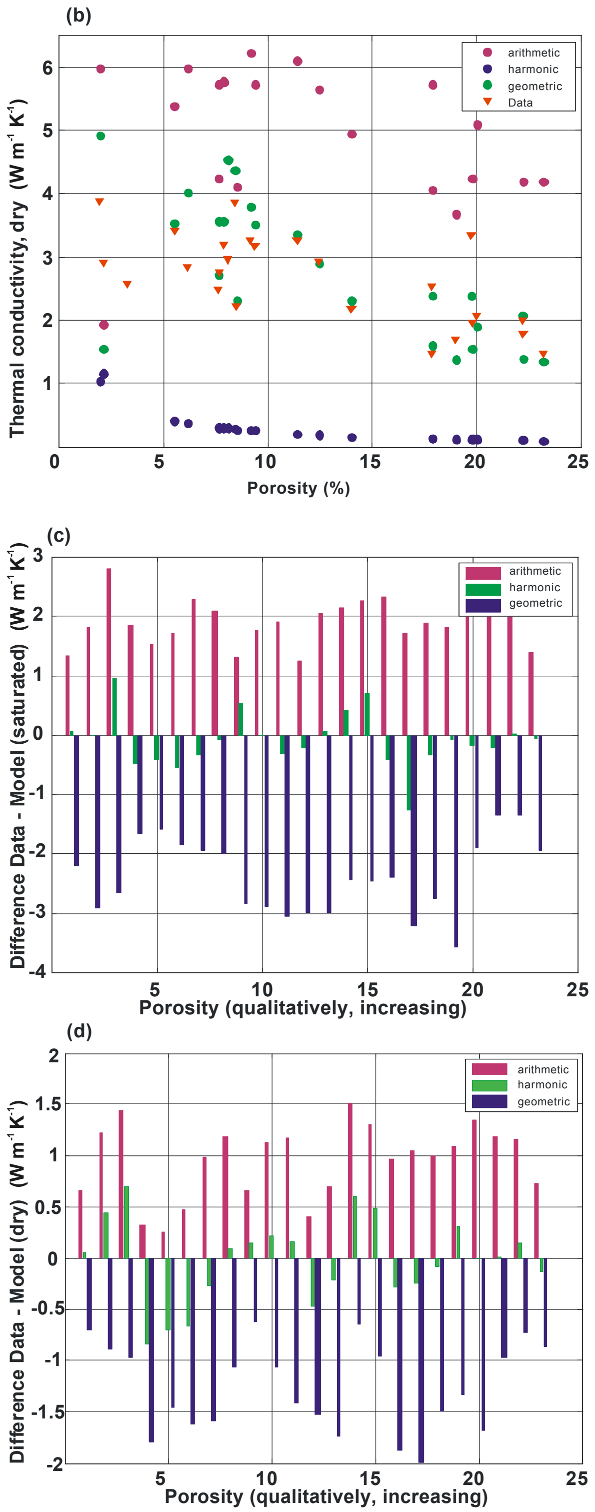


Figure 5: Comparison of the measured and calculated thermal conductivities for saturated (a) and dry (b) samples. Fig. (c) and (d) show the deviation of the calculated values form the measured data.

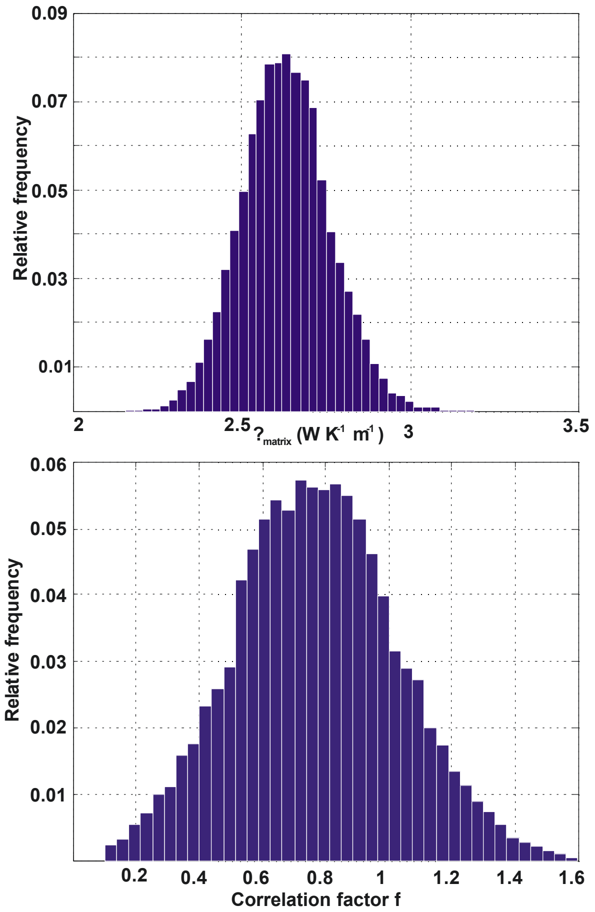


Figure 6: Results of Monte Carlo simulation for calculating the matrix thermal conductivity and the *f*-factor after the Asaad's-Model for limestone.

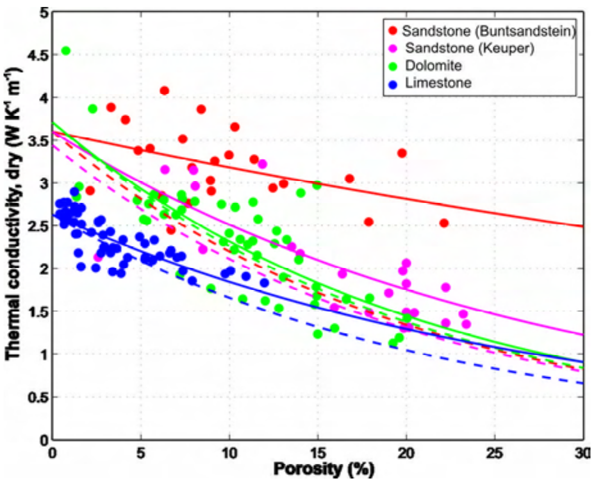


Figure 7: Rock thermal conductivity prediction using the Monte Carlo results and Asaad's model (bold lines) compared with the measured data (dots) and the calculated data from the geometric mean (dashed lines).

4 CONCLUSION

The geometric mixing law was confirmed as a fast and robust estimator for thermal conductivity, especially for limestones and dolomites regardless of their stratigraphic age and genetic origin. In a more sophisticated approach, the data were further used to compare and to calibrate theoretical models for thermal conductivity prediction. Rock type specific parameters were determined describing the relations between rock matrix, porosity, rock morphology, and the effective thermal conductivity. This grouping by rock type and rock generation allows an enhanced prediction of thermal properties of the mesozoic strata.

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