SOME COMMENTS ON THE ESTIMATION OF GEOTHERMAL GRADIENTS FROM THE DEPTHS OF BOTTOM SIMULATING REFLECTORS

Timothy A. Minshull∗
School of Ocean and Earth Science
National Oceanography Centre, Southampton
University of Southampton
European Way, Southampton, SO14 3ZH
UNITED KINGDOM

ABSTRACT
The phase boundary between hydrate and free gas is marked in seismic reflection profiles from the deep ocean by a “bottom simulating reflector” (BSR). The pressure at the BSR may be estimated from its depth and, if the phase boundary is known and the geotherm is assumed to be linear, or the variation of thermal conductivity with depth is known, geothermal gradients can then be estimated. The calculation of the geothermal gradient is prone to several uncertainties (e.g., in seafloor temperature and time-to-depth conversion), but the main contribution to the absolute uncertainty is the uncertainty in the phase boundary resulting from uncertainties in the composition both of the pore fluid and of the hydrate-forming gas. In the absence of direct sampling, these compositions are unknown. It is commonly assumed that the hydrate-forming gas is pure methane, but a wide range of other gases may be present and may perturb the phase boundary, as may variations in pore fluid salinity. Use of the wrong phase boundary in calculations of geothermal gradient will introduce an artificial correlation between the geothermal gradient and seafloor and BSR depth. If lateral variations in the geothermal gradient are negligible or uncorrelated with seafloor depth, this correlation will disappear when the correct phase boundary is used. In these circumstances, a straight line or smooth curve fit to the estimates of the temperature difference between the BSR and the seabed, as a function of depth below the seabed, will pass through the origin only if the correct phase boundary is used. I use this constraint to develop an approach to estimation of the geothermal gradient that is less sensitive to compositional uncertainties and can be applied when the BSR is densely sampled in a region with significant seabed relief.

Keywords: gas hydrates, heat flow, geotherm

INTRODUCTION
The presence of methane hydrate beneath the seafloor is most commonly inferred from the presence of “bottom simulating reflectors” (BSRs) marking the phase boundary between hydrate and free gas [1, 2]. If the composition of the hydrate-forming gas is known and the salinity of the pore-fluid is known, the temperature at the BSR may be estimated from its depth. Hence, given measurements of or assumptions regarding the seafloor temperature and sediment thermal conductivity, the geothermal gradient and heat flow may be estimated [3]. Direct measurement of heat flow in the deep ocean is difficult and expensive, with heat flow probes typically penetrating only the upper few metres, where the geothermal gradient may be perturbed by bottom currents or geologically recent changes in ocean
temperature. Such measurements only allow the geothermal gradient to be determined in a few isolated locations, and continuous transects are not possible. Mapping the depth of the BSR in seismic reflection profiles is a powerful method for determining the geothermal gradient over a broad area and has therefore been widely used. The method is, however, vulnerable to a range of errors, both systematic and stochastic [4]. These errors include picking errors, uncertainties in the seabed temperature, and uncertainties in the seismic velocity used for depth conversion. One of the largest uncertainties is in the choice of phase boundary, which is influenced by the gas and pore fluid composition [5] and by capillary effects in fine-grained sediments [6]. Here I show how a poor choice of phase boundary can lead to systematic regional trends in inferred geothermal gradient that are merely artifacts of the method, and how in certain circumstances the BSR depth data themselves can be used to identify and eliminate such systematic errors. I illustrate both conclusions using BSR picks from an extensive hydrate province in the eastern Black Sea [7].

ESTIMATION OF GEOTHERMAL GRADIENTS

The estimation of geothermal gradient involves the following steps:

1. The seabed and BSR are picked.
2. The sub-seabed BSR two-way-time is converted to a depth interval.
3. The BSR depth is converted to pressure, normally with an assumption that pressure is hydrostatic.
4. The pressure is converted to temperature using an assumed phase boundary.
5. The geothermal gradient is calculated by dividing the temperature difference between the seabed and BSR by the depth difference.

The final step assumes that the geothermal gradient is linear. The gradient will decrease with depth if the thermal conductivity increases with depth, if there is significant advective heat transport, or if the seabed temperature has recently decreased. It will increase with depth if recent sedimentation is very rapid or the seabed temperature has recently increased. In the following analysis, I will assume that such effects are small or cancel each other out, such that the geotherm is approximately linear.

Steps 2-3 above may generate systematic errors, but in many cases the main contributor to systematic errors is likely to be step 4. From a comparison of borehole temperature measurements at the BSR with predicted phase boundaries, Hyndman et al. [8] concluded that the phase boundary for pure methane and fresh water provided the best fit. Some more recent studies have concluded that it is more appropriate to use a seawater salinity [4]. These differing assumptions may change the inferred temperature at the phase boundary by 1°C or more (Figure 1). The presence of gases other than methane can introduce even larger changes. It is also quite possible to use erroneous phase boundaries. For example, the empirical fits to experimental data of [5] are commonly used, but these fits are not valid if extrapolated beyond the range of the corresponding experimental data (Figure 1).

Because the phase boundary is a non-linear function of pressure and hence of depth, in a region of constant geothermal gradient an error in the choice of or computation of the phase boundary will lead to an artificial relationship between the water depth and the inferred geothermal gradient (Figure 2). For example, if the pore fluid at the BSR is fresh (due to hydrate dissociation) but the phase boundary for seawater
is used, the geothermal gradient will be underestimated and will appear to increase with increasing water depth and BSR depth. Conversely, if the gas is pure methane but a phase boundary for a more mixed gas is used, the geothermal gradient will be overestimated and will appear to decrease with increasing water depth and BSR depth. If the seafloor temperature varies significantly with water depth, the behaviour will be more complicated. Step 5 above assumes that the geotherm is linear; an artificial correlation between BSR depth and inferred heat flow also results if the geotherm is non-linear.

The effect of such assumptions is best illustrated by an example. Here I use a dataset from the eastern Black Sea (Figure 3). The Eastern Black Sea Basin was formed by rifting in the early Tertiary [11]. The most highly stretched parts of the basin correspond to the deepest water [11], but given the age of the basin, any systematic variation of lithospheric heat flow with water depth is expected to be small. The thickest sediments are also in the centre of the basin, any increase in lithospheric heat flow towards the centre of the basin may be compensated at least in part by sedimentation effects [12]. BSRs are widespread in the easternmost part of the basin (Figure 4) where there are dramatic local variations in water depth due to the presence of canyon systems. The BSR depth has been mapped in an industry three-dimensional seismic survey acquired within this region [7] using two 3090 cu. in. airgun arrays and ten 480-channel, 6-km-long hydrophone streamers with 100 m spacing (Figure 3).

The BSR was picked at 16560 locations within this survey and its depth computed using velocities estimated using a “dip moveout” approach that accounts for reflector dips. The geothermal
gradient was first estimated by assuming that the hydrate-forming gas was pure methane and that the pore fluid had seawater salinity. In this calculation, a seabed temperature of 9°C was assumed; the temperature of Black Sea bottom-water varies less than 1% from this value over the depth range of the survey [13]. I also assume that perturbations to the phase boundary by capillary effects [6] can be neglected. The calculation gives a plausible result for the geothermal gradient, though perhaps values in the shallowest part of the survey are rather low. However, if the inferred geothermal gradient is plotted against the water depth, a correlation emerges (Figure 5). The correlation is also present if the inferred gradient is plotted against the BSR depth (Figure 6).

In a region of rough topography, isotherms follow the seabed in the shallowest sediments and flatten with depth. The net effect is that the geothermal gradient is reduced at topographic highs and increased in topographic lows. This effect was simulated using a thermal model with a constant-temperature upper boundary condition and a constant heat-flux lower boundary condition. The model was applied to a bathymetric profile across the steepest topography in our survey area (Figure 3). These calculations resulted in lateral variations in the geothermal gradient of only ±3% at the seabed and ±1.5% at a typical BSR depth of 300 m below the seabed. This effect is therefore much too small to explain the observed correlation. However, such correlation is precisely what we would expect if the chosen fluid composition were too saline (Figure 2).

The present-day Black Sea has a salinity that is much lower than the global ocean because it has strong freshwater input from rivers and only a very limited link to the global ocean through the Bosphorus. Although the pore fluid salinity at the depth of the BSR within the survey area is unknown, pore fluids from deep boreholes in the central Black Sea have salinities of c. 0.5% [14]. If the geothermal gradient is re-calculated using this salinity, the correlation with BSR depth is much reduced (Figure 7).

Hydrate sampled by gravity coring about 20 km north of our survey area has pure methane composition [15]. However, a “thermogenic front” has been described at the recent TPAO-BP borehole HPX-1 within our survey area, with significant higher hydrocarbons beneath [16]. Therefore a plausible alternative composition for the hydrate-forming gas at depth includes a significant percentage of higher hydrocarbons. If a 95% methane and 5% ethane composition is used, the strong correlation between BSR depth and inferred geothermal gradient returns, but now...
the geothermal gradient increases as the BSR depth decreases (Figure 8). Again, this behaviour is exactly as expected if the phase boundary corresponds to the wrong gas composition (Figure 2).

If there is no geological reason for a systematic correlation of geothermal gradient with BSR depth, the above observations suggest that the correct phase boundary will be one that minimizes the correlation between the inferred geothermal gradient and the BSR depth. One way of determining the correct phase boundary to use would be therefore to try a range of gas and pore fluid compositions and choose the composition that minimizes the correlation. An equivalent approach that is more intuitive is to dispense with step 5 of the calculation and instead to use the BSR picks to construct a regional geotherm (Figure 9).

Figure 7: Estimated geothermal gradient using a phase boundary for pure methane and pore water with 0.5% salinity. Correlation coefficient is 0.19.

Figure 8: Estimated geothermal gradient using a phase boundary for pore water with 0.5% salinity and a gas comprising 95% methane and 5% ethane. Correlation coefficient is -0.73.

Figure 9: Method for constructing the geotherm in an area where it can be assumed that lateral variations are small. Filled circles, squares and diamonds mark computed temperature differences from the seabed for the three phase boundaries used in Figure 2, and solid, dashed and dotted lines mark linear regressions on these values. Horizontal lines correspond to BSR depths at the three locations shown in Figure 2, and thin lines mark the geothermal gradients for the corresponding BSR depths and assumed phase boundaries. Triangle marks the origin. Modified from [7].

One approach would be to plot each BSR pick at its observed depth and at the corresponding temperature for an assumed phase boundary. If the geotherm is linear and the correct phase boundary has been used, a linear regression on the resulting dataset would intersect the temperature axis at the correct seabed temperature. If the phase boundary is incorrect, the intercept will be at a different temperature. The correct phase boundary may therefore be determined by trying a range of possibilities for different gas composition or pore water salinity and choosing a phase boundary that results in the correct intercept on the temperature axis. This approach is mathematically equivalent to choosing the phase boundary that
minimizes the correlation between BSR sub-bottom depth and inferred geothermal gradient. There may not be an unique solution, in that different combinations of gas composition and salinity may yield very similar phase boundaries, so the composition may not be uniquely determined, but errors in the geothermal gradient due to choice of phase boundary will be substantially reduced.

If the seabed temperature varies significantly across the survey area, the regression could be done on the temperature difference from the seabed rather than the temperature itself. If the geotherm was non-linear, for example because of conductivity variations with depth or advective heat flow, in principle a curve could be fitted rather than a straight line, though in most real applications such curvature will be a second-order effect.

A wide range of assumed gas compositions and pore water salinities can be explored in this way to determine which combinations result in a reasonable temperature intercept, and also the sensitivity of the inferred geothermal gradient to the assumed composition and salinity (Figure 12). The composition and salinity cannot be uniquely determined, but for this particular dataset, we may conclude that if the salinity is low, less than about 2% higher hydrocarbons can be present in the gas, but larger amounts of higher hydrocarbons could be present if the pore fluid salinity is similar to that of the global ocean. The inferred geothermal gradient from this method is relatively insensitive variations in assumed salinity and gas composition, compared to the sensitivity when applying the standard method of Yamano [3].

Because it is constant, we can use directly the seabed temperature in the regression. If we use pure methane gas and a seawater salinity, the temperature intercept is well below 9°C (Figure 10), while if we use pure methane and a salinity of 0.5%, the temperature intercept is much closer to 9°C (Figure 11).

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Figure 10: Dots mark temperatures inferred at the BSR depth assuming a pure methane hydrate composition and seawater salinity. Solid line marks a least-squares linear regression on these values. Filled triangle marks the seafloor temperature of 9°C. Modified from [7].

Figure 11: Regression as in Figure 10 but for a salinity of 0.5%. Modified from [7].

**CALIBRATION WITH BOREHOLE DATA**

Data from borehole HPX-1 [16], which lies within the area of Figure 3, provide an opportunity to test the approach developed in this paper (Figure 13). Temperature measurements are only available in deeper parts of the borehole, but the geotherm of Figure 11 provides a remarkably good fit to these data. A regression that included all the borehole measurements and the seabed temperature would result in a slightly higher geothermal gradient, but such a regression would fit the seabed temperature poorly, and it seems likely that the measurements beyond 2.5 km depth are disturbed, perhaps by fluid flow.

The fit to a linear geotherm is surprising because we would expect the geotherm to be curved over this depth range because of variations in thermal
conductivity with depth, sedimentation effects [12], and the increased bottom-water temperature since glacial times [13]. There may however be trade-offs between these effects since the first results in a decrease in geothermal gradient with depth, while the third causes an increase in geothermal gradient with depth and the second also causes an increase with depth because sedimentation rates in the Pleistocene have been particularly high [17].

**DISCUSSION AND CONCLUSIONS**

Heat flow estimation from hydrate BSRs is subject to a range of systematic and random errors [4]. The method developed above reduces significantly the uncertainty resulting from uncertainties in the phase boundary used in the calculation, and provides some constraint on what that phase boundary should be and therefore what combinations of gas composition and pore fluid salinity may be present.

The example application described above makes use of a 3D seismic dataset, and the method may be most readily applied to 3D data. The acquisition of such datasets in hydrate provinces is becoming increasingly common. The method may also be applied any dataset where the seabed relief is the dominant control on the BSR depth beneath the seabed. The method may still work if there are other strong controls on this depth, such as real lateral changes in geothermal gradient, as long as such changes are uncorrelated with the bathymetry. These real variations will just add scatter to plots such as that shown in Figure 11.

The method will not work where significant variations in geothermal gradient are strongly correlated with water depth over the region of the survey. This scenario may arise for profiles extending many tens of kilometres downslope at young continental margins where heat flow increases oceanwards towards a nearby mid-ocean ridge, or at subduction zones where heat flow decreases landward due to thickening of an accretionary wedge. However, even where the conditions for validity of the method may not be valid, if a dataset is densely sampled I recommend that a plot such as Figure 5 is created and if a strong correlation is observed, that use of an inappropriate phase boundary is considered as a possible origin for such correlation.

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