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A Computational Method for Determining Segmental and Overall Geothermal Gradients and Geothermal Heat Flow Values

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ABSTRACT

A new computational method is presented which calculates geothermal heat flow values and geothermal gradients with more precision than permitted by previously published techniques. The data required are: geothermal temperature at a known depth, mean surface temperature, the rock types in the stratigraphic column and the thermal resistivity values for the different types of rocks. This method is valuable in areas that have no measured gradient values. Basic equation used was the Fourier heat transfer equation $\dot{Q}/A = -1/\rho_i\ (\partial T/\partial x)$ where $\dot{Q}/A$ is heat flux in μcal/(cm^2 s), ρ_i is thermal resistivity (°C s cm/μcal) and $\partial T/\partial x$ is the x component of the temperature gradient (°C/cm). The thermal resistivity was allowed to vary linearly with temperature $\rho_i = \rho_i^{\circ}\ [1 + K_i\ (T - 30)]$ where ρ_i is thermal resistivity of the lithographic segment « i » at a temperature T, ρ_i° is thermal resistivity at 30 °C and K_i is the temperature coefficient of thermal resistivity. The procedure consisted of intergrating the combined equation for heat flux in terms of temperature dependent resistivity.

Two iterative solutions were used to simplify the calculations: exact and approximate. The heat flux for each well was assumed to be 1.0 HFU and segmental temperatures were calculated from the bottom (arbitrarily) up, until a surface temperature was obtained. The calculated surface temperature could then be compared with the mean surface temperature (MST). Correction in the heat flux value was made until the calculated surface temperature and MST agreed. An analysis of three deep Appalachian test wells was made and the results showed the critical importance of lithographic ordering and the temperature dependence of thermal resistivity upon calculated geothermal quantities.

Introduction

Individual geothermal gradients and heat flux values are important for predicting surface or *in situ* temperature effects which result from thermal perturbations. Some perturbations result from thermal recovery of heavy oil, *in situ* shale oil or coal conversion, or geothermal energy extraction. In addition, the individual thermal effects are often accumulated into various types of regional geothermal surveys, such as geothermal gradient and heat flow maps. These maps are then correlateable with historical geologic factors, geophysical factors and phenomena, geochemical observations, and large-scale plate tectonic theories in order to formulate a theoretical thermal model of the earth's crust (Schubert, Anderson 1974). Some former solutions to the problem of determining local geothermal gradients and heat fluxes have lacked some of the refinement recommended here (Joyner 1960; Grisafi, Rieke, Skidmore 1974). In these former solutions the actual lithographic column was replaced by a regional or local characteristic column composed of rock with intermediate thermal properties. This replacement simplified the calculation of heat flux values or geothermal gradients but the simplification gave averaged answers which lost a large degree of local detail.

In other simplifications (Grisafi, Rieke, Skidmore 1974), segmental values of thermal resistivity have been grouped rather than ordered naturally, have been averaged over temperature, or have been presumed constant with temperature. As will be shown, each of these assumptions has an effect upon heat flow values as well as overall and segmental geothermal gradient values. These effects are compared by means of the computational methods proposed by the authors.

The methods presented here provide two improved solutions to the steady state conductive heat transfer problem. These solutions, however still have several constraints. The constraints are:

- the thermal resistance consists of horizontal stacked semi-infinite slabs so that heat flow lines are parallel outward and are unaffected by edge effects,
- the lithographic segments although differing from each other are internally homogeneous and isotopic,
- the heat generated or absorbed in a segment is negligible,
- the thermal resistivity (or conductivity) values vary with each segment and change instantaneously at the segmental boundary, and
- the thermal resistivity varies from segment to segment and within a segment increases linearly with temperature (Joyner 1960).

Equations governing heat flow by conduction under these constraints have been written and solved by two approaches, namely, exactly and approximately. In both the exact and approximate solutions the heat flow equation was solved by formally integrating the heat equation and manipulating that result. The exact solution used the thermal resistivity function exactly, whereas the approximate solution used the arithmetic mean thermal resistivity for a lithologic segment. The

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exact solution was applied to the lithographic column and the column was artificially altered in the following ways:

- inverted,
- rock types, i.e. sandstones, limestones and shales, together,
- rock types grouped together and inverted, and
- thermal resistivity held constant at ρ^0 for 30 °C for a given rock type ($K_i = 0$).

Mathematical approach

The data used for these calculations are:

- mean surface temperature,
- thermal properties of extant rock types,
- lithologic character of the stratigraphic column (rock type, sequence, and thickness),
- bottom hole temperatures and well depth. Good subsurface temperature data are often not available.

Uncertainty is greatest in bottom hole temperature measurements which may have been obtained for thermal non-equilibrium situations. SCHOEPPEL and GILARRANZ (1966) have shown that the maximum logged temperatures, when properly recorded, provide better basic data than previously realized. In addition the rock type was inexactly described owing to mixtures of different lithologies, e.g., silty sandy shale.

Data used in the illustrative computations were extracted from well logs of exploratory wells drilled in West Virginia. Description of each well and the location are presented in Table 1. With these data, the heat flow per unit area can be calculated using the Fourier heat transfer equation

$$\frac{\dot{Q}}{A} = -\frac{1}{\rho}\frac{\partial T}{\partial x} \qquad (1)$$

where $\frac{\dot{Q}}{A}$ is the x-direction (upward) heat flow per unit area in μcal/(cm² s), ρ is the thermal resistivity (°Ccms/μcal), ∂T is the temperature difference (°C) across a slab thickness ∂x (cm). The negative sign governs the convention from the second law of thermodynamics; i.e., that heat flows from hotter to cooler regions.

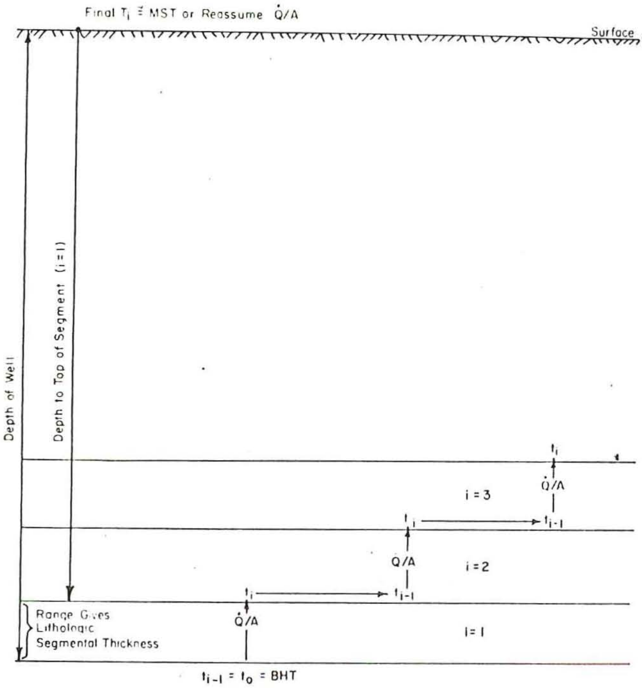

FIG. 1. — *Physical form of solution.*

TABLE 1. — *Basic data used to demonstrate computation method.*

A. WELL No. 1

Randolph Co., Huttonville District, WV (Randolph No. 103 *)
Elev. 2036 feet; 38° 45′ N; 79° 55′ W
MST = 12.8 °C BHT = 119 °C

Segment number	Depth range (ft)		Thickness of segment (cm)	Lithology	Resistivity at 30 °C (°C s cm/μcal)	K (°C⁻¹)
1	0	2280	69494.40	Sh	296	0.001
2	2280	2310	914.40	LS	162	0.003
3	230	2480	5181.60	Sh	250	0.001
4	2480	2695	6553.20	LS	184	0.003
5	2695	2830	4114.80	SS	95	0.003
6	2830	3460	19202.40	LS	162	0.003
7	3460	4906	44074.08	LS+SS+Sh	170	0.001
8	4906	5703	24292.56	Sh	296	0.001
9	5703	5917	6522.72	Impure SS	157	0.003
10	5917	7310	42458.64	Sandy Sh	211	0.001
11	7310	10118	85587.84	Sh	296	0.001
12	10118	13121	91531.44	LS	162	0.003

B. WELL No. 2

Springfield District; (Hampshire No. 12 *)
Elev. 900 feet; 39° 30′ N, 78° 35′ W
MST = 12.8 °C BHT = 82.2 °C

Segment number	Depth range (ft)		Thickness of segment (cm)	Lithology	Resistivity at 30 °C (°C s cm/μcal)	K (°C⁻¹)
1	0	295	8991.60	Sh	296	0.001
2	295	660	11125.20	Impure SS	157	0.003
3	660	2360	51816.00	LS	162	0.003
4	2360	2560	6096.00	SS+Sh	157	0.001
5	2560	2760	6096.00	Sh+LS	221	0.001
6	2760	3140	11582.40	SS+Sh+LS	157	0.001
7	3140	3188	1463.04	Impure SS	157	0.001
8	3188	3780	18044.16	Sh	296	0.001
9	3780	3850	2133.60	Impure SS	157	0.003
10	3850	4144	8961.12	Impure SS	157	0.001
11	4144	5600	44378.88	Impure SS	157	0.003
12	5600	6510	27736.80	Impure SS	157	0.001
13	6510	8000	45415.20	Sh	296	0.001
14	8000	9300	39624.00	Sandy Sh	211	0.001
15	9300	14000	143256.00	LS	162	0.003

C. WELL No. 3

Marshall Co., Liberty District, WV; (Marshall No. 539 *)
Elev. 1423 feet; 39° 50′ N; 80° 30′ W
MST = 12.8 °C BHT = 115 °C

Segment number	Depth range (ft)		Thickness of segment (cm)	Lithology	Resistivity at 30 °C (°C s cm/µcal)	K (°C−1)
1	0	280	8534.4	Impure SS	157	0.003
2	280	450	5181.60	Sh	296	0.001
3	450	560	3352.80	Impure SS	157	0.003
4	560	650	2743.20	Impure SS	157	0.001
5	650	730	2438.40	Impure SS	157	0.003
6	730	780	1524.00	LS+Sh	162	0.003
7	780	940	4876.80	Sh	296	0.001
8	940	1120	5486.40	LS	162	0.003
9	1120	2280	35356.80	Sh	296	0.001
10	2280	2370	2743.20	LS	162	0.003
11	2370	2620	7620.00	Impure SS	157	0.003
12	2620	2973	10759.44	Sh	296	0.001
13	2973	2993	609.60	Impure SS	157	0.003
14	2993	3170	5394.96	Sh	296	0.001
15	3170	3205	1066.80	Impure SS	157	0.003
16	3205	3240	1066.80	Sh	296	0.001
17	3240	3285	1371.60	Impure SS	157	0.003
18	3285	3310	762.00	Sh	296	0.001
19	3310	3350	1219.20	Impure SS	157	0.003
20	3350	3520	5181.60	Sh	296	0.001
21	3520	3540	609.60	Impure SS	157	0.003
22	3540	7575	122986.80	Sh	296	0.003
23	7575	7802	6918.96	LS	162	0.003
24	7802	7890	2682.24	Impure SS	157	0.003
25	7890	9780	57607.20	LS+DO	162	0.003
26	9780	10150	11277.60	Sh	296	0.001
27	10150	10190	1219.20	DO	162	0.003
28	10190	10470	8534.40	Impure SS	157	0.003
29	10470	12400	58826.40	Sh	296	0.001
30	12400	13800	42672.00	Sh+LS	221	0.001
31	13800	14040	7315.20	LS	162	0.003
32	14040	16095	62636.40	DO	162	0.003
33	16095	16275	5486.40	Impure SS	157	0.003
34	16275	16512	7223.76	LS	162	0.003

* West Virginia Geological and Economical Survey well numbers.

The major mathematical problem when employing the Fourier heat transfer equation is that the thermal resistivity is a function of temperature of the material. According to JOYNER (1960) a linear relation between temperature and thermal resistivities of different rocks exists and can be expressed as

$$\rho_i = \rho_i^{\circ} (1 + K_i (T - 30))$$

where ρ_i° is the thermal resistivity at 30 °C, K_i is the temperature coefficient of thermal resistivity (°C^{-1}), and T is the temperature in °C.

The variation from linearity of the T vs x expression is determined by the change in thermal resistivity. Thus, a thicker segment with a higher temperature coefficient would tend to deviate more from a linear T vs x relation.

Values of $\frac{\dot{Q}}{A}$ were calculated for each of the three exploratory wells described in Table 1 using both the exact and approximate methods. These values are listed in Table 2 and the two methods, for these cases, give identical results. Results upon heat flow of various assumptions about the lithographic column, calculated exactly, are presented in Table 3. As expected, significant changes occur in HFU. Maximum value changes at $K = 0$ reflect lower resistivities which result from the neglect of the resistivity temperature dependence. Other changes occur with inversion of extant stacking order, grouping by K, and inverted grouping by K (Table 3). The need for precise and detailed lithographic stacking order, as well as thickness and rock type, is obvious.

The same factors which influence heat flow also determine segmental geothermal gradients. Table 4 shows the effect upon each segmental gradient of each of the transpositions described. Inversion places a segment into a different temperature range and thermal

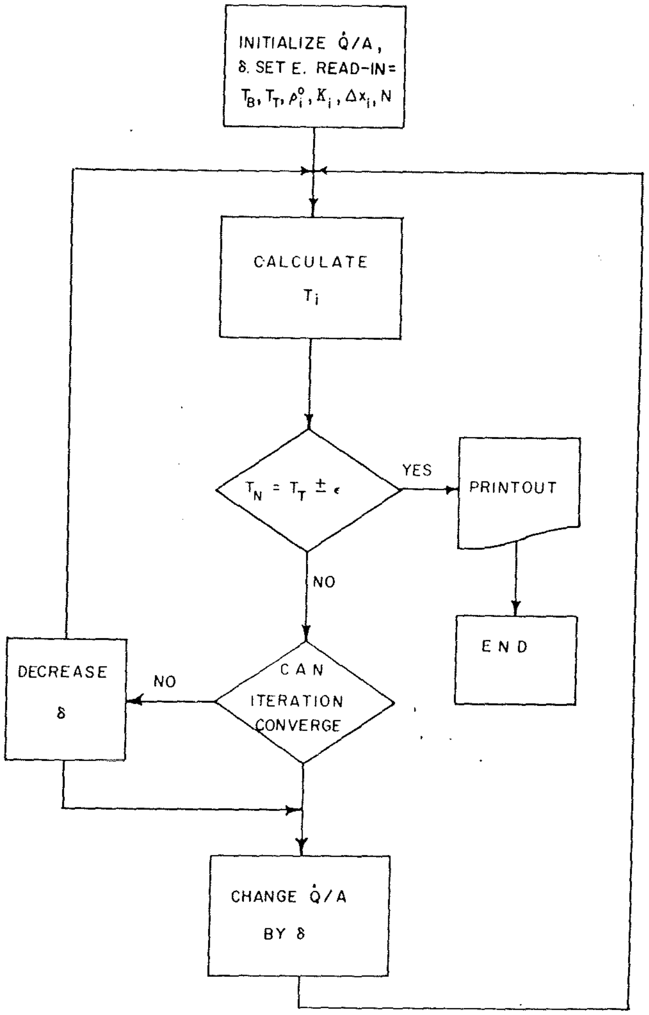

FIG. 2. — *Logic for computation of heat flow ($\dot{Q}/A$).*

TABLE 2. — *Values of heat flow ($\dot{Q}/A$) for three test wells calculated by two different methods. Lithology is in normal stratigraphic sequence for each well.*

Well No.	1	2	3
$\dot{Q}/A$ µcal/(cm² s)	(12 lithologic segments)	(15 lithologic segments)	(34 lithologic segments)
Exact	1.25	0.82	0.74
Linear approximation in ρ_i	1.25	0.82	0.74

TABLE 3. — *Heat flow ($\dot{Q}/A$) values exactly calculated for the three test wells employing different stratigraphic arrangement for the various lithologic units.*

Lithologic unit arrangement	1	2	3
	(12 lithologic segments)	(15 lithologic segments)	(34 lithologic segments)
Normal order	1.25	0.82	0.74
Inverted order	1.27	0.85	0.74
Grouped by K (K = .001 first)	1.27	0.85	0.75
Grouped by K (K = .003 first)	1.24	0.82	0.72
Normal order K = 0	1.32	0.85	0.79

resistivity range while neglect of temperature dependence lowers resistivity and changes geothermal gradient. Segmental interlayer temperatures and effective resistivites (not shown) varied slightly for the lithographic transpositions described.

Additional contributions could be made by extending the resistivity function in temperature to the quadratic and by determining effective surface temperatures and heat flow values in the field.

Conclusion

A simple method was devised for computing heat flux, segmental and overall geothermal gradients and effective thermal resistivities for lithographic columns from data comprising bottom hole temperature, depth, mean surface temperatures, rock types, thermal resistivity at 30 °C and variation in thermal resistivity with the temperature coefficient of thermal resistivity.

Results on three test wells show that use of an average (arithmetic mean) thermal resistivity in a segment leaves exact values unaltered while neglect of K, and various rearrangements of lithographic segments change important values significantly.

The computational method was programmed using FORTRAN IV. The program and complete outputs for the three test wells are available upon request from the authors. A sample output is presented in Table 5.

TABLE 4. — *Descriptions of three wells used to demonstrate computation method.*

Lithologic segment	Exact solution	Inverted order	Grouped by K (0.001 first)	Grouped by K (0.003 first)	Normal order $K = 0$
		A. RANDOLPH No. 103			
1	2.49	2.02	2.02	2.47	2.15
2	2.74	2.09	2.17	2.10	2.15
3	2.75	2.76	2.78	2.70	2.80
4	2.17	2.19	2.17	2.33	2.08
5	3.81	3.91	3.86	3.75	3.92
6	2.17	2.27	2.20	2.13	2.25
7	2.11	2.40	2.10	2.38	2.15
8	1.23	1.42	1.23	1.39	1.26
9	2.39	2.75	2.37	2.68	2.44
10	3.16	3.38	3.38	3.12	3.31
11	2.08	2.45	1.96	2.54	2.15
12	3.68	4.06	4.06	3.65	3.92
		B. HAMPSHIRE No. 12			
1	1.50	1.50	1.34	1.41	1.38
2	1.79	1.79	1.79	1.86	1.79
3	2.48	2.49	2.52	2.58	2.52
4	1.31	1.31	1.34	1.36	1.34
5	1.32	1.32	1.34	1.31	1.34
6	1.29	1.29	1.34	1.39	1.34
7	1.31	1.30	1.34	1.30	1.34
8	2.44	2.44	2.44	2.63	2.52
9	1.29	1.29	1.29	1.40	1.34
10	1.29	1.29	1.29	1.40	1.33
11	1.82	1.82	1.82	1.97	1.88
12	1.29	1.29	1.29	1.40	1.34
13	1.30	1.30	1.30	1.33	1.38
14	1.24	1.24	1.24	1.27	1.34
15	2.40	2.40	2.40	2.65	2.52
		C. MARSHALL No. 539			
1	1.50	1.50	1.13	1.40	1.28
2	1.45	1.45	1.11	1.36	1.24
3	1.48	1.48	1.15	1.38	1.28
4	1.46	1.46	1.16	1.37	1.28
5	1.74	1.74	1.62	1.72	1.74
6	2.31	2.31	2.20	2.35	2.33
7	1.34	1.34	1.20	1.29	1.24
8	1.38	1.38	1.24	1.34	1.28
9	2.29	2.29	2.22	2.37	2.33
10	1.35	1.35	1.26	1.32	1.28
11	1.30	1.30	1.24	1.27	1.24
12	1.34	1.34	1.28	1.30	1.28
13	2.34	2.34	2.44	2.28	2.33
14	1.20	1.19	1.35	1.16	1.24
15	2.21	2.20	2.30	2.38	2.33
16	1.19	1.19	1.35	1.16	1.24
17	2.21	2.21	2.32	2.39	2.33
18	1.19	1.19	1.35	1.16	1.24
19	2.22	2.20	2.31	2.39	2.33
20	1.19	1.19	1.36	1.16	1.24
21	2.21	2.21	2.31	2.38	2.33
22	1.18	1.18	1.39	1.16	1.24
23	2.20	2.19	2.31	2.38	2.33
24	1.16	1.16	1.38	1.14	1.24
25	1.18	1.18	1.45	1.16	1.28
26	2.16	2.16	2.34	2.39	2.33
27	1.15	1.15	1.48	1.16	1.28
28	2.15	2.15	2.36	2.41	2.33
29	1.14	1.14	1.49	1.16	1.28
30	1.11	1.11	1.44	1.12	1.24
31	1.14	1.14	1.26	1.28	1.24
32	1.11	1.11	1.44	1.12	1.24
33	2.14	2.14	2.37	2.41	2.33
34	1.10	1.10	1.45	1.12	1.24

TABLE 5. — *Sample printout for well No. 1: normal order, exact solutions.*

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DELTA =  0.50E-07   HEAT FLOW IS  1.25 MICROCALORIES/CM**2/SEC.

      N =  12    TBOT = 0.1190000E 03        TTOP = 0.1280000E 02

      AVERAGE Q OVER INTERVAL  1.25 COMPARISON WITH THE CALCULATED VALUE   -0.00 PER CENT



LEVEL   TEMPERATURE      GRADIENT      RHO AVE    THICKNESS       TOP TEMP    DELTA TEMP      RHO 30        K

  1       96.16         -0.25E-03      199.70     0.9153E 05       96.16     -0.228E 02      162.00      0.30E-02
  2       77.84         -0.21E-03      171.23     0.8559E 05       77.84     -0.183E 02      162.00      0.10E-02
  3       66.17         -0.27E-03      219.86     0.4246E 05       66.17     -0.117E 02      211.00      0.10E-02
  4       64.75         -0.22E-03      173.70     0.6523E 04       64.75     -0.142E 01      157.00      0.30E-02
  5       55.49         -0.38E-03      304.92     0.2429E 05       55.49     -0.926E 01      296.00      0.10E-02
  6       45.93         -0.22E-03      173.52     0.4407E 05       45.93     -0.956E 01      170.00      0.10E-02
  7       41.88         -0.21E-03      168.76     0.1920E 05       41.88     -0.405E 01      162.00      0.30E-02
  8       41.37         -0.12E-03       98.31     0.4115E 04       41.37     -0.506E 00       95.00      0.30E-02
  9       39.82         -0.24E-03      189.85     0.6553E 04       39.82     -0.156E 01      184.00      0.30E-02
 10       38.18         -0.32E-03      252.25     0.5182E 04       38.18     -0.164E 01      250.00      0.10E-02
 11       37.99         -0.21E-03      165.93     0.9144E 03       37.99     -0.190E 00      162.00      0.30E-02
 12       12.40         -0.37E-03      294.58     0.6949E 05       12.40     -0.256E 02      296.00      0.10E-02
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