

CONF - 770847 -- 10

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Abstract

The thermal conductivity of several rocksalt materials has been determined. Some of the materials were core samples from well AEC 8, Carlsbad, New Mexico. These samples ranged from nearly pure halite (NaCl) to nearly pure anhydrite (CaSO_4). Core sample crystallite size ranged from about 3 centimeters to essentially packed salt sand ($\approx 0.5\text{mm}$). The samples exhibited thermal conductivities from ≈ 1.5 to 7.5 W/mK which depended upon purity and grain size.

A one meter cube of rocksalt from the Mississippi Chemical Company's S.E. New Mexico potash mine was obtained for other experiments. The thermal conductivity of one sample from each of the orthogonal directions of the cube was measured. This material had a high conductivity of $\approx 8.5 \text{ W/mK}$ and was very isotropic. A core of rocksalt from the Morton Salt Company, Paynesville, Ohio had a thermal conductivity of 6 W/mK , which is in the upper band of the results on cores from well AEC 8.

Finally, a concrete made with salt sand and rocksalt aggregate was determined to have a conductivity of $\approx 2 \text{ W/mK}$.

A longitudinal heat flow apparatus was used to determine the thermal conductivity. An analysis of the experiment gave an accuracy within $\pm 15\%$ on geological samples and within $\pm 10\%$ on 304 stainless steel.

*This work supported by the Department Of Energy

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Published in Proceedings of the International Conference on Thermal Conductivity, 15th, 1977, Ottawa

pages 263-276

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Introduction

Salt beds are geological formations that have lain undisturbed by seismic activity for millions of years. Because of this fact, these salt beds are attractive sites for the disposal of the radioactive wastes that would be produced by the large scale production of electricity by atomic reactors. The construction of a waste disposal facility requires a complete characterization of the salt formation and an analysis of the interactions of the waste and waste containers with the salt surroundings. These thermal conductivity measurements form a small part of that characterization and analysis.

Materials

Well AEC 8

Generalized descriptions of the core sections from well AEC 8 near Carlsbad, New Mexico, are given in Table 1. These descriptions are based on visual examination as well as some x-ray diffraction analysis. Core compositions varied from about 95% halite (NaCl) to 95% anhydrite (CaSO_4). Some cores contained other foreign materials such as calcite, clay and sandstone. The color of the cores ranged from white and opaque for core 527; through dark gray (smokey) and translucent for core 837; to reddish brown with both opaque and translucent grains for core 281. The crystallite sizes varied between 0.5mm to 3 cm. Core densities averaged 2170kg/m^3 with a 15% spread.

Paynesville, Ohio

One core section (10cm long) from Paynesville, Ohio was measured. No information is available about its composition or location. It is very similar in appearance to AEC 8 core 837.

Mississippi Formation

Several cubes of rocksalt were obtained from the Mississippi Chemical Company's S.E. New Mexico potash mine. These cubes, 1 meter on a side, were used in bench heating experiments. Three samples, corresponding to the orthogonal directions, were taken from one cube and labeled 'X', 'Y' and 'Z'. This material is salmon in color. The three samples are indistinguishable from

one another. The densities for samples X, Y and Z are 2156, 2090 and 2157 kilogram per cubic meter, respectively.

The blocks are composed of halitic rock with 1-2% sylvite (KCl). The halite crystal size varies from 2-3 mm to 1 cm with some crystals as large as 2 cm. Crude layers are evident based on crystal size and varying degrees of translucency. The layers are approximately one centimeter thick and sometimes contain fracturing parallel to the layers. The sylvite is slightly milky and is commonly outlined by a halo of orange iron oxide. A few small (0.5 mm) fluid inclusions were noted--but are not abundant. The halite does not show any well defined foliation. The halite crystal cross-sections are polygonal on faces normal to the bedding.

Saltcrete (concrete)

The composition of the concrete made with salt sand and rocksalt aggregate is given in Table II.

TABLE II
Saltcrete
1560 Kg/m³

Composition in Percent by Volume

| | |
|------------------------|--------------|
| Portland Cement Type 3 | 13.93 |
| Saltsand | 31.10 |
| Coarse Salt: | |
| #8 Sieve to 1/4 inch | 16.65 |
| 1/4 to 1/2 inch | 15.37 |
| Brine | 3.66 |
| Water | <u>19.29</u> |
| | 100.00 |

Concretes of this nature are of interest for several reasons. They may be used for stemming bore holes, grouting instrument packages in place of backfilling around construction or cannisters. The composition of the concrete is varied in an attempt to match the properties of the surrounding strata.

TABLE I. WELL AEC 8 CORE DESCRIPTIONS

| Depth <u>M</u> | Density <u>Kg/m³</u> | |
|-------------------|------------------------------------|---|
| 281 | 2180 | Roughly equigranular (up to 8 mm) reddish halite crystals (50% of rock) are set in a fine grained reddish sandstone consisting mainly of quartz and feldspar. Crude layering of sandstone and halite exists. Minor anhydrite is present. |
| 504 | 2300 | Calcite banded anhydrite (95%) which is finely crystalline (>.5 mm). Clear neomorphic halite (5%) is concentrated in small lenticular areas where banding has been contorted. |
| 527 | --- | Massive appearing, finely crystalline anhydrite (95%) of rock with some poorly developed bedding. Halite (>5%) is dispersed through the rock. |
| 560 | 2220 | Halite (95%) consisting of large (up to 3 cm) crystals which vary from clear to light reddish color. Fluid inclusions (1-3 mm) are common in this halite. Some interstices are filled with a pink-colored anhydrite. Some minor polyhalite and unidentified clay minerals (especially along crudely horizontal surfaces). |
| 628 | 2180 | Large (1-2 cm) halite crystals with common small fluid inclusions (up to 2-3 mm) for 85% of rock. Anhydrite and calcite comprise about 15% of the rock, fill the interstices, and also form some crude bedding planes through the rock. |

TABLE I. WELL AEC 8 CORE DESCRIPTIONS
(continued)

| Depth | Density | |
|----------|-------------------------|--|
| <u>M</u> | <u>Kg/m³</u> | |
| 646 | 2180 | Finely crystalline anhydrite and calcite, without apparent microscopic structure, forms about 75% of rock; coarsely crystalline (up to 1 cm) neomorphic halite has formed generally vertical masses through the anhydrite, and is about 25% of the rock. Halite has a texture where individual masses appear to crudely radiate about dispersed centers or upward from laminations in the anhydrite. |
| 777 | 2120 | Very similar to 504m'; 90% calcite banded anhydrite with about 10% halite. |
| 837 | 2000 | Medium (2-4 mm) to coarsely crystalline (1-2 cm) clear halite (95% of rock). The halite is foliated at an angle of about 30° from the horizontal. About 5% of the rock consists of anhydrite in disseminated and lenticular forms. |
| ? | 2210 | Morton Co., Paynesville, Ohio, similar to core 837 meters, AEC 8. |

Experimental Method

A longitudinal heat flow apparatus was used to determine the thermal conductivities of the materials of this report. The apparatus was designed specifically for use with geological core sections. One feature of design is that cores of different diameters and length may be measured without effecting a change in the equipment.

The core sample rests upon a nichrome wound heater constructed of zirconia tiles. Thermocouples are placed in drilled holes along the sample length and into the centerline. A heat flux transducer is placed on the top flat end of the sample. A piece of asbestos paper cushions the transducer from the upper cold plate. The upper cold plate may be used to apply pressure to the stack, to insure proper interface contact, by a screw arrangement. A schematic of the apparatus is shown in Figure 1. Not shown in Figure 1 is lead foil tape usually affixed to the top flat sample face to insure intimate contact between the sample and the heat flux transducer. The entire sample stack is surrounded by a powered silica insulation.

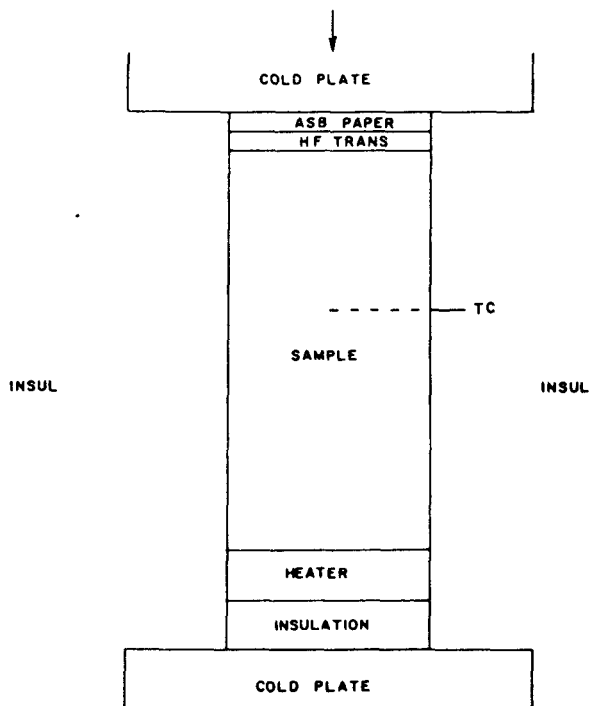


Figure 1. Schematic of Thermal Conductivity Apparatus

The measurement procedure consists of applying constant power to the heater and allowing time for thermal equilibrium to be established. Once equilibrium is established, the heat flux transducer and thermocouple outputs are recorded. The thermal conductivity is then calculated from the equation

$$\lambda = \frac{Q/A}{dT/dX} \quad (1)$$

where

λ = thermal conductivity

Q/A = heat flux (transducer output)

dT/dX = temperature gradient (thermocouples output and location).

Analysis

The experiment has been analyzed using the finite differencing heat transfer code CINDA.¹ An auxiliary code, HEATMESH-71,² was used to generate node and conductor data required by CINDA. In the analysis, the experimentally measured thermal conductivity was input to the code as was either (i) the experimental sample hot face temperature or (ii) the transducer determined flux. The temperature gradient produced by the code was then compared to the experimental temperature gradient. The agreement between analysis and experiment has varied from 2 to 14% for geological materials. Part of this variation is believed to be due to the nonuniformity of some of the materials. Experiments on a sample of 304 stainless steel have yielded results that are within $\pm 5\%$ ($300 \leq T \text{ (K)} \leq 400$) and $\pm 10\%$ ($400 \leq T \text{ (K)} \leq 500$) of the recommended values³ for that material.

CINDA requires re-coding for each change in sample dimensions. In addition to this, there was a desire to be able to check each data point, as it was taken, on the time-sharing terminal in the laboratory. For this purpose, an analytical solution was used. The experiment may be described as a pin protruding from a plane surface heated through its base and losing heat out of its curved surface and other end. The differential equation governing this configuration is

$$\frac{d^2\theta}{dx^2} - m^2\theta = 0 \quad (2)$$

where

$$\Theta = T - T_s$$

$$m = \sqrt{\frac{hC}{\lambda A}}$$

T = temperatures at x

T_s = temperature of surroundings

h = heat transfer coefficient at surface

C = circumference

A = cross sectional area

λ = thermal conductivity

Chapman⁴ gives the general solution to this equation as

$$\Theta = B e^{-mx} + D e^{mx} \quad (3)$$

where B and D are arbitrary constants evaluated (or specified) by the boundary conditions. Eq. (3) is more conveniently expressed in terms of the hyperbolic functions:

$$\frac{\Theta}{\Theta_o} = \frac{T - T_s}{T_o - T_s} = \frac{\cosh m(L - x) + H \sinh m(L - x)}{\cosh mL + H \sinh mL} \quad (4)$$

where

T_o = temperature of base

L = sample length

$$H = \frac{h_e}{\lambda m}$$

h_e = heat transfer coefficient at sample end.

All of the heat dissipated by the sample was conducted through the base ($x = 0$). Thus the heat flow rate, Q is given by

$$Q = - \lambda A \left(\frac{dT}{dx} \right)_{x=0} \quad (5)$$

Introduction of the temperature distribution from Eq. (4) yields

$$Q = \lambda mA(T_o - T_s) \frac{\sinh mL + H \cosh mL}{\cosh mL + H \sinh mL} \quad (6)$$

If h_e is allowed to equal zero, then H becomes zero and Eq. (6) reduces to the heat flow rate out of the curved surface only

$$Q = \lambda mA(T_o - T_s) \tanh mL \quad (7)$$

Thus by using equation (4), (6) and (7), we may calculate the temperature gradient and the hot and cold face heat fluxes. Estimates of h and h_e are determined from a knowledge of the thermal conductivity of the powdered insulation and of the heat flux transducer. The experimental hot and cold face temperatures and the experimental thermal conductivity are used in these equations to yield an analytical temperature gradient and heat fluxes which are compared to their experimental counterparts.

The above technique does not actually give an accuracy figure but it does establish whether or not the data is self-consistent - a valuable aid to the technician who must decide whether to accept that data point and proceed or to look for trouble.

Results

The thermal conductivities of the cores that contained mostly salt are shown in Figure 2; those of mostly anhydrite in Figure 3 and the saltcrete in Figure 4. Data for the mutually perpendicular samples from the one meter cube of Mississippi rocksalt are shown in Figure 5.

Two of the cores from well AEC 8 and one of the Mississippi samples contained brine inclusions. These inclusions caused the samples to decrepitate - violently in two cases. The decrepitations were accompanied by a loud report and powdered insulation was thrown into the air. Core AEC 8, 527 was crumbled when the experiment was disassembled. When the sample crumbled is not known, therefore, all of the data for this sample is suspect. The Mississippi 'Y' sample decrepitated within moments after the power was turned off after taking the last data point. The sample cracked nearly in two about one

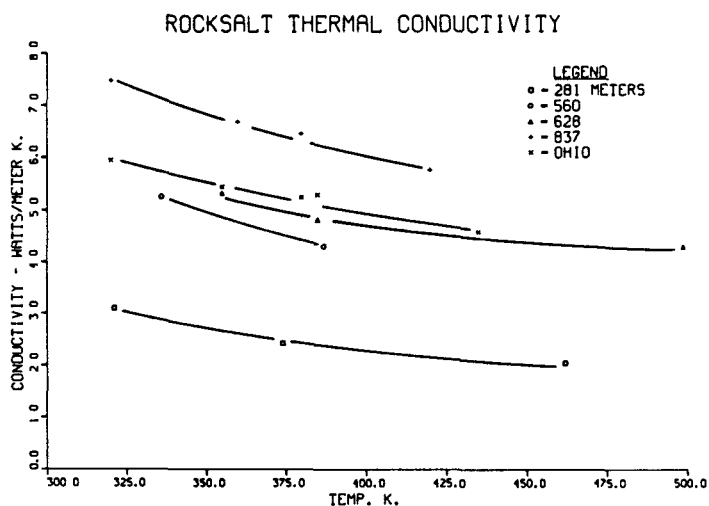


Figure 2. Thermal Conductivity of Well AEC8 Cores Containing 50% or More Halite.

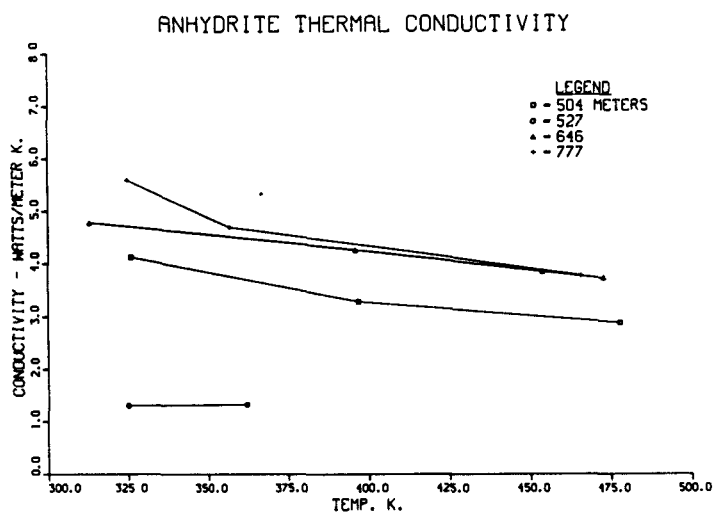


Figure 3. Thermal Conductivity of Well AEC8 Cores Containing 50% or More Anhydrite.

SALICRETE THERMAL CONDUCTIVITY

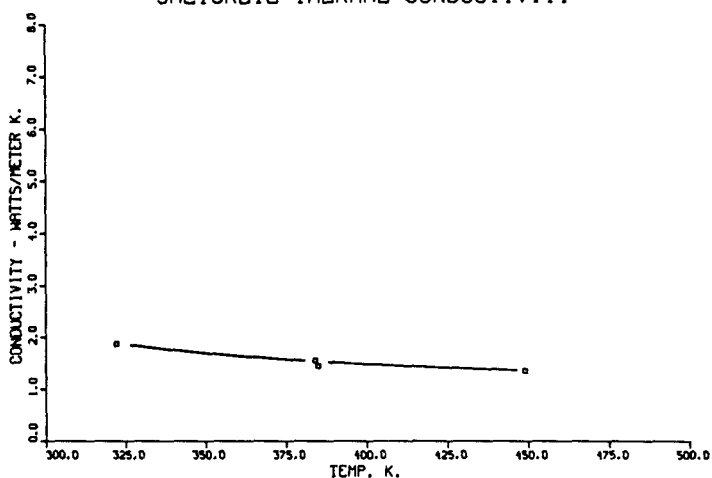


Figure 4. Thermal Conductivity of A Concrete Made with Saltsand and Rocksalt Aggregate.

ROCKSALT THERMAL CONDUCTIVITY

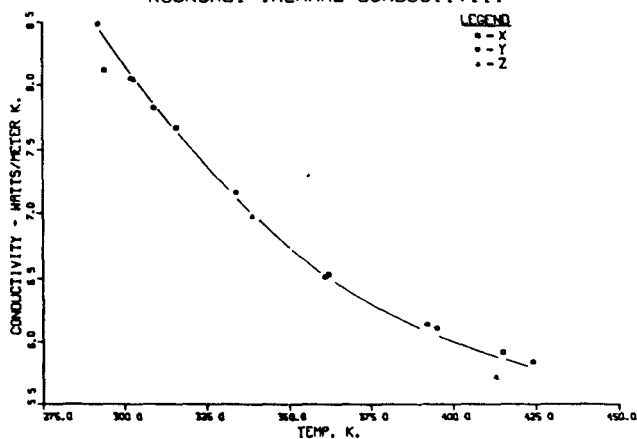


Figure 5. Thermal Conductivity of a One Meter Cube of Rocksalt From Mississippi Chemical Co. S.E. New Mexico Potash Mine. Measured in the Orthogonal Directions.

inch from the hot face. The temperature at that location was approximately 525K. Core AEC 8, 560 also decrepitated.

Discussion of Results

Salts

The thermal conductivity of solid, nonmetallic materials is influenced primarily by purity and grain size. Heat is transported in these materials principally by phonons (lattice vibrations). Phonons are scattered (resisted) by grain boundaries and impurity atoms. Those cores, therefore, that had the larger grain size and the higher purity exhibited the higher thermal conductivity. Phonon transport is characterized by a $\frac{1}{T}$ relationship. Halite

and anhydrite can range from opaque to transparent - again depending on grain size and purity. At higher temperatures, heat may be transported through transparent materials by radiation. Radiant conduction is characterized by a T^3 relationship. The three orthogonal samples had the same thermal conductivity and yielded enough data to test the above relationships. A non-linear least squares routine⁵ was used to fit the data to an equation of the form

$$\lambda = \frac{b_1}{T - b_2} + b_3 T^3$$

where b_1 , b_2 and b_3 are parameters (constants) to be determined. The first term on the right in the equation provides the lattice conduction while the second term gives the radiant conduction. The least squares routine gave the following equation:

$$\lambda = \frac{1549.9}{T - 100} + 0.13199 \times 10^{-7} T^3 \quad (8)$$

290 < T < 450

where

λ = thermal conductivity, Watts per meter Kelvin

T = temperature, Kelvin.

Thirteen of the experimental data points within one percent of the curve generated by this equation. The other two data points are within 2.2% and 2.8%, respectively. Stephens and Maimoni⁶ present an equation for Carey mine rocksalt from Winfield, La., where b_1 is 1423.2 and b_3 is 0.35581×10^{-8} .

A vertical traverse of a salt bed would go from dirty, impure salt at the edges to clean salt at the center. Herrin and Clark⁷ have investigated the temperature gradients in the salt section of the Permian Salado formation of West Texas and Eastern New Mexico and have concluded that the effective thermal conductivity of the formation is 5.44 W/mK at 300 K. The average of the range of values for the current study is 5.75 W/mK at room temperature.

Saltcrete

The behavior of the saltcrete is typical of concretes in general. The value of the conductivity is a function of the density which in turn is a function of the particular aggregate and sand used. J. P. Moore⁸ et al., show an increase by a factor of 12 in the thermal conductivity of concretes as the density varies from 400 to 2400 Kg/m³. They also show a steady decline in the conductivity as a function of drying time -- reaching a constant value at about 200 days. The decrease was 21%. Other than the effect caused by water loss, the thermal conductivity of concretes is insensitive to temperature over the range of normal usage.

Conclusions

The thermal conductivity of a number of core sections of rocksalts has been investigated. Room temperature values for the thermal conductivity ranged from 3 to 8.5 W/mK with the purer materials having the higher values. No anisotropy was found in the thermal conductivity of purer rocksalt when mutually perpendicular samples were measured.

The dirty rocksalts are not being considered for radioactive waste isolation and the data was collected as base line information only. For the cleaner rocksalts, the thermal conductivity should be investigated to somewhat higher temperatures because this may influence the value of the thermal radiation conduction parameter b_3 in the equation (8).

REFERENCES

- 1 Chrysler Improved Numerical Differencing Analyzer, CINDA-3G, TN-AP-67-287, Space Div., Chrysler Corp., New Orleans, LA, 1967.
- 2 HEATMESH-71: A Computer Code for Generating Geometrical Data Required for Studies of Heat Transfer in Axisymmetric Structures, SCL-DR-72004, V. K. Gabrielson, Sandia Laboratories, Albuquerque, NM, 1972.
- 3 Thermal Conductivity, Metallic Elements and Alloys, Thermo-Physical Properties of Matter. Vol. 1, the TPRC Data Series, Y. S. Touloukian et al., IFI Plenum, NY, 1970, p. 1175.
- 4 Heat Transfer, 2nd ed., Alan A. Chapman, p. 59, MacMillan Co., NY, 1967.
- 5 TJMARI - a Fortran Subroutine for Nonlinear Least Squares Parameter Estimation, T. H. Jefferson, SLL-73-0305, Sandia Laboratories,
- 6 Thermal Conductivity of Rocksalt, D. R. Stephens and A. Maimoni, UCRL-6894 Rev. II, Lawrence Radiation Laboratory, California, 1964.
- 7 Heat Flow in West Texas and Eastern New Mexico, E. Herrin and S. Clark, Jr., Geophysics, Vol. XXI, No. 4, p. 1087, 1956.
- 8 Some Thermal Transport Properties of a Limestone Concrete, J. P. Moore et al., ORNL-TM-2644, Oak Ridge National Laboratory, 1969.

Acknowledgement

The author wishes to thank Dennis Powers, R. E. Stinebaugh and P. L. Nelson for furnishing the cores and their descriptions and A. J. Anaya for sample preparation and set-up.